A Review of Homogenization Techniques for Heterogeneous Materials

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By

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Objective

The effective properties of macroscopic homogeneous composite materials can be derived from the microscopic heterogeneous material structures using homogenization techniques. Several models for determination of the bounds of the effective properties and for the effective properties are available in literature. The objective of this work is the review of different homogenization techniques for random heterogeneous microstructures. The methods have to be applied to the meso-scale model of concrete and compared with each other.

The following problems are to be addressed:

- Literature research about models for determination of the bounds of effective material properties (Voigt / Reuss Approximation, Hashin-Shtrikman Variational principles).
- Literature research about classical homogenization models (Self Consistent Method, Mori-Tanaka Method).
- Linear elastic simulation of several samples of a two phase random material RVE (simplified concrete grain structure) in 2D (plane stress / plane strain) using Ansys.
- Determination and comparison of effective material properties of the RVE for different boundary conditions (displacements, tractions). Three loading conditions have to be used to generate the full stiffness matrix, uni-axial tension in the two in-plane directions and an in-plane shear.
- Investigation of sensitivity of obtained effective properties due to different finite elements and element sizes.
- Comparison of the effective properties, which were derived from RVE with the results of the classical models.

Contents

1. Introduction to Mechanics of Heterogeneous Materials

Introduction:

Mechanics of materials, in present notion, started some one-hundred years ago with pioneering work by Reuss and Voigt. It was developed further with time and was applied increasingly. In recent years, research activities were given a boost because of the tremendous multiplication of computational resources. The activities have also been accelerated by the introduction of novel high performance materials like composites, layered compounds, and foam-type structures. However, not only these are the subjects to intense research, but also 'conventional' materials such as concrete, metals, alloys, ceramics, and polymers. Computational modeling aims at understanding the physical mechanisms which govern the behavior of a material. Once having gained such knowledge, it can be utilized for design, improvement, and tailoring of materials. Moreover, components and structures made from such materials can be investigated in greater detail with respect to their loading response. And, thinking about product development, the number of prototypes can be reduced by guiding the way towards promising solutions.

Mechanics of materials is an interdisciplinary field combining elements from mathematics, mechanics, and materials science.

The present work is dedicated to computational (i.e. numerical and analytical) modeling of heterogeneous materials, primarily to matrix-inclusion type composites. The modeling of the entire behavior is far beyond the scope of this work, which would require the treatment of a huge number of different properties, mechanisms, and phenomena. Analytical as well as numerical methods are employed within the framework of continuum mechanics of materials. Theoretical foundations and applications are presented for both approaches; advantages and drawbacks are addressed. Although the models have been set up for simulation of cement aggregate composites, application is not restricted to that family of materials. As long as the assumptions underlying the modeling are met, different material systems can be investigated equivalently.

A primary task in mechanics of materials is the prediction of material's behavior. This means, on the one hand, to estimate the effective (or overall) properties from the composition, commonly referred to as homogenization. On the other hand, most approaches allow for localization, i.e. to estimate the local load state within the individual constituents as response to an overall applied (far field) load. A number of mechanisms are active, coupled to each other and interacting with each other, building a complex system which governs the behavior.

Understanding the physics as well as the mathematics of the models (at least to a certain extent) provides the basis for gaining proper results from modeling and simulation. As mentioned above, prediction of overall properties can be regarded as the first step. Identification of the governing mechanisms and assessing their effect on the material behavior leads one step further. Bringing together this knowledge with service requirements allows for functional oriented materials design. Such tools at hand can guide the way to promising candidate materials with the potential to markedly reducing the number of prototypes and development time. This applies not only to materials but also can be extended straightforward to structures and components made from composite materials.

Transition between Length Scales:

The length-scale at which a problem is considered is of great importance in mechanics of materials. Each material has features of a structure when studied at sufficiently high spatial resolution, and any structure has material type features when viewed from afar. Typically, a material is an inhomogeneous agglomeration of constituents, provided the viewer zooms in close enough, e.g. particles and matrix material in a composite, gravel and cement in concrete, etc. At the length scale of the constituents, their behavior is described by some continuum type material models. At the scale of micro-mechanical investigations, the interaction of the various phases is taken into account. This way, for the greater length-scale, a unique constitutive behavior is extracted which typically cannot be captured fully by standard closed form continuum models. An illustrative way for denoting these different length-scales are the micro, meso, and macro scale. Among these the level of components or structural parts is called macro scale. At the meso scale sub-domains are regarded with locally varying loads and/or compositions. Finally, the

interaction of the constituents is accounted for at the micro scale [5]. Within the present work mechanics of materials, typically, provides the transition from the micro to the meso scale (homogenization) and vice versa (localization).

1.1 Inhomogeneous Materials:

Many industrial and engineering materials as well as the majority of “natural" materials are inhomogeneous, i.e. they consist of dissimilar constituents (or “phases") that are distinguishable at some (small) length scale. Each constituent shows different material properties and/or material orientations and may itself be inhomogeneous at some smaller length scale(s). Typical examples of inhomogeneous materials are composites, concrete, polycrystalline materials, porous and cellular materials, functionally graded materials, wood, and bone. An important aim of theoretical studies of multiphase materials lies in homogenization, i.e. in deducing their overall (“effective" or “apparent") behavior (e.g. stiffness, thermal expansion and strength properties, heat conduction and related transport properties, electrical and magnetic properties, electromechanical properties,…..) from the corresponding material behavior of the constituents (and of the interfaces between them) and from the geometrical arrangement of the phases [25].

1.2 The Concept of Homogenization:

At a sufficiently fine scale, all materials are heterogeneous, even those said be homogeneous. In order to be convinced of this suffices to start at the level of atoms and molecules. If the usual engineering materials had to be characterized at this level of observation the task would be overwhelming. To overcome this difficulty, engineers introduce the hypothesis of continuity of a material. This hypothesis implies a notion of statistical average in which the actual constitution of the material is idealized by considering the material to be continuous. Once the continuity model is admitted, the concept of homogeneity is deduced from it. A homogeneous medium is then characterized by properties that are identical at every point.

At the engineering level character of heterogeneity appears whenever the physical or mechanical properties of a material are functions of a point. The variations of the properties can be of two types: either continuous, or discontinuous as in the case of

composite materials. In this case the properties of the material vary from point to point in a discontinuous manner at the interfaces between its various phases. Each phase is assumed to be homogeneous and isotropic.

In the case of a phase 1 dispersed with in phase 2 there exists in general a characteristic dimension of the heterogeneity. For example, in the case of a composite material made of fibers this dimension would be the average distance between the fibers. This dimension is in fact an idealized description of a statistical distribution inside the actual heterogeneous material. On the other hand, there generally exists a scale of size δ at which the properties of the material can be averaged to a good approximation. This means that, in this case, the properties measured in a sample of size δ are independent of the place (of the point) within material at which the sample was taken. In terms of such a concept the material can then be considered as being effectively homogeneous, and the problems of designing structures can be solved by considering the averaging properties measured on the scale δ. In the case where there exists such a scale (intermediate between the microscopic scale—that of the constituents—and the scale of the structure) it is said that the material can be *homogenized*. One then speaks of *macroscopic homogeneity* (as opposed to the scale of constituents, which is called microscopic), or of *statistical homogeneity*. The concept of rendering "homogeneous" a "heterogeneous" material is called *homogenization*.

1.3 Homogenized Moduli:

The notion of homogenization having been introduced, it is now possible to express the homogenized mechanical properties of a heterogeneous material. These properties are determined for an element of volume V and size δ. In composite literature, such a sample volume is known as **Representative Volume Element (RVE)** of the material [6, 9]. When a composite specimen is under external load, micro stresses and strains are induced throughout the specimen. Ideally, the micro fields should be computed exactly, given the specimen and its matrix-inclusion microstructure. According to the statistical homogeneity assumption, an appropriate RVE can be defined and isolated. On the RVE boundary, there exist definitive surface displacements and surface tractions. Within the RVE, there exist definitive stress field σ_{ij} and strain field ε_{ij} .

Through homogenization, the composite specimen is regarded as a body of an effective homogeneous material, whose mechanical behavior is described by a definitive constitutive law. This constitutive law can be determined based on the detailed fields in the selected RVE through an "averaging" procedure:

Specifically, if the exact micro fields σ_{ij} and ε_{ij} in the RVE are known under the applied load, the averaged stresses and strains over the RVE are given by:

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV \qquad i = 1 \ldots 6 \tag{1.1}$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \qquad i = 1 \ldots 6 \tag{1.2}$$

Where V is the volume of the RVE. The averages are then treated as the effective stress and strain fields in the homogenized RVE. The relations between σ_{ij} and ε_{ij} determine the "effective" constitutive law. When linear elasticity is assumed, the generalized Hook's law applies:

$$\bar{\sigma}_{ij} = C_{ijkl}\bar{\varepsilon}_{kl} \tag{1.3}$$

or

$$\bar{\varepsilon}_{ij} = S_{ijkl}\bar{\sigma}_{kl} \tag{1.4}$$

In the above, C_{ijkl} and S_{ijkl} are the effective stiffness and the effective compliance for the homogenized composite respectively.

Thus in order to determine the homogenized properties of a heterogeneous material it is necessary to calculate the average stress and strain over the RVE by means of (1.1) and (1.2), and then to deduce from them the stiffness and compliance constants with the help of (1.3) and (1.4). If this problem appears to be simple in principle to solve, it is particularly complex in practice. In fact in order to apply equations (1.1) and (1.2) it is necessary first to find the exact solutions of the stress and strain fields σ_{ij} and ε_{ij} at each point of a heterogeneous material. These exact solutions can be obtained only in the case of simple and idealized geometric models, and some what away from reality.

1.4 Stress-Strain relations for anisotropic materials:

The generalized Hooke`s law relating stresses to strains can be written in contracted notation as

$$\sigma_i = C_{ij}\varepsilon_j \qquad i, j = 1...6 \tag{1.5}$$

where σ_i are the stress components shown on a three-dimensional cube in x, y, and z coordinates in Figure 1, C_{ij} is the stiffness matrix, and ε_j are the strain components.

