Fracture Mechanics of Concrete Structures,
Proceedings FRAMCOS-2, edited by Folker H. Wittmann,
AEDIFICATIO Publishers, D-79104 Freiburg (1995)

REPRESENTATIVE VOLUMES OF CEMENTITIOUS MATERIALS

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Abstract
Representative volume is redefined from statistical point of view. First, a representative relationship is established among three parameters: the local volume under consideration, V, a effective property corresponding to the volume, Ω_V, and the coefficient of variation of the effective property, ρ_Ω. Then, an arbitrary level of the variation can be set, any V_O corresponding to a variation below that level may be considered to be acceptable as representative volume. The present study focus on ρ_Ω due to variation in local volume fraction, which depends on the local microstructural configuration, and can be described by autocorrelation function of internal structure of the composite. The autocorrelation function is formulated based on a morphological model called mosaic pattern. The representative volume of effective bulk modulus of a two phase composite, concrete, is determined as an example.

1 Introduction

Representative volume (RV) of a composite material has been defined as the minimum volume on which the measured properties of the composite material can be considered to be equivalent to the real effective properties of the composite. RV is important not only for experimental determination of materials properties, but also for theoretical analyses of various properties of the materials. However, a general and quantitative description on RV of composite materials has not been developed simply because the complexity of the problem. In fact, RV is not a very well defined quantity, and, there is no distinct value of RV in the sense of the definition. Because one cannot say that an effective property of a composite measured from a sample with a given volume represents the real effective property perfectly, while another result from a sample with 90% volume of the first one does not represent the property at all.

In the present study, we first define a representative relationship, which is the relationship among three parameters: the volume under consideration, V, a property corresponding to the volume, Ω_v, and the variation of the property, ρ_Ω. Under this definition, a property of a composite measured based on a given volume may predict the real property with 20% variation, while the same property measured based on a larger volume may have only 10% variation. Actually, the asymptotic trend of the variation is very clear. It decreases monotonically with increasing size of the volume, and approaches to a constant as the size of the volume approaches to infinity.

Now that the representative relationship is a continuous function in terms of the variation, an arbitrary level of the variation can be set, which may be called the acceptance level or the critical level. Any volume corresponding to a variation below that level may be considered to be acceptable as RV, otherwise should be rejected. This is the new definition of RV proposed in the present study. One of the advantages of the definition is that the adequate RV can be quantitatively evaluated upon different requirements on degree of variation of measurements, which is important not only for theoretical analysis but also for engineering practice.

The fundamental question, now, is how to determine the variation of a material property, ρ_Ω, under certain volume. For a composite material, there are two possible sources that induce variations in the effective property, namely, uncertainty of properties of each constituent phase, and uncertainty of the local microstructural configuration, such as local volume fraction of aggregate in the case of concrete. Apparently, the variation of local volume fraction depend on the size of the local volume. In general, with increasing size of the local volume, the statistics obtained based on the local volume will asymptotically approach the value of the global average. Similarly, the variation of properties of the aggregate and the cement paste depend also on the local volume. But as the local volume increases, variations of local properties approach not to zero but to certain constants, which are inherent variations of the properties of aggregate and cement paste measured as single phase.

The main purpose of this paper is to establish a theoretical model for quantitative evaluation of the RV for cementitious materials. Focus will be made on the effect of variation in local volume fraction, because it is important for fracture analysis of concrete. In fracture analysis, the local volume fraction of aggregate around a crack tip has dominant effect on the resistance to crack growth, but the local volume fraction is different with the one used in mixing design for the specimen. This local heterogeneity of the internal structure explains size effect and large scattering in fracture testing. Since local heterogeneity is related to the morphological features of the internal structure of concrete, a morphological model, called mosaic pattern (Xi and Jennings, 1995) , is adopted in the present study. A simplified method for evaluation of morphological parameters of two phase composites is provided, and as an example, RV for effective bulk modulus of concrete are demonstrated.