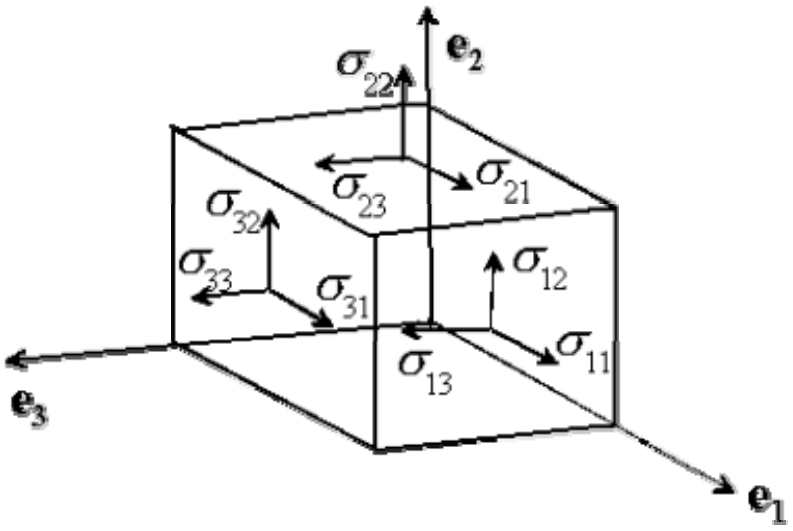

Figure 1: *Stresses on an element*

The stiffness matrix, C_{ij}, has 36 constants in Equation (1.5). However, less than 36 of the constants can be shown to actually be independent for elastic materials when important characteristics of the strain energy are considered. So because of symmetry, the stiffness and compliance matrix are each determined by 21 independent constants.

With the foregoing reduction from 36 to 21 independent constants, the stress-strain relations are

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix} \tag{1.6}$$

as the most general expression within the framework of linear elasticity. Actually, the relations in equation (2.2) are referred to as characterizing anisotropic materials because there are no planes of symmetry for material properties.

If there is one plane of material symmetry, the stress-strain relations reduced to

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{31}\\ \tau_{12}\end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16}\\ & C_{22} & C_{23} & 0 & 0 & C_{26}\\ & & C_{33} & 0 & 0 & C_{36}\\ & & & C_{44} & C_{45} & 0\\ & & & & C_{55} & 0\\ & & & & & C_{66}\end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix} \tag{1.7}$$

where the plane of symmetry is $z = 0$ (1-2 plane). Such a material is termed as *monoclinic* and has 13 independent elastic constants.

If there are two orthogonal planes of symmetry for a material, symmetry will exist relative to a third mutually orthogonal plane. The stress-strain relations in coordinates aligned with principal material directions are

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{31}\\ \tau_{12}\end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0\\ & C_{22} & C_{23} & 0 & 0 & 0\\ & & C_{33} & 0 & 0 & 0\\ & & & C_{44} & 0 & 0\\ & & & & C_{55} & 0\\ & & & & & C_{66}\end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix} \tag{1.8}$$

and are said to define an *orthotropic* material. Note that there is no interaction between normal stresses $\sigma_1, \sigma_2, \sigma_3$ and shearing strains $\gamma_{23}, \gamma_{31}, \gamma_{12}$ such as occurs in anisotropic materials. Similarly, there is no interaction between shearing stresses and normal strains. Note also that there are now only nine independent constants in the stiffness matrix.

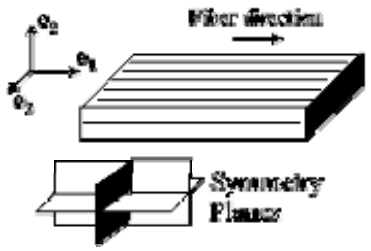

Figure 2: *Orthotropic Symmetry*

If at every point of a material there is one plane in which the mechanical properties are equal in all directions, and then the material is called *transversely isotropic*. If for example, the 1-2 plane is the plane of isotropy, then the 1 and 2 subscripts on the stiffnesses are interchangeable. The stress-strain relations have only *five* independent constants:

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{31}\\ \tau_{12}\end{bmatrix}=\begin{bmatrix}C_{11} & C_{12} & C_{13} & 0 & 0 & 0\\ & C_{11} & C_{13} & 0 & 0 & 0\\ & & C_{33} & 0 & 0 & 0\\ & & & C_{44} & 0 & 0\\ & & & & C_{44} & 0\\ & & & & & (C_{11}-C_{12})/2\end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix} \tag{1.9}$$

if there is an infinite number of planes of material symmetry, then the forgoing relations simplify to the *isotropic* material relations with only *two* independent constants in the stiffness matrix:

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{31}\\ \tau_{12}\end{bmatrix}=\begin{bmatrix}C_{11} & C_{12} & C_{12} & 0 & 0 & 0\\ & C_{11} & C_{12} & 0 & 0 & 0\\ & & C_{11} & 0 & 0 & 0\\ & & & (C_{11}-C_{12})/2 & 0 & 0\\ & & & & (C_{11}-C_{12})/2 & 0\\ & & & & & (C_{11}-C_{12})/2\end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix} \tag{1.10}$$

1.5 Strain-Stress relations for anisotropic materials:

The strain-stress relations for the five most common material property symmetry cases are shown in Equations (1.11) to (1.15):

Anisotropic (21 independent constants):

$$\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix}=\begin{bmatrix}S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16}\\ & S_{22} & S_{23} & S_{24} & S_{25} & S_{26}\\ & & S_{33} & S_{34} & S_{35} & S_{36}\\ & & & S_{44} & S_{45} & S_{46}\\ & & & & S_{55} & S_{56}\\ & & & & & S_{66}\end{bmatrix}\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \tau_{23}\\ \tau_{31}\\ \tau_{12}\end{bmatrix} \tag{1.11}$$

Monoclinic (13 independent constants) (for symmetry about $z = 0$)

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\ & S_{22} & S_{23} & 0 & 0 & S_{26} \\ & & S_{33} & 0 & 0 & S_{36} \\ & & & S_{44} & S_{45} & 0 \\ & & & & S_{55} & 0 \\ & & & & & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} \tag{1.12}$$

Orthotropic (9 independent constants):

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ & S_{22} & S_{23} & 0 & 0 & 0 \\ & & S_{33} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{55} & 0 \\ & & & & & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} \tag{1.13}$$

Transversely Isotropic (5 independent constants):

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ & S_{11} & S_{13} & 0 & 0 & 0 \\ & & S_{33} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{44} & 0 \\ & & & & & 2(S_{11} - S_{12}) \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} \tag{1.14}$$

Where the 1-2 plane is a symmetry plane in which the compliances are isotropic and in the 3-direction (transverse to the symmetry plane), the compliances are different.

Isotropic (2 independent constants):

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ & S_{11} & S_{12} & 0 & 0 & 0 \\ & & S_{11} & 0 & 0 & 0 \\ & & & 2(S_{11}-S_{12}) & 0 & 0 \\ & & & & 2(S_{11}-S_{12}) & 0 \\ & & & & & 2(S_{11}-S_{12}) \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{23} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} \tag{1.15}$$

One of the major objectives in studying the strain-stress relations are to be able to conclude what deformation response occurs because of a specific applied stress.

1.6 Stress-strain relations for a plane stress in an orthotropic material in principal directions:

The basics developed in the preceding sections are applicable to the solutions of any arbitrary elastic problem for a composite material. In the case where the elasticity problem can be reduced to a two-dimensional elasticity problem, so a plane stress state is defined by setting

$$\sigma_3 = 0\,, \qquad \tau_{23} = 0\,, \qquad \tau_{31} = 0 \tag{1.16}$$

so that

$$\sigma_1 \neq 0\,, \qquad \sigma_2 \neq 0\,, \qquad \tau_{12} \neq 0 \tag{1.17}$$

The plane stress state is not a merely an idealization of reality, but instead is a practical and achievable objective of how we must use a RVE in its plane.

When referred to the principal material directions, a plane stress state is characterized by:

$$\sigma_i \neq 0 \quad \text{if } i = 1,2,6 \qquad \text{and} \qquad \varepsilon_i \neq 0 \text{ if } i = 1,2,3,6 \tag{1.18}$$

$$\sigma_i = 0 \text{ if } i = 3,4,5 \qquad \text{and} \qquad \varepsilon_i = 0 \text{ if } i = 4,5 \tag{1.19}$$

The elastic equations can be written in one of the two forms:

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & 0 \\ S_{12} & S_{22} & 0 \\ 0 & 0 & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_{21} \\ \tau_{12} \end{bmatrix} \tag{1.20}$$

with

$$\varepsilon_3 = S_{13}\sigma_1 + S_{23}\sigma_2 \tag{1.21}$$

where

$$S_{11} = \frac{1}{E_1} \quad S_{22} = \frac{1}{E_2} \quad S_{12} = -\frac{\nu_{12}}{E_1} = -\frac{\nu_{21}}{E_2} \quad S_{66} = \frac{1}{G_{66}} \tag{1.22}$$

or

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \tau_{12} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{12} & Q_{22} & 0 \\ 0 & 0 & Q_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \gamma_{12} \end{bmatrix} \tag{1.23}$$

with

$$\varepsilon_3 = -\frac{1}{C_{33}}(C_{13}\varepsilon_1 + C_{23}\varepsilon_2). \tag{1.24}$$

where Q_{ij} are the so called reduced stiffness for a plane stress state in the $1-2$ plane.

$$Q_{ij} = C_{ij} - \frac{C_{i3}C_{j3}}{C_{33}} \qquad i, j = 1,2,6 \tag{1.25}$$

The term C_{63} is zero because no shear-extension coupling exists for an orthotropic material in principal material directions. For the orthotropic material Q_{ij} are:

$$Q_{11} = \frac{S_{22}}{S_{11}S_{22} - S_{12}^2} \qquad Q_{22} = \frac{S_{11}}{S_{11}S_{22} - S_{12}^2}$$

$$Q_{12} = \frac{S_{12}}{S_{11}S_{22} - S_{12}^2} \qquad Q_{11} = \frac{1}{S_{66}} \tag{1.26}$$

or, in terms of the engineering constants,

$$Q_{11} = \frac{E_1}{1 - \nu_{12}\nu_{21}} \qquad Q_{22} = \frac{E_2}{1 - \nu_{12}\nu_{21}}$$

$$Q_{12} = \frac{\nu_{12}E_2}{1 - \nu_{12}\nu_{21}} = \frac{\nu_{21}E_1}{1 - \nu_{12}\nu_{21}} \qquad Q_{66} = G_{12} \tag{1.27}$$

2. Analytical Techniques for Heterogeneous Materials

In this section various models and bounds for elastic predictions of two-phase composites are reviewed. The methods comprise rules of mixture, Hashin-Shtrikman type bounds, Mori-Tanaka type models, and classical self-consistent schemes. Their relations among each other and to specific micro-topologies are discussed as well as their range of applicability.

Concrete grain structure form part of the class of composites known as particulate composites. The particles of dispersed component of the composite (aggregates) are distributed in three dimensions. Hence, accurate models of these composites should be three-dimensional. However, for simplicity, we primarily explore two-dimensional models in this work.

Table 1 shows the elastic moduli of concrete grain structure. These data are used to assess the predictions of some of the techniques discussed in this work.

Material	Volume Fraction	Young's Modulus	Poisson's Ratio	Bulk Modulus	Shear Modulus
Mortar	65%	37900	0.18	19739	16059
Aggregate	35%	89900	0.18	46823	38093

Table 1: *Elastic moduli of Concrete grain structure.*

2.1 Rule of Mixtures:

The rule of mixture models are derived from the mechanics of materials approach. The key feature of the mechanics of materials approach is that certain specifying assumptions must be made regarding the mechanical behavior of a composite material in order to get an effective solution. A typical RVE is shown in Figure 3.

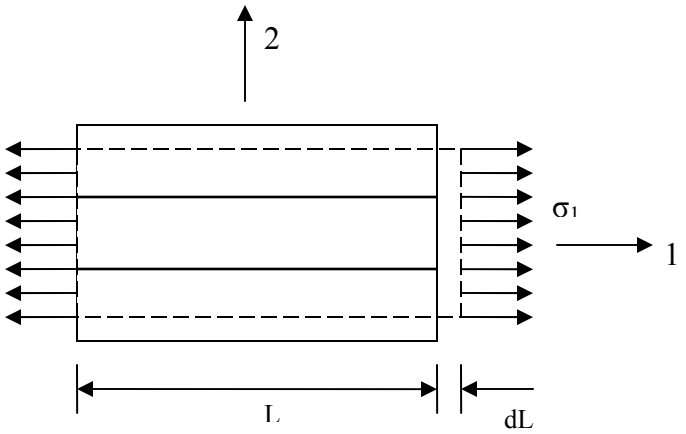

Figure 3: *RVE loaded in the 1-Direction*

It consists only the fiber and the matrix. This representation is applicable to both the $x_1 - x_2$ and $x_1 - x_3$ planes, and it is valid for a transversely isotropic symmetry. The only defining parameters are elastic constants and the volume fraction of the phases, and were independent of the phase geometry and spatial distribution. On the basis of this RVE, one can predict four elastic constants E_1, E_2, ν_{12} and G_{12}.

Determination of E_1:

The associated boundary conditions to find the E_1 is an axial strain ε_1 in the fiber direction.

$$\varepsilon_1 = dL / L \tag{2.1.1}$$

where ε_1 applies for both the bodies and matrix according to the basic assumption that the strain throughout the bulk material is uniform (iso-strain) after *Voigt (1889)* [7]. Then, if both constituent materials behave elastically, the stress in the fiber direction are

$$\sigma_f = E_f \varepsilon_1 \qquad\qquad \sigma_m = E_m \varepsilon_1 \tag{2.1.2}$$

The average stress σ_1 acts on cross-sectional area *A of the RVE,* σ_f acts on the cross-sectional area of the fibers A_f, and σ_m acts on the cross-sectional area of the matrix A_m. Thus the resultant force on the RVE is

$$P = \sigma_1 A = \sigma_f A_f + \sigma_m A_m \tag{2.1.3}$$

By substitution of Equation (2.1.2) in Equation (2.1.3) and recognition from macro-mechanics that

$$\sigma_1 = E_1 \varepsilon_1 \tag{2.1.4}$$

apparently

$$E_1 = E_f \frac{A_f}{A} + E_m \frac{A_m}{A} \tag{2.1.5}$$

But the volume fraction of the fibers and matrix can be written as

$$V_f = \frac{A_f}{A} \qquad V_m = \frac{A_m}{A}$$

Thus,

$$E_1 = E_f V_f + E_m V_m \tag{2.1.6}$$

Determination of E_2:

To determine the E_2, the associated boundary condition is to transverse stress σ_2 normal to the fiber direction. It is assumed that, the same transverse stress σ_2 is to be applied to both the fiber and the matrix [8].

The strains in the fiber and in the matrix are, therefore, found from the stress:

$$\varepsilon_f = \frac{\sigma_2}{E_f} \quad , \quad \varepsilon_m = \frac{\sigma_2}{E_m} \tag{2.1.7}$$

The transverse dimension over which, on average, ε_f acts is approximately $V_f W$, where as ε_m acts on $V_m W$. Thus, the total transverse deformation is

$$dW = \varepsilon_2 W = V_f W \varepsilon_f + V_m W \varepsilon_m \tag{2.1.8}$$

$$\varepsilon_2 = V_f \frac{\sigma_2}{E_f} + V_m \frac{\sigma_2}{E_m} \tag{2.1.9}$$

but from the macroscopic stress-strain relation

$$\sigma_2 = E_2 \varepsilon_2 = E_2 \left[V_f \frac{\sigma_2}{E_f} + V_m \frac{\sigma_2}{E_m} \right] \tag{2.1.10}$$

Where upon

$$\frac{1}{E_2} = \frac{V_f}{E_f} + \frac{V_m}{E_m} \tag{2.1.11}$$

Determination of ν_{12}:

The so called major Poisson's ratio ν_{12} is determined by an approach similar to the analysis for E_1.

$$\nu_{12} = \nu_m V_m + \nu_f V_f \tag{2.1.12}$$

Determination of G_{12}:

The in-plane shear modulus of modulus of lamina G_{12} is determined by presuming that the shearing stresses on the fiber and on the matrix are the same. So this condition yields the axial shear modulus G_{12}:

$$\frac{1}{G_{12}} = \frac{V_f}{G_f} + \frac{V_m}{G_m} \tag{2.1.13}$$

Where G_f and G_m are the shear modulus of the fiber and matrix, respectively.

The rule of mixture provides a quick estimation of the effective moduli in a simple way. The four constants describe the composites under plane-stress conditions. Since the fiber packing in the $2-3$ plane is omitted in the RVE description, the effective moduli in the $2-3$ plane cannot be determined. Moreover, in solving the B-V problems, one-dimensional stress state is assumed. These simplifications lead to inaccurate micro stress and strain fields in the RVE.

Using the Young's modulus, Poisson's ratio and Shear modulus of the components of concrete grain structure in Table 1, we can calculate the Voigt and Reuss bounds on the effective moduli of the composite. These values are shown in Table 2.

Elastic Moduli	E_{11}	E_{22}	G_{12}
at 35% Vol.Fraction	56100	47520	20135

Table 2: *The Effective Elastic Moduli from the Voigt and Reuss bounds*

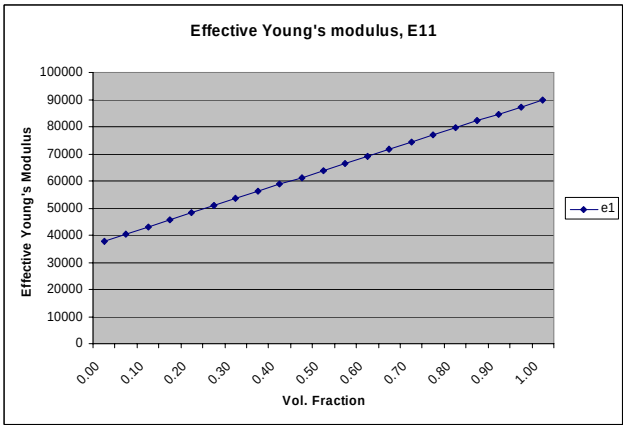

Figure 4: *Variation of* E_{11} *as a function of Volume Fraction*

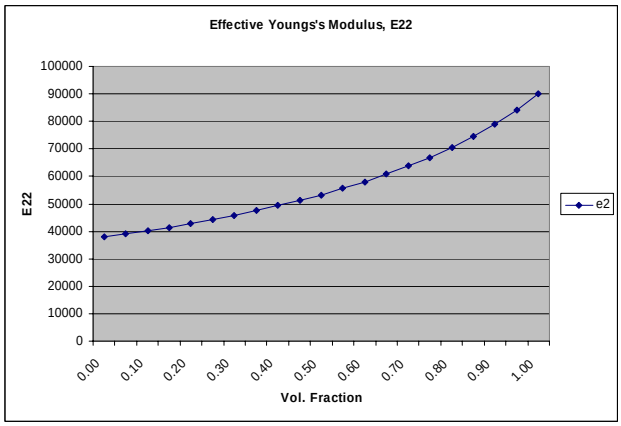

Figure 5: *Variation of* E_{22} *as a function of Volume Fraction*

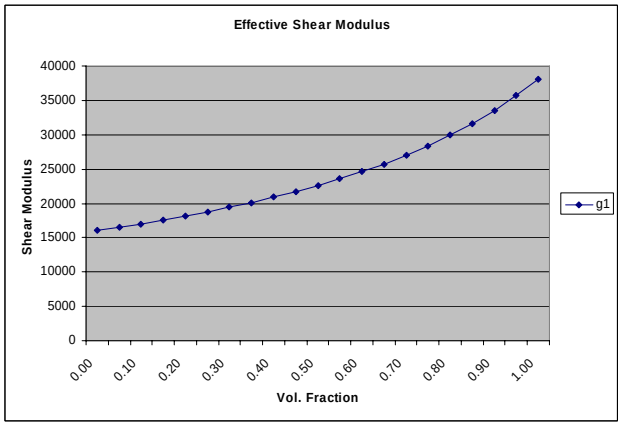

Figure 6: *Variation of* G_{12} *as a function of Inclusion Volume Fraction*

2.2. Variational Bounding Techniques

Paul was apparently the first to use the Variational bounding techniques of linear elasticity to examine the bounds on the moduli of the multiphase materials. These bounding models involve the application of the minimum energy principles to set the bounds for the effective moduli [9]. Development of these approaches is as follows:

Suppose the exact boundary conditions on the selected RVE could be specified; the induced micro fields can be computed exactly. The averaged stresses $\overline{\sigma}_{ij}$ and strains $\overline{\varepsilon}_{ij}$ are expressed through (1.1) and (1.2); and the strain energy stored in the RVE is given by

$$U = \frac{1}{V}\int_V \frac{1}{2}\sigma_{ij}\varepsilon_{ij}dV \tag{2.2.1}$$

where V is the volume of the RVE.