2 Criterion for determination of representative relationships

Let us denote Ω_v as an effective property of a composite in a finite volume V. Ω_v, depends on three types of parameters. The first type is local volume fractions of the phases, τ_k ; the second is corresponding properties of the constituent phases, Ω_i, which is the averaged value over the local volume V; and the third is related properties of the phases averaged over V, Ψ_j. Ω_v and these three types of parameters can be written in a general functional form as follows

$$\Omega_v = g(\Omega_i, \Psi_j, \tau_k) \tag{1}$$

where i = 1,2, ..., m, m = the total number of phases in the composite; j = 1,2, ..., M; k = 1,2, ..., m-1, since only m-1 of local volume fractions are independent; g is a functional form which depends on various factors such as the property to be studied, the type of composite under investigation, and the theory employed to establish Eq. 1. Since Ω_i, Ψ_j, and τ_k, are considered to be random variables, Ω_v, as a function of these random variables, is a random variable too. According to probabilistic theory, the mean value and variance of Ω_v can be written in general forms

$$E\{\Omega_v\} = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} g(\Omega_i, \Psi_j, \tau_k) f(\Omega_i, \Psi_j, \tau_k) d\Omega_i d\Psi_j d\tau_k \tag{2}$$

$$\sigma_\Omega^2 = E\{\Omega_v^2\} - [E\{\Omega_v\}]^2 \tag{3}$$

in which $f(\Omega_i, \Psi_j, \tau_k)$ is the joint probability density function for the random variables; E{.} is the expectation operator; σ_Ω is the standard deviation of Ω_v. The mean value, Eq. 2, can be evaluated easily because $E\{\Omega_V\}$ must equal to the global average Ω

$$E\{\Omega_v\} = \Omega = g(\bar{\Omega}_i, \bar{\Psi}_j, \phi_k) \tag{4}$$

in which $\bar{\Omega}_i$, $\bar{\Psi}_j$, and ϕ_k are global averages of Ω_i, Ψ_j, and τ_k, respectively. Actually, we are more interested in the second order information in a dimensionless form, that is, the coefficient of variation, ρ_Ω, which can be obtained by combining Eqs. 3 and 4

$$\rho_\Omega = \frac{\sigma_\Omega}{E\{\Omega_v\}} = \frac{\left\{E\{\Omega_v^2\} - [E\{\Omega_v\}]^2\right\}^{1/2}}{g(\bar{\Omega}_i, \bar{\Psi}_j, \phi_k)} \tag{5}$$

ρ_Ω depends on $f(\Omega_i, \Psi_j, \tau_k)$ and $g(\Omega_i, \Psi_j, \tau_k)$. $g(\Omega_i, \Psi_j, \tau_k)$ represents physical relationships among the effective properties, the local properties of each constituent phase, and the local volume fractions. $f(\Omega_i, \Psi_j, \tau_k)$ characterizes the statistical features of these random variables. As one can see clearly that Eq. 5 is exactly the representative relationship that we are looking for. To evaluate Eq. 5, both $f(\Omega_i, \Psi_j, \tau_k)$ and $g(\Omega_i, \Psi_j, \tau_k)$ must be determined first.

Determination of effective properties of composite materials based on the properties of their constituents, i.e. $g(\Omega_i, \Psi_j, \tau_k)$, has long been a major research topic in composite mechanics. A wide variety of mathematical models has been developed to evaluated many different effective materials properties. However, all these methods have been developed to evaluate the effective properties of composites presumably with a very large volume, much larger than any possible size of RV. Then, the methods will be valid for all kinds of composites.

As a simple example of $g(\Omega_i, \Psi_j, \tau_k)$, Hashin and Shtrikman bounds (lower bound only) for bulk modulus of a two phase composite is listed as following (Hashin and Shtrikman, 1963)

$$K_1^* = K_1 + \frac{1-\tau_1}{\dfrac{1}{K_2 - K_1} + \dfrac{3\tau_1}{3K_1 + 4G_1}} \tag{6}$$

in which K_1^* is the lower bound for effective bulk modulus of the composite; K_1 and K_2 are bulk moduli of the two phases with $K_2 > K_1$; G_1 is the shear moduli of the phase 1.

The exact solutions for $f(\Omega_i, \Psi_j, \tau_k)$ are very difficult to determine in most of the cases. For practical engineering problems, however, we are interesting in the variations close to mean values rather than extreme values. This provides us an alternative to evaluate σ_Ω^2 approximately. In fact, assuming only the local volume fractions are random variables, an approximate evaluation of σ_Ω^2 can be obtained by linearization of $g(\Omega_i, \Psi_j, \tau_k)$ around the mean values (Ditlevsen, 1981)

$$\sigma_\Omega^2 = \sum_{k=1}^{m-1}\sum_{l=1}^{m-1} \frac{\partial g(\Omega_i, \Psi_j, E\{\tau_k\})}{\partial \tau_k} \frac{\partial g(\Omega_i, \Psi_j, E\{\tau_l\})}{\partial \tau_l} Cov(\tau_k, \tau_l) \tag{7}$$