Now, for the composite (i.e. the RVE) as a continuum, the stresses and strains in the RVE under the same boundary conditions are given by (1.1) and (1.2); the associated strain energy stored therein is given by

$$\overline{U} = \frac{1}{V}\int_V \frac{1}{2}\overline{\sigma}_{ij}\overline{\varepsilon}_{ij}dV \tag{2.2.2}$$

Now, if the energies in (2.2.1) and (2.2.2) are equal, the effective constants in the homogenized RVE are uniquely determined. Since the exact boundary conditions on the RVE are unknown before the true micro fields are obtained, a linear displacement condition may be prescribed on the RVE boundary

$$u_i^0 = \varepsilon_{ij}^0 x_j, \tag{2.2.3}$$

where ε_{ij}^0 are the boundary strains. This results in a uniform strain field ε_{ij}^0 in the homogenized RVE. Moreover, the associated stress field is computed through the generalized Hook's law: $\overline{\sigma}_{ij} = C_{ijkl}\varepsilon_{kl}^0$. The field is also uniform throughout the RVE. The strain energy stored therein is given by

$$\overline{U}^{\varepsilon^0} = \frac{1}{V}\int_V \frac{1}{2}C_{ijkl}\varepsilon_{kl}^0\varepsilon_{ij}^0 dV \tag{2.2.4}$$

Now, if the micro fields in the RVE under the same boundary condition in (2.2.3) are solved, the stored energy U^{ε^0} is computed using (2.2.1). It follows from the principle of minimum potential energy that

$$\overline{U}^{\varepsilon^0} \le U^{\varepsilon^0} \tag{2.2.5}$$

By the equality in (2.2.5), the upper bounds for the effective stiffness in C_{ijkl} are determined.

Alternatively, a uniform surface traction may be prescribed on the RVE:

$$T_i^0 = \sigma_{ij}^0 n_j \tag{2.2.6}$$

This produces a uniform stress field σ_{ij}^0 in the RVE as a continuum. The corresponding Strain field is computed through $\overline{\varepsilon}_{ij} = S_{ijkl}\sigma_{kl}^0$. The latter is also uniform throughout the RVE. The stored strain energy is given by

$$\overline{U}^{\sigma^0} = \int_V \frac{1}{2} S_{ijkl}\sigma_{kl}^0\sigma_{ij}^0 dV \tag{2.2.7}$$

The micro fields in the RVE under the same boundary condition of (2.2.6) can be solved rigorously; the stored strain energy U^{σ^0} is computed again through (2.2.1). It follows from the principle of minimum complementary energy that

$$\overline{U}^{\sigma^0} \le U^{\sigma^0} \tag{2.2.8}$$

The upper bounds for the effective compliance in S_{ijkl} are determined by the equality of (2.2.8). The inverse of S yields C; the upper bounds for S_{ijkl} correspond to the lower bounds for C_{ijkl}.

Paul was the first to use the bounding techniques. His work was directed toward analysis of the elastic moduli of alloyed metals rather than toward composite materials. Accordingly the treatment is for an isotropic composite material made of different isotropic constituents. The composite material is isotropic because the alloyed constituents are uniformly dispersed have no preferred orientation. Obviously, the bounds are far apart.

Hashin [10] and *Hashin and Shtrikman* [11] attempted to tighten the *Paul's* bounds to obtain more useful estimates of moduli for isotropic heterogeneous materials.

According to Hashin [10], the bounds for the effective elastic moduli will be derived by assuming that the particles are spherical and that the action of whole heterogeneous material on any one inclusion is transmitted through a spherical shell, which lies wholly in the matrix. The included spheres never touch one another in the model, although clearly as the volume percentage of particles increases, so does the likelihood of particle contact. Moreover, lack of contact might imply perfect particle spacing, an unlikely situation from the practical stand point.

Hashin and Shtrikman [11] further extended their work by involving the *elastic polarization tensor*, to the derivation of upper and lower bounds for the effective elastic moduli of quasi-isotropic and quasi-homogeneous multiphase materials of arbitrary phase geometry. When the ratios between the different phase moduli are not too large the bounds derived are close enough to provide a good estimate for the elastic moduli. For the particulate two phase composite materials these bounds, lower (K_1^*) and upper (K_2^*) can be written as

$$K_1^* = K_1 + \frac{V_2}{\frac{1}{K_2 - K_1} + \frac{3V_1}{3K_1 + 4G_1}} \tag{2.2.9}$$

$$G_1^* = G_1 + \frac{V_2}{\frac{1}{G_2 - G_1} + \frac{6(K_1 + 2G_1)V_1}{5G_1(3K_1 + 4G_1)}} \tag{2.2.10}$$

$$K_2^* = K_2 + \frac{V_1}{\frac{1}{K_1 - K_2} + \frac{3V_2}{3K_2 + 4G_2}} \tag{2.2.11}$$

$$G_2^* = G_2 + \frac{V_1}{\frac{1}{G_1 - G_2} + \frac{6(K_2 + 2G_2)V_2}{5G_2(3K_2 + 4G_{21})}} \tag{2.2.12}$$

where $K_2 > K_1;\ G_2 > G_1; V_2 + V_1 = 1$.

Using the Young's modulus, Bulk Modulus and Shear modulus of the components of concrete grain structure in Table 1, we can calculate the upper and lower bounds on the effective moduli of the composite at *35% volume fraction* of inclusion material. These values are shown in Table 3.

Elastic Moduli	*Bulk Modulus*	*Shear Modulus*
Upper Bound	27325	22143
Lower Bound	26378	21380

Table 3: *Hashin-Shtrikman upper and lower bounds for concrete structure*

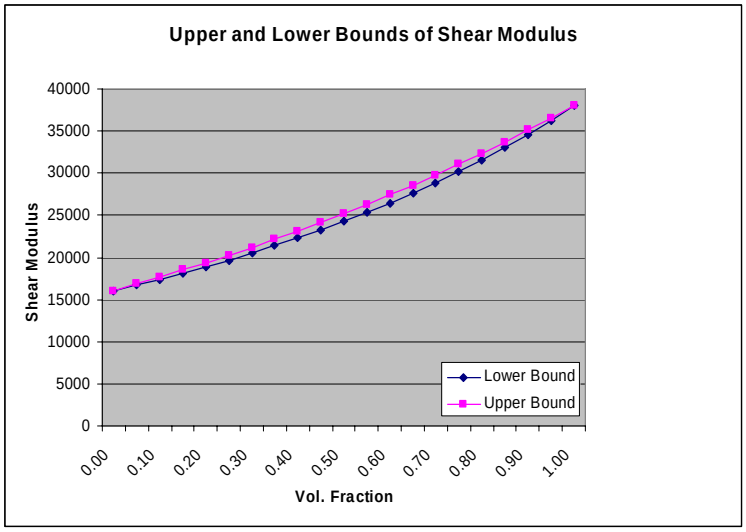

Figure 7: *Variation of* K_1^* *and* K_2^* *with Inclusion Volume Fraction*

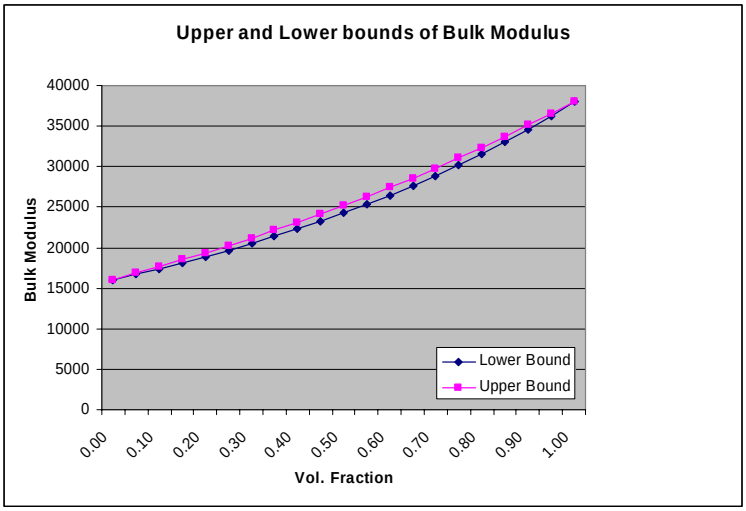

Figure 8: *Variation of* G_1^* *and* G_2^* *with Inclusion Volume Fraction*

2.3. Self Consistency Method

Predictions of macroscopic properties of two-phase solid composites have mostly been restricted to stating universal bounds on various overall elastic moduli *(Hashin 1965)*. Such bounds depend only on the relative volumes and do not reflect any geometry, except when one phase consists of continuous aligned fibers *(Hashin and Rosen 1964)*. However when one phase is dispersion of ellipsoidal inclusions, not necessarily dilute, a much more direct approach is available. This is the self consistency Method of *Hershey (1954)* and *Kroner (1957)* was originally proposed for aggregates of crystals and then reviewed and elaborated by *Hill (1965)*[14].

The method draws on the familiar solution to an auxiliary elastic problem. In particular, it assumes that interaction of phases is accounted for by imagining each phase to be an inclusion embedded in a homogeneous medium that has the over all properties (C, S) of the composite. To proceed, denote here the inclusion and matrix by subscripts 1 and 2 respectively. From the elementary relations between the phase and the overall averages of stress:

$$V_1(\bar{\sigma}_1 - \bar{\sigma}) + V_2(\bar{\sigma}_2 - \bar{\sigma}) = 0 \tag{2.3.1}$$

The basic postulate of the Self Consistent Method suggests that

$$\bar{\sigma}_1 - \bar{\sigma} = C^*(\bar{\varepsilon} - \bar{\varepsilon}_1) \tag{2.3.2}$$

and from Equation (2.3.1),

$$\bar{\sigma}_2 - \bar{\sigma} = C^*(\bar{\varepsilon} - \bar{\varepsilon}_2) \tag{2.3.3}$$

Evidently, both the phases are regarded on the same footing (concentration factors for both the inclusion and the matrix are derived from the same C^*). It means that the same overall moduli are predicted for another composite in which the roles of the phases are reversed.

Equations (2.3.2) and (2.3.3), which may as well now be taken together, can be rearranged as

$$(C^* + C_1)\bar{\varepsilon}_1 = (C^* + C_2)\bar{\varepsilon}_2 = (C^* + C)\bar{\varepsilon} \tag{2.3.4}$$

The above equation is can be solved for the effective stiffness of the composite for various particle shapes. This procedure is called "Self Consistent Scheme". These self consistent approximations have been found to generate excellent effective properties at low concentrations of the dispersed component. However, at high concentrations when the modulus contrast between the components is large, these methods do not perform well.

For particulate composite containing a dispersion of elastic spheres, the self-consistent scheme leads to two equations in K^* and G^* which have to be solved iteratively. These are:

$$K^* = K_2 + \frac{V_1 K^* (K_1 - K_2)}{K^* + \left(\frac{3K^*}{3K^* + 4G^*}\right)(K_1 - K^*)} \tag{2.3.5}$$

$$G^* = G_2 + \frac{V_1 G^* (G_1 - G_2)}{K^* + \left(\frac{6K^* + 12G^*}{15K^* + 10G^*}\right)(G_1 - G^*)} \tag{2.3.6}$$

where

$K^* \equiv$ effective bulk modulus of the composite material,

$G^* \equiv$ effective shear modulus of the composite material,

$K_1 \equiv$ bulk modulus of the inclusion material,

$G_1 \equiv$ shear modulus of the inclusion material,

$K_2 \equiv$ bulk modulus of the matrix material,

$G_2 \equiv$ shear modulus of the matrix material, and,

$V_1 \equiv$ volume fraction of the inclusion material.

For the components of concrete grain structure, these equations leads to the effective bulk and shear moduli are shown in Table 4

Elastic Moduli	Shear Modulus	Bulk Modulus
at 35% Vol.fraction	21042	26667

Table 4: *Self Consistent Scheme prediction for Concrete Structure*

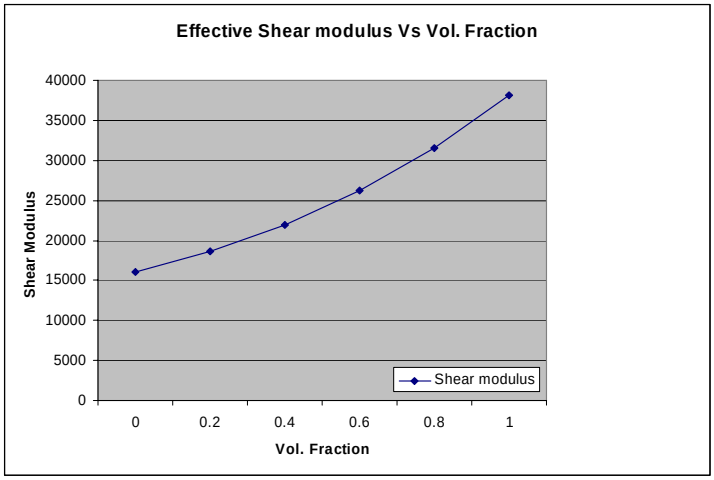

Figure 9: *Variation of K^* with Inclusion Volume Fraction*

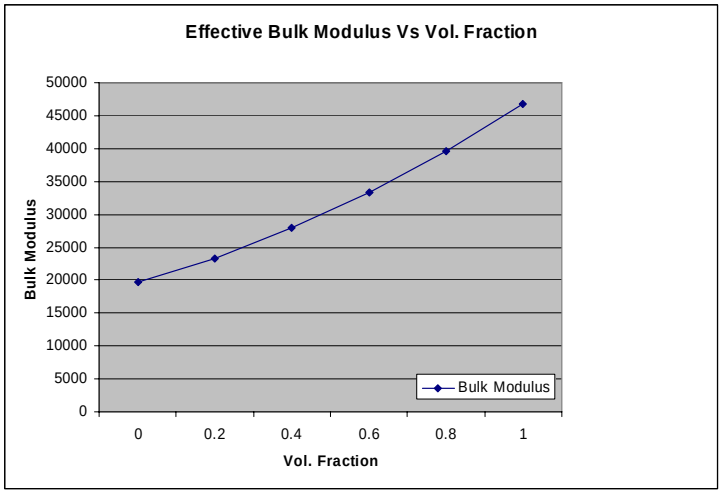

Figure10: *Variation of G^* with Inclusion Volume Fraction*

2.4 Mori-Tanaka (reformulated by Benveniste 1987):

The Mori-Tanaka method (Mori and Tanaka, 1973) was originally concerned with calculating the average internal stress in matrix of a material containing precipitates with eigenstrains [16]. Benveniste (1987) reformulated it so that it could be applied to composite materials [17]. He considered anisotropic phases and ellipsoidal phases. From the homogeneous boundary conditions on the displacements and tractions

$$u(S) = \varepsilon^0 x\,, \qquad \sigma(S) = \sigma^0 n \tag{2.4.1}$$

where $u(S)$ and $\sigma(S)$ denote the displacements and traction vectors respectively, S is the external surface of the composite, ε^0 and σ^0 are constant strain and stress tensors, and n denotes the exterior normal to the surface S. These dual set of boundary conditions is useful in defining the effective stiffness and compliance tensors of composite media.

Under the set of equations (2.4.1), we respectively have

$$\bar{\varepsilon} = V_1\bar{\varepsilon}^{(1)} + V_2 < \bar{\varepsilon}^{(2)} >= \varepsilon^0 \tag{2.4.2}$$

$$\bar{\sigma} = V_1\bar{\sigma}^{(1)} + V_2 < \bar{\sigma}^{(2)} >= \sigma^0 \tag{2.4.3}$$

Where $< \bar{\varepsilon}^{(2)} >$ and $< \bar{\sigma}^{(2)} >$ are the overall possible average orientation dependent strain and stress tensors in a typical individual inclusion, $\bar{\varepsilon}^{(1)}$ and $\bar{\sigma}^{(1)}$ are the average quantities in the matrix, and finally $\bar{\varepsilon}$, $\bar{\sigma}$ denote the overall average strain and stress tensors.

The effective stiffness tensor C^* is defined as

$$\bar{\sigma} = C^*\bar{\varepsilon} \tag{2.4.4}$$

and with the idea of a concentration matrix we have that the effective properties can be defined as

$$C^* = C^{(1)} + V_2\left(C^{(2)} - C^{(1)}\right)A_{2,} \tag{2.4.5}$$

Where $C^{(1)}$ and are the stiffness tensors of the phases, and the orientation dependent tensor $A_{2,}$ called 'concentration factor' in the literature, is defined through

$$\bar{\varepsilon}^{(2)} = A_2\varepsilon^0 \tag{2.4.6}$$

We define the concentration tensor, A_2 , from the dilute approximation, as

$$A_2 \equiv T \tag{2.4.7}$$

Where T can be written in terms of Eshelby's tensor, P , as

$$T = \left[I + P\left[C^{(1)}\right]^{-1}\left(C^{(2)} - C^{(1)}\right)\right]^{-1} \tag{2.4.8}$$

Where I is the fourth order identity tensor. This approximation, due to the dilute model, neglects particle interactions and so is most valid at dilute concentrations. To extend this method assume that there exits a tensor such that

$$\bar{\varepsilon}^{(2)} \approx M\bar{\varepsilon}^{(1)} \tag{2.4.9}$$

Using Equations (2.4.5), (2.4.6) and (2.4.9)

The approximation in this method is that

$$M = T \tag{2.4.10}$$

therefore

$$C^* = C^{(1)} + V_2(C^{(2)} - C^{(1)})T(V_1 I + V_2 T)^{-1} \tag{2.4.11}$$

and similarly for the effective compliance tensor. Benveniste also showed that these results are consistent in the sense that

$$S^* = \left(C^*\right)^{-1} \tag{2.4.12}$$

Finally,

$$\frac{\varepsilon_{kk}^{(2)}}{\varepsilon_{kk}^{0}} = \left(3K_1 + 4G_1\right)/\left(3K_2 + 4G_1\right) \tag{2.4.13}$$

and the effective bulk modulus is

$$K^* = K_1 + V_2(K_2 - K_1)\frac{K_1}{(1-V_2)(K_2 - K_1)\alpha_1 + K_1} \tag{2.4.14}$$

and

$$\alpha_1 = \frac{3K_1}{(3K_1 + 4G_1)} \tag{2.4.15}$$

For the components of concrete grain structure, these equations leads to the effective bulk is shown in Table 5

Effective Moduli	Bulk Modulus
at 35% Vol.Fraction	26378

Table 5: *Mori-Tanaka Scheme prediction for Concrete Structure*

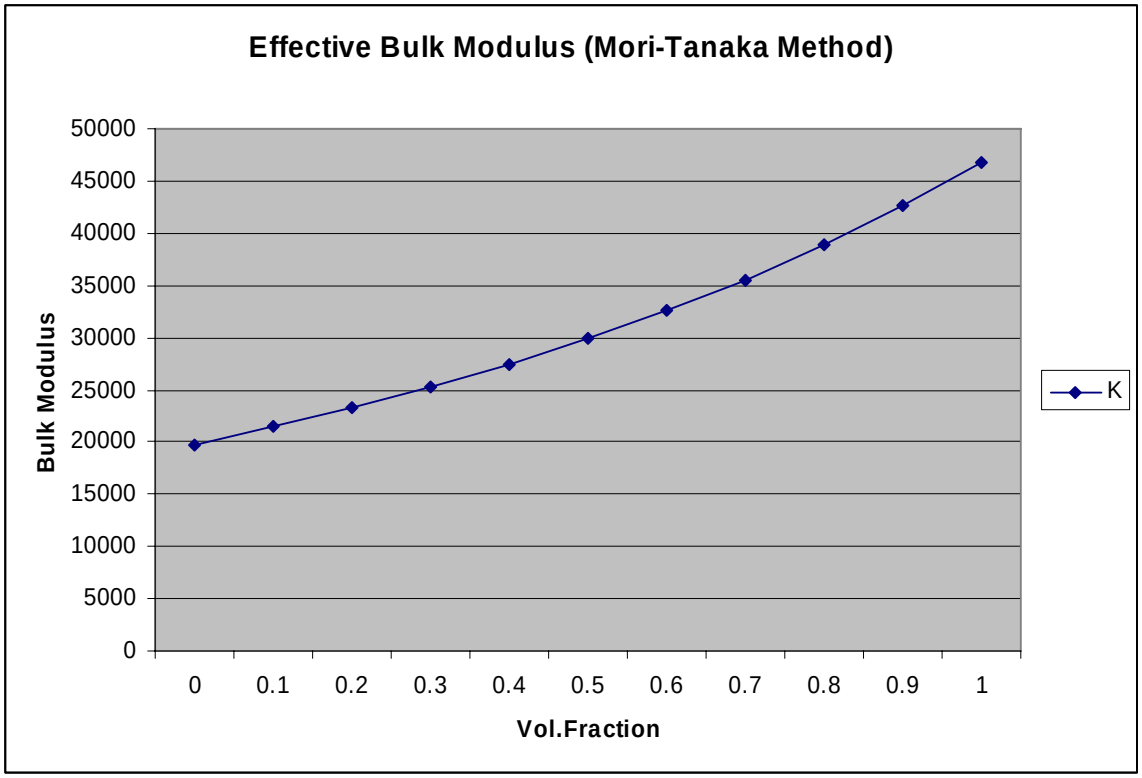

Figure 11: *Variation of* K^* *with Inclusion Volume Fraction*

3. Numerical Techniques for Heterogeneous Materials

3.1 Introduction

Even if analytical and semi analytical models have been developed to homogenize composites, they are often reduced to specific cases. Numerical models seem to be a well suited approach to describe the behaviour of these materials, because there is no restriction on the geometry, on the material properties, on the number of phases in the composite, and on the size. Therefore finite element method has been used to determine the effective properties of the composites. Hence the prediction of the mechanical effective properties has been an active research area for the few decades. Except for the experimental studies, either micro- or macro mechanical methods are used to obtain the overall properties of composites. Micromechanical method provides overall behaviour of the matrix-inclusion composites from known properties of their constituents (inclusion and matrix) through an analysis of Representative Volume Element (RVE) or a unit-cell model. In the macro mechanical approach, on the other hand, the heterogeneous structure of the composite is replaced by a homogeneous medium with anisotropic properties. The advantage of the micromechanical approach is not only the global properties of the composites but also various mechanisms such as damage initiation and propagation, can be studied through the analysis.