in which $Cov(\tau_k, \tau_l)$ is the covariance of the local volume fractions. Assuming τ_k are mutually independent random variables, $Cov(\tau_k, \tau_l) = 0$ for $k \neq l$. For a two phase composite, by denoting $Cov(\tau_1, \tau_1) = \sigma_\tau^2$ Eq. 7 can be further simplified as

$$\sigma_\Omega = \left(\frac{\partial g(\Omega_i, \Psi_j, E\{\tau_1\})}{\partial \tau_1} \right) \sigma_\tau \tag{8}$$

Now, one can see from Eqs. 7-8 that the problem that determination of variance of an effective property, σ_Ω^2, has been transformed into another problem, that is, the determination of the variance of local volume fraction.

3 Variation of local volume fraction

Variation of local volume fractions is related to the microstructural configurations of the material under investigation. It depends on many factors, such as the size of the local volume, the global volume fractions of the constituent phases, and the coarseness of the grains. Obviously, a quantitative evaluation on σ_τ^2 requires a mathematical model that includes all these influential factors. A method developed by Lu and Torquato (1990) will be used in the present study for evaluation of σ_τ^2.

$$\sigma_\tau^2 = \frac{1}{V_0^2} \int \left[R_x(r) - \phi_1^2 \right] V_2^{\text{int}}(r, R_0)\, dr \tag{9}$$

in which V_0 is the local volume; R_0 is the shape factor of V_0; r is the distance between the centroids of two local volumes; $R_x(r)$ is the autocorrelation function of the microstructure; $V_2^{\text{int}}(r,R_0)$ is the intersection volume of two identical local volumes, it is a function of r and R_0. When the local volume is a sphere with diameter R_0, the intersection volume of two spheres with a center to center spacing r can be easily determined

$$V_2^{\text{int}} = \frac{\pi R_0^3}{6}\left[1-\frac{3r}{2R_0}+\frac{r^3}{2R_0^3}\right] \tag{10}$$

Autocorrelation function is the second order information of the spatial arrangement of randomly distributed constituent phases. In the present study, the autocorrelation functions for multiphase composites developed based on mosaic patterns will be used (Xi, 1995). Figs. 1 and 2 show two different kinds of mosaic patterns, the one on Fig. 1 is called L-mosaic, and the other one on Fig. 2 is S-mosaic.

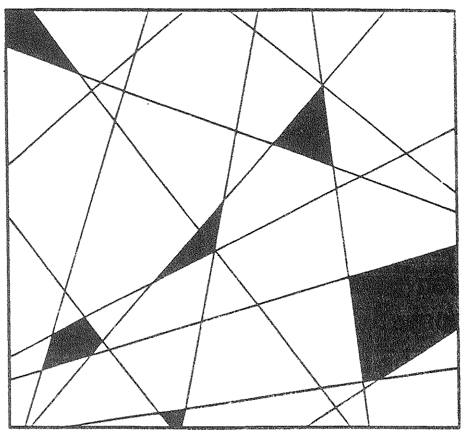

Fig. 1 Generated 2D and two phase L-mosaic pattern

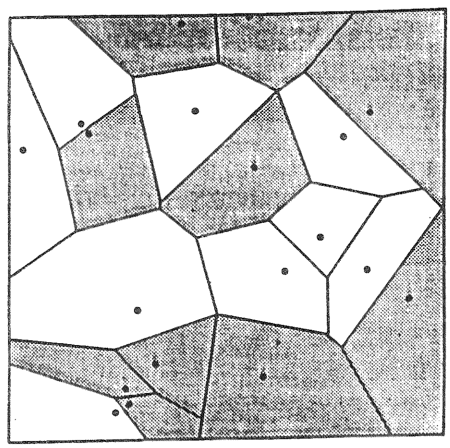

Fig. 2 Generated two dimension and two phase S-mosaic pattern

Two dimensional polygons in the figures are called basic cells of mosaics. The methods to construct these mosaic patterns can be seen in literature (Xi and Jennings, 1995; Kumar, 1992; Pielou, 1977). From Figs. 1 and 2, it is clear that L-mosaic may be used for the concrete with crushed stones, and S-mosaic for river gravels. The autocorrelation functions for two phase L- and S-mosaic are (Xi, 1995)

$$R_x^L(r) = \phi_1^2 + \left(\phi_1 - \phi_1^2\right)e^{-\lambda r} \tag{11a}$$

$$R_x^S(r) = \phi_1^2 + \left(\phi_1 - \phi_1^2\right)(1 + \lambda r)e^{-2\lambda r} \tag{11b}$$

in which the superscripts L and S represent L- and S-mosaic, respectively. Parameter λ in Eq. 11 is called coarseness of grain structures, it is the number of segments of the basic cells on unit length when a 2D mosaic is cut by a transect. λ is independent with the volume fraction, and is a measure of the grain sizes of the mosaic.