Uni-directional fiber composites can be analyzed by using Asymptotic Homogenization Method. Inclusion problems can be analyzed by self-consistent methods. Although other analytical methods are also available, all these methods are restricted by the geometry of the inclusion, the number of phases, the material properties etc. In order to overcome all these difficulties, numerical methods (e.g. FEM techniques) have been developed to evaluate the effective coefficients of composites.

However, actual microstructures of composites are difficult to obtain and simulate, most finite element simulations of the micromechanics of composites have involved square or hexagonal arrays of fibers in two dimensions. With decreasing computational costs, complex two-dimensional and three-dimensional problems in the micromechanics of composites are being investigated with finite elements.

3.2 The Representative Volume Element:

Primary to use of numerical approximations of the effective properties of composite is the concept of representative volume element (RVE). Square or cubic RVEs are used for most numerical approximations because of the ease of numerically solving boundary values problems with these geometries. The difficulties involved in generating statistical information about particle distributions and concentrations leads to difficulties in the rigorous determination of RVE sizes. Hence, for most applications, RVE sizes have been rather arbitrary.

Sab [18] has shown that if an RVE exists for a random composite material, the homogenized properties of the material can be calculated by the simulation of one single realization of the medium. The "ergodic" hypothesis, which assumes that the ensemble average is equal to the volume average, has been used to arrive at this conclusion. The ensemble average is the mean of a large number of realizations of the microstructure. The volume average, on the other hand, is the average as the RVE volume becomes infinitely large compared to the volume of a particle. However, such a realization may lead to an extremely large RVE and a more practical approach is to simulate a large number of different realizations on smaller RVEs so that bounds on the effective properties are obtained.

3.3 Random Distribution in Two Dimensions:

Models using regular arrays of fibers provide reasonably good approximations of the effective elastic properties of fiber composites. However, for particulate composites, it is not true and the complex microstructure has to be taken into account. This implies that three-dimensional models are required. The high computational cost involved in modeling particulate composite microstructures in three dimensions leads to the development of two-dimensional techniques that perform well for some of these composites.

Ramakrishnan et al. [19] have used a generalized plane strain approach to model particulate metal matrix composites. The composite considered in the study had a maximum volume fraction of 40% of particles. Particles of various shapes and sizes were

randomly distributed in two-dimensional square RVE. The effective Young's modulus was determined by the application of a uniform unidirectional displacement. The effective bulk modulus was determined by applying equal displacements in the orthogonal directions. The effective Poisson's ratio was determined from the effective bulk and Young's moduli. It is observed that the shape of the particles do not have any significant effect on the effective elastic moduli even though many particles have sharp acute angles and therefore high stress concentrations. Periodic boundary conditions are not used in the approach. The RVE size is also chosen arbitrarily. The use of the bulk modulus to determine the Poisson's ratio assumes that the material is isotropic. However, the two-dimensional approximation automatically implies that each particle extends continuously in the out-of-plane direction and hence makes the material anisotropic.

Random distributions of particles in two dimensions have also been studied by Theocaris et al. [20] in the context of determining the effective Poisson's ratio. Finite element simulations were carried out on a unit cell. Periodic boundary conditions and uniform pre-stresses were applied to the unit cell. The effective elastic properties were determined using a strain energy match between a cell simulating the microstructure and as equivalent homogeneous cell.

3.4 Homogeneous boundary conditions:

In classical lamination theory the composite lamina is modelled as a homogeneous orthotropic medium with certain effective moduli that describe the 'average' material properties of the composite. To describe this macroscopically homogeneous medium, macro-stress and macro-strain are derived by averaging the stress and strain tensor over the volume of the RVE:

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV \tag{3.1}$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \tag{3.2}$$

The equivalence between the actual heterogeneous composite medium and the homogeneous medium given by the average stresses and strains and the effective elastic constants needs to be reviewed. For this purpose we subject the RVE to appropriate

boundary displacements ($u_i(S) = \bar{\varepsilon}_{ij} x_j$) or boundary tractions ($t_i(S) = \bar{\sigma}_{ij} n_j$) to produce uniform strains ($\bar{\varepsilon}_{ij}$) and uniform stresses ($\bar{\sigma}_{ij}$) in a homogeneous medium.

The total strain energy U stored in the volume V of the effective medium is:

$$U = \frac{1}{2} \bar{\sigma}_{ij} \bar{\varepsilon}_{ij} V \tag{3.3}$$

The strain energy stored in the heterogeneous RVE of the volume is:

$$U' = \frac{1}{2} \int_V \sigma_{ij} \varepsilon_{ij} dV \tag{3.4}$$

$$= \frac{1}{2} \int_V \sigma_{ij} (\varepsilon_{ij} - \bar{\varepsilon}_{ij} + \bar{\varepsilon}_{ij}) dV \tag{3.5}$$

$$= \frac{1}{2} \int_V \sigma_{ij} (\varepsilon_{ij} - \bar{\varepsilon}_{ij}) dV + \frac{1}{2} \bar{\varepsilon}_{ij} \int_V \sigma_{ij} dV \tag{3.6}$$

$$= \frac{1}{2} \int_V \sigma_{ij} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial \bar{u}_i}{\partial x_j} \right) dV + \frac{1}{2} \bar{\sigma}_{ij} \bar{\varepsilon}_{ij} V \tag{3.7}$$

Subtracting equation (3.3) from equation (3.7) yields:

$$U' - U = \frac{1}{2} \int_V \sigma_{ij} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial \bar{u}_i}{\partial x_j} \right) dV \tag{3.8}$$

Using the equilibrium equation:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{3.9}$$

we can write equation (3.8) as:

$$U' - U = \frac{1}{2} \int_V \frac{\partial}{\partial x_j} \left[\sigma_{ij} (u_i - \bar{u}_i) \right] dV \tag{3.10}$$

The volume integral in equation (3.10) can be converted in to a surface integral by using Gauss theorem. Thus:

$$U' - U = \frac{1}{2} \int_S \sigma_{ij} (u_i - \bar{u}_i) n_j dS \tag{3.11}$$

where S is the surface and n the unit outward normal. On the surface S:

$$u_i = \bar{u}_i \tag{3.12}$$

Thus:

$$U' - U = 0 \tag{3.13}$$

The average stress and strain quantities defined in equations (3.1) and (3.2) thus ensure equivalence in strain energy between the equivalent homogeneous material and the original heterogeneous material. These average quantities will be used in the subsequent analysis to determine composite moduli.

3.5 Finite Element Analysis of concrete grain RVE:

In general the object is regarded as a large-scale/macroscopic structure. The common approach to model the macroscopic properties of composites is to create a representative volume element (RVE) or a unit-cell that captures the major features of the underlying microstructure. The mechanical and physical properties of the constituent material are always regarded as a small-scale/micro structure. One of the most powerful tools to speed up the modelling process, both the composite discretization and the computer simulation of composites in real conditions, is the homogenization method. The main idea of the method is to find a globally homogeneous medium equivalent to the original composite, where the strain energy stored in both systems is approximately the same. In this paper we limit ourselves to a quasi-static analysis of concrete grain structures with perfectly bonded elliptic shaped aggregate particulates. Here we choose elliptic shaped aggregate particulates of different sizes. The Figure 12 shows the schematic diagram of the RVE selected from the heterogeneous concrete block having dimensions of 100 x 100mm. The particles of dispersed component of the composite (aggregates) are distributed in three dimensions. Hence, accurate models of these composites should be three-dimensional. However, for simplicity, we primarily explore two-dimensional models in this work.

In the FE analysis of concrete grain particulate composite, the material is assumed to be *orthotropic* and for simplified analysis *plane stress state* is taken into account. A plane stress state is defined by setting

$$\sigma_3 = 0\,, \qquad \tau_{23} = 0\,, \qquad \tau_{31} = 0 \tag{3.14}$$

so that

$$\sigma_1 \neq 0\,, \qquad \sigma_2 \neq 0\,, \qquad \tau_{12} \neq 0 \tag{3.15}$$

The plane stress state is not a merely an idealization of reality, but instead is a practical and achievable objective of how we must use a RVE in its plane.

When referred to the principal material directions, a plane stress state is characterized by:

$$\sigma_i \neq 0 \quad \text{if } i = 1,2,6 \qquad \text{and} \qquad \varepsilon_i \neq 0 \text{ if } i = 1,2,3,6 \tag{3.16}$$

$$\sigma_i = 0 \text{ if } i = 3,4,5 \qquad \text{and} \qquad \varepsilon_i = 0 \text{ if } \quad i = 4,5 \tag{3.17}$$

The elastic equations can be written in one of the two forms:

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & 0 \\ S_{12} & S_{22} & 0 \\ 0 & 0 & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_{21} \\ \tau_{12} \end{bmatrix} \tag{3.18}$$

with

$$\varepsilon_3 = S_{13}\sigma_1 + S_{23}\sigma_2 \tag{3.19}$$

where

$$S_{11} = \frac{1}{E_1} \quad S_{22} = \frac{1}{E_2} \quad S_{12} = -\frac{\nu_{12}}{E_1} = -\frac{\nu_{21}}{E_2} \quad S_{66} = \frac{1}{G_{66}} \tag{3.20}$$

or

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \tau_{12} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{12} & Q_{22} & 0 \\ 0 & 0 & Q_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \gamma_{12} \end{bmatrix} \tag{3.21}$$

with

$$\varepsilon_3 = -\frac{1}{C_{33}}(C_{13}\varepsilon_1 + C_{23}\varepsilon_2). \tag{3.22}$$

where Q_{ij} are the so called reduced stiffness for a plane stress state in the $1-2$ plane.

$$Q_{ij} = C_{ij} - \frac{C_{i3}C_{j3}}{C_{33}} \qquad i, j = 1,2,6 \tag{3.23}$$

The term C_{63} is zero because no shear-extension coupling exists for an orthotropic material in principal material directions. For the orthotropic material Q_{ij} are:

$$Q_{11} = \frac{S_{22}}{S_{11}S_{22} - S_{12}^2} \qquad Q_{22} = \frac{S_{11}}{S_{11}S_{22} - S_{12}^2} \tag{3.24}$$

$$Q_{12} = \frac{S_{12}}{S_{11}S_{22} - S_{12}^2} \qquad Q_{11} = \frac{1}{S_{66}} \tag{3.25}$$

or, in terms of the engineering constants,

$$Q_{11} = \frac{E_1}{1 - \nu_{12}\nu_{21}} \qquad Q_{22} = \frac{E_2}{1 - \nu_{12}\nu_{21}} \tag{3.26}$$

$$Q_{12} = \frac{\nu_{12}E_2}{1 - \nu_{12}\nu_{21}} = \frac{\nu_{21}E_1}{1 - \nu_{12}\nu_{21}} \qquad Q_{66} = G_{12} \tag{3.27}$$

3.6 Calculation of different effective coefficients of cement concrete composites using RVE:

In the following we consider aggregate particulates embedded in a soft cement paste material (Mortar). In both the analytical and numerical modeling, we are assuming that the particulates and matrix are perfectly bonded.

3.6.1 Calculation of C_{11} and C_{12}

The Figure 12 shows the boundary conditions applied to the RVE in order to predict the effective coefficients C_{11} and C_{12}. To find these two effective coefficients the boundary conditions have to be applied to the RVE in such a way that, except the strain in the X direction, all other mechanical strains are zero. As a load, uniform unidirectional displacement (prescribed displacement condition) is applied on the edge A_1. The displacements in normal direction on the edges B_1 and B_2 are constrained to be zero. So that the strain in the X-direction is the only one, having finite value and all other strains are equal to zero. Then the averaged strain

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \tag{3.28}$$

Where ε_{ij} is the stain in each element of the FE model in X-direction, and average stress

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV \tag{3.29}$$

Where σ_{ij} is the stress in each element of the FE model in X-direction.

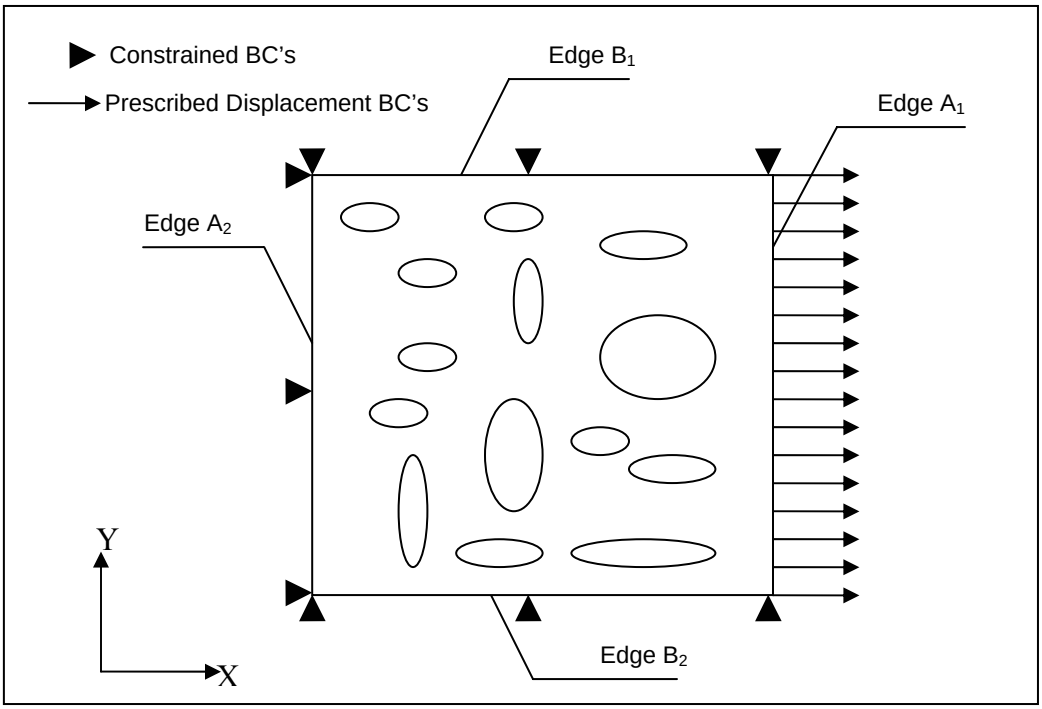

Figure 12: *Boundary Conditions applied to the RVE for evaluation of* C_{11} *and* C_{12}

So average stress $\bar{\sigma}_{ij}$ and the average strain $\bar{\varepsilon}_{ij}$ in the X-direction have been evaluated and inserted in to the constitutive equation to find the effective coefficient C_{11}. Therefore

$$C_{11} = \frac{\bar{\sigma}_{11}}{\bar{\varepsilon}_{11}} \tag{3.30}$$

To find the effective coefficient C_{12}, consider the average stress in Y-direction and average strain in X-direction and insert into constitutive equation. Therefore

$$C_{12} = \frac{\bar{\sigma}_{22}}{\bar{\varepsilon}_{11}} \tag{3.31}$$

3.6.2 Calculation of C_{22} and C_{12}

The Figure 13 shows the boundary conditions applied to the RVE in order to predict the effective coefficients C_{22} and C_{12}. To find these two effective coefficients the boundary conditions have to be applied to the RVE in such a way that, except the strain in the Y- direction, all other mechanical strains are zero. As a load, uniform unidirectional displacement (prescribed displacement condition) is applied on the edge B_1. The displacements in normal direction on the edges A_1 and A_2 are constrained to be zero. So that the strain in the Y-direction is the only one, having finite value and all other strains

are equal to zero. Then the averaged strain and the average stress in the Y-direction have to be evaluated in the similar to the above.

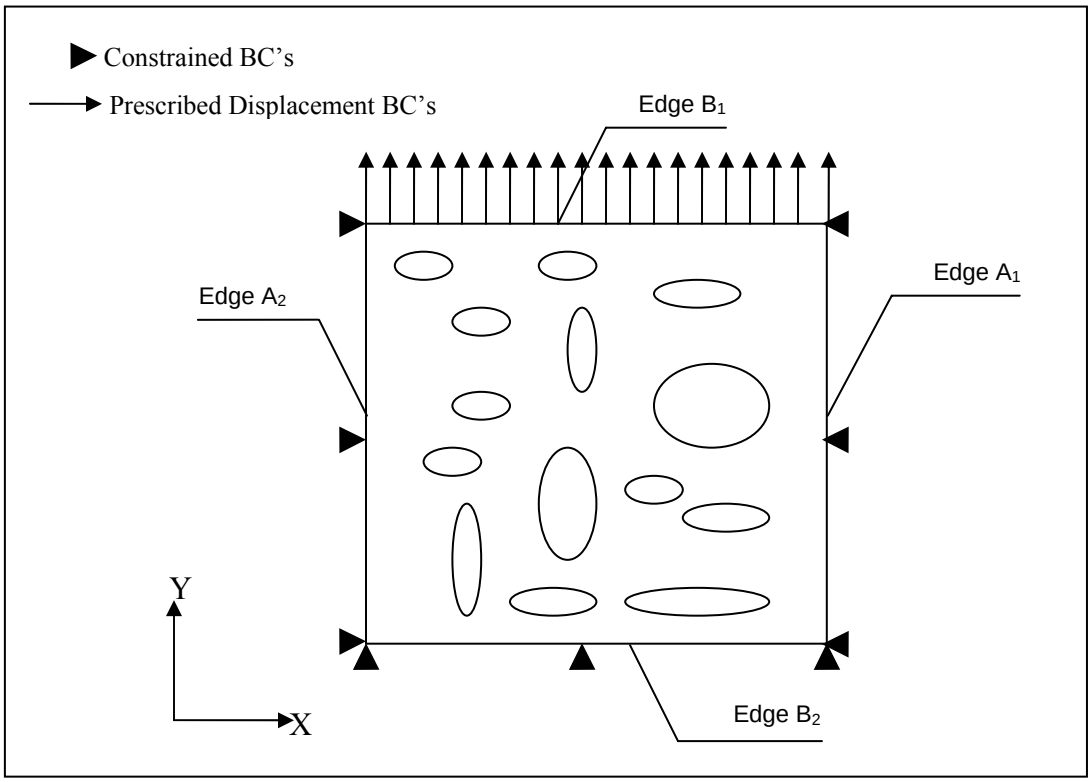

Figure 13: *Boundary Conditions applied to the RVE for evaluation of* C_{22} *and* C_{12}

With the average stresses and average strains, we can compute C_{22} from the constitutive relation:

$$C_{22} = \frac{\bar{\sigma}_{22}}{\bar{\varepsilon}_{22}} \tag{3.32}$$

Similarly C_{12} can be found as the ratio of

$$C_{12} = \frac{\bar{\sigma}_{11}}{\bar{\varepsilon}_{22}} \tag{3.33}$$

3.6.3 Calculation of C_{66}

The Figure 14 shows the boundary conditions applied to the RVE in order to predict the effective coefficient C_{66}. To find this effective coefficient the boundary conditions have to be applied to the RVE in such a way that, The lower corner node of the RVE is fixed in order to prevent the rigid body rotation and prescribed displacement BC's are applied

as shown in the Figure 14. On solving the problem, all the stresses and strains are equal to zero except the stress σ_{12} and strain ε_{12}. Then the averaged strain and the average stress have to be evaluated. From the constitutive relation, we can find the C_{66}.

$$C_{66} = \frac{\bar{\sigma}_{12}}{\bar{\varepsilon}_{12}} \tag{3.34}$$

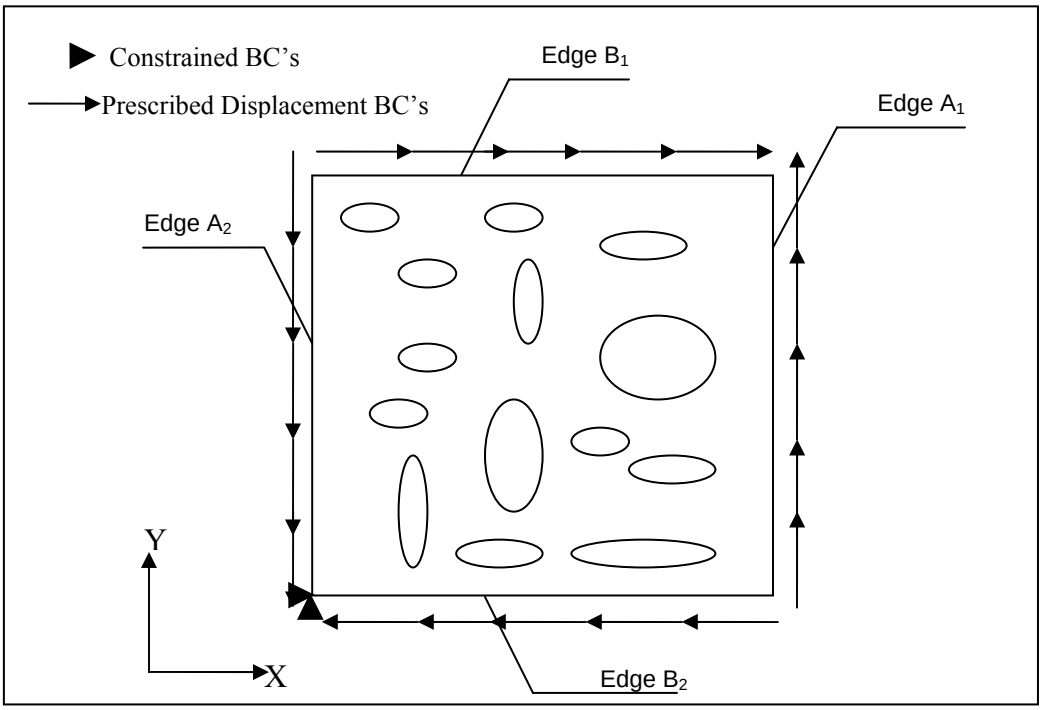

Figure 14: *Boundary Conditions applied to the RVE for evaluation of* C_{66}

Using the relations given in (3.26) and (3.27), we can deduce the effective elastic moduli $E_1, E_2, \nu_{12}, \nu_{21}$ and G_{12} for the given concrete grain composite. These values are shown in Table 6.