4 Influential factors on representative relationships

The representative relationship (RR) for a two phase composite material (m = 2) can be established by combining Eq. 5, 8 and 9

$$\rho_\Omega = \frac{1}{g(\bar{\Omega}_i, \bar{\Psi}_j, \phi_1)} \left[\left(\frac{\partial g(\Omega_i, \Psi_j, E\{\tau_1\})}{\partial \tau_1} \right)^2 \frac{1}{V_0^2} \int \left[R_x(r) - \phi_1^2 \right] V_2^{\text{int}}(r, R_0)\, dr \right]^{1/2} \tag{12}$$

Consider the effective bulk modulus shown in Eq. 6 as an example. From Eq. 12, the complete expression for the RR of effective bulk modulus of a two phase composite (L-mosaic) is

$$\rho_\Omega = \frac{\partial K_1^*}{\partial \phi_1} \frac{1}{K_1^*} \left\{ \frac{-24}{\xi^3} \left(\phi_1 - \phi_1^2\right) \left[e^{-\xi} \left(3 + \frac{21}{\xi} + \frac{60}{\xi^2} + \frac{60}{\xi^3} \right) + \left(-2 + \frac{9}{\xi} - \frac{60}{\xi^3} \right) \right] \right\}^{1/2} \tag{13}$$

where $\xi = \lambda R_0$, called characteristic number.

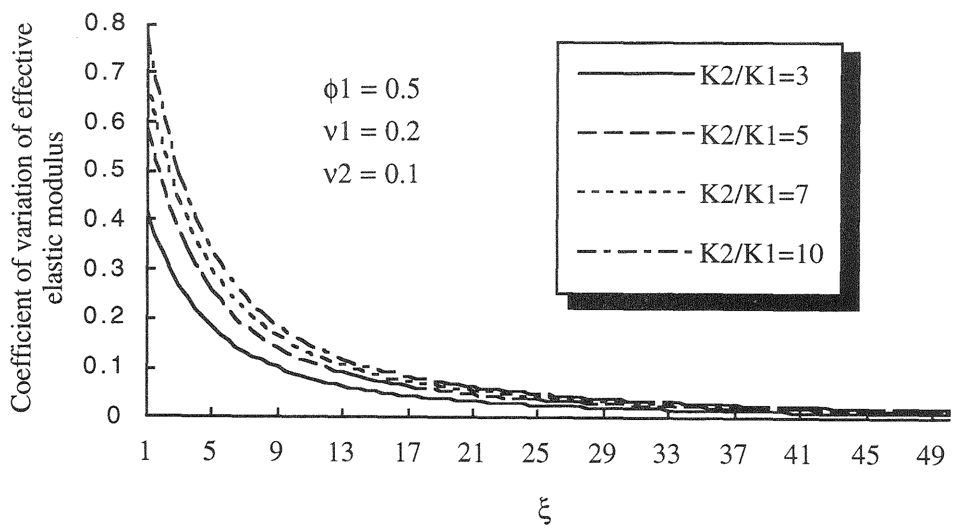

Fig. 3 ξ and the coefficient of variation of effective bulk modulus.

Fig. 3 shows curves of ρ_Ω verses characteristic number ξ at ϕ_1 = 0.5. Also, the effect of bulk moduli on ρ_Ω is analyzed by taking K_2/K_1 = 3,5,7,10, respectively. Poisson's ratio for the two phases are assumed to be ν_2 = 0.1 for phase 2 and ν_1 = 0.2 for phase 1, and thus $G_1/K_1 = 3(1-2\nu_1)/2(1+\nu_2)$ = 0.818. From Fig. 3, one can see that the effect of K_2/K_1 is significant especially when ξ is small. The effect of Poisson's ratio has shown to be negligible.

Eq. 13 is based on the effective bulk modulus of a two phase composite. RR and characteristic number for any other effective properties of composite materials can be obtained in a similar manner. Then the RV for any of the effective properties can be determined when λ is known. The main progress made in the present study is that the estimation on RV is not based on qualitative analysis or probabilistic reasoning but on rigorous theoretical modeling. Derivation of Eq. 13 is completely analytical, and there is no free parameters involved in the derivation that must be determined by curve fitting.

5 Representative volumes of cementitious materials

Once the characteristic number is obtained for a property of a composite material, the determination of λ becomes a major concern. λ can be determined by image analysis method which, however, is not available in many cases. It is therefore desirable to develop a method for evaluation of λ based solely on those parameters of initial mixing design that can be easily assessed in most of practical engineering laboratories. Next, portland cement concrete will be taken as an example to demonstrate how to determine λ and RV without using image analysis method.

Initial parameters in concrete mixing design that are needed for determination of coarseness λ are volume fraction of aggregate ϕ_a and grading curve of the aggregate (particle size distribution). From the latter, the average size of aggregates, E{D}, can be obtained. In one dimension case where a transect cutting through the sample of the concrete, the same ϕ_a can be obtained as $\phi_a = E\{L_a\}/[E\{L_a\}+E\{L_{cp}\}]$, in which $E\{L_a\}$ is the average length of the aggregate segments on the transect, $E\{L_{cp}\}$ is the average length of the cement paste segments on the transect. Then the coarseness λ can be evaluated as (Xi, 1994; Xi and Jennings, 1995) $\lambda = \lambda_{cp} + \lambda_a = 1/E\{L_{cp}\} + 1/E\{L_a\} = 1/[E\{L_a\}(1-\phi_a)]$.

Now, one must realize that $E\{L_a\}$ is not the average size of the aggregates, E{D}, obtained from sieve analysis, because $E\{L_a\}$ is the average segment length of aggregates on transects used for one dimension mosaic analysis. While the sieve analysis gives the average size of aggregates in three dimension. As a first approximation, $E\{L_a\} \approx (2/\pi)\ E\{D\}$ (Xi and Jennings, 1995). The final expression of coarseness λ for concrete is

$$\lambda = \frac{\pi}{2\ E\{D\}} \frac{1}{1-\phi_a} \tag{14}$$

As an example, let us take $\phi_a = 0.7$ and E{D} = 0.7 inch (for coarse aggregate), then from Eq. 14, $\lambda = 7.48$. According to Fig. 3 with $v_1/v_2 = 2$, $v_2 = 0.1$, and $K_2/K_1 = 7$, for variation of bulk modulus of concrete below 5%, the corresponding characteristic number $\xi = 23$, and thus acceptable RV = R_0 = $\xi/\lambda = 3$ inch. It is exactly the diameter of the most commonly used cylinder size for concrete testing although the standard cylinder size is 6 inch. We now know from the present example that the minimum variation of 3 inch cylinder test for concrete is about 5%, and the actual scattering must be larger than 5%, because variations due to random sources other than local volume fraction of aggregate are not included in this example. Eq. 14 is valid not only for concrete but also for any two phase composites.

6 Conclusions

1. Representative volume is defined from statistical point of view. First, a representative relationship is established among three parameters: the local volume under consideration, V, an effective property corresponding to the volume, Ω_V, and the coefficient of variation of the effective property, ρ_Ω. Then, an arbitrary level of the variation can be set. Any volume corresponding to a variation below that level may be considered to be acceptable as representative volume, otherwise should be rejected.

2. The variation of an effective property is due mainly to two sources, namely, uncertainty of the properties of constituent phases, and uncertainty of the local microstructural configuration. The present study focus on the latter one, particularly on the variation in local volume fractions. The variation of the local volume fractions depends on autocorrelation function of internal structure of the composite under consideration, which has been formulated based on a morphological model, called mosaic pattern. Two controlling parameters of the resulting representative relationship are volume fractions of constituent phases and characteristic number ξ, $\xi = \lambda\ R_0$, where R_0 is the size of the local volume and λ is coarseness of the mosaic, i.e. the coarseness of the grain structure of the composite.

3. The representative relationship of effective bulk modulus of a two phase composite is determined as an example. A simplified method is developed to evaluate λ for a two phase composite. A numerical example shows that for commonly used concrete composition, the representative volume (diameter) for concrete cylinder test should not be smaller than 3 inch, if variation of the measured property (bulk modulus) is required to be less than 5% (variations due to random sources other than local volume fraction of aggregate are not included in this example).

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