Elastic Moduli	E_1	E_2	ν_{12}	ν_{21}	K_{12}	G_{12}
35% Vol.Fraction	49446	49657	0.1846	0.1854	26079	20727.5

Table 6: *The Effective Elastic Moduli from the FE analysis*

Further the given FE model has been investigated for the sensitivity of effective properties due to different finite elements and element sizes. The results are shown in Table 7.

Effective Coefficient	*Type of ANSYS Element*				
	Shell63	*Plane 42*		*Plane82*	
		Plane stress	*Plane strain*	*Plane stress*	*Plane strain*
C11	51134	51199	53874	51230	53779
C12	9482	9493	11978	9513	12000
C22	51415	51417	53970	51350	54006
C66	20727	20727	20751	20777	20802

Table 7: *Effective coefficients of the composite for different ANSYS elements*

3.7 Comparison of shear and bulk moduli, which were derived from RVE with the results of the classical models:

Elastic Moduli	Voigt Bounds	Reuss Bounds	H-S Bounds		Self Consistency Method	Mori-Tanaka Method	FE Analysis
			Lower	Upper			
Shear Moduli	23771	20315	27589	28577	21042	-	20727
Bulk Moduli	29218	24750	34048	35258	26667	26378	26079

Table 8: *Effective coefficients of the composite from different models*

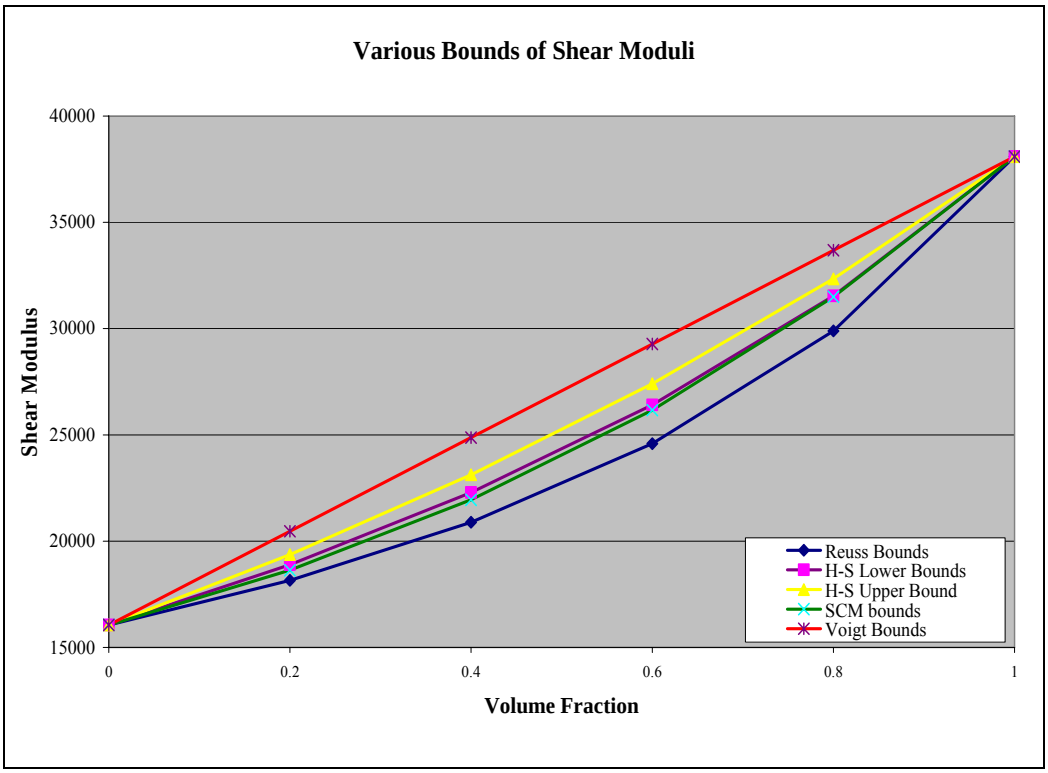

Figure 15: *Shear moduli of composite from various models*

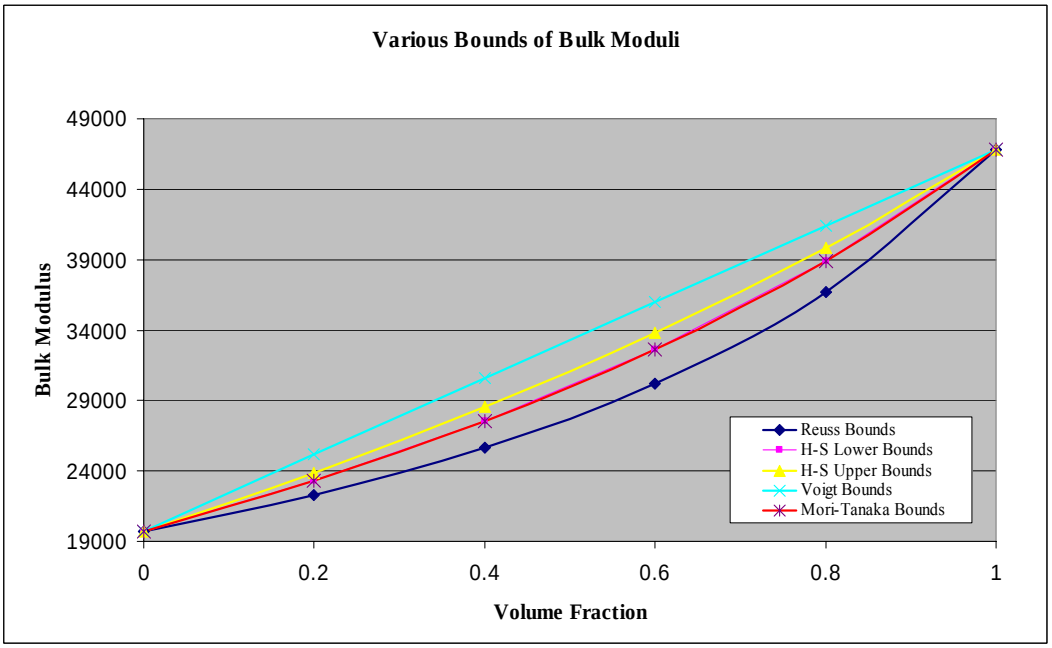

Figure 16: *Bulk moduli of composite from various models*

Appendix –A

FORTRAN Programs:

```
!  SELF_CONSISTANT_GEN.f90
!  SELF_CONSISTANT_GEN      - Entry point of console application.
!****************************************************************************
*
!  PROGRAM: SELF_CONSISTANT_GEN
!****************************************************************************
*
      program SELF_CONSISTANT_GEN

      ! Variables

      real k1,k2,kf,gf,vf
      real g1,g2,km,gm,vm,em,ef,p
      integer l
      kf=46823
      km=19740
      gf=38093
      gm=16059
      p=0.18
      k2=km
      g2=gm
      k1=0
      g1=0
      l=0
            open(1,file='scm.txt')

! Body of SELF_CONSISTANT_GEN

do   vf = 0 ,1, .2
       vm=1-vf
       l=0
      do while(l= =0)
        k1=km+(vf*k2*(kf-km)/(k2+(3*k2/(3*k2+4*g2)*(kf-k2))))
        g1=gm+(vf*g2*(gf-gm)/(g2+((6*k2+12*g2)/(15*k2+10*g2)*(gf-g2))))
        if((abs(k2-k1)/k2 < .00001) .and.(abs(g2-g1)/g2 < .00001))then
               l=1
            else
               k2=k1
               g2=g1
           endif
           end do
      write(1,*) vf,k1,g1,vm
end do

end program SELF_CONSISTANT_GEN
```

```
!  MORI_TANAKA.f90
!
!  FUNCTIONS:
!     MORI_TANAKA      - Entry point of console application.

!****************************************************************************
*
!
!  PROGRAM: MORI_TANAKA
!
!  PURPOSE:  Entry point for the console application.
!
!****************************************************************************
*

      program MORI_TANAKA

      implicit none

      ! Variables

      real k1,k2,g1,k3,v1,v2,a1
      integer i
      k1=19739.6
      k2=46822.9


      g1=16059

      open(2,file='mori.txt')

      ! Body of MORI_TANAKA

             v1=0
      v2=1-v1
      a1=(3*k1)/(3*k1+4*g1)
            do i = 0,20
      k3=k1+v1*(k2-k1)*(k1/((1-v1)*(k2-k1)*a1+k1))

      write(2,*) k3,v1,v2

      v1=v1+.05
      v2=1-v1
      end do
      end program MORI_TANAKA
```

Appendix –B

Ansys Input code:

```
/TITLE, Effective Coefficient C11
*ULIB, macbib,mac
/prep7
*USE, Ellipse,12.095026,8.303226,74.750660,41.057244,85.709053
*USE,Ellipse,11.944055,10.591417,26.799589,42.271072,20.528009
*USE,Ellipse,3.924256,3.085529,76.636222,66.679598,36.844768
*USE,Ellipse,6.828546,4.798289,44.447548,60.751316,142.398584
*USE,Ellipse,6.222256,5.694589,16.043153,63.133226,90.792615
*USE,Ellipse,6.327580,5.252574,22.970233,15.324275,149.582462
*USE,Ellipse,6.556206,5.925137,56.597664,73.431478,119.127973
*USE,Ellipse,8.658090,6.830494,15.514891,87.840601,170.546966
*USE,Ellipse,7.586546,5.747628,61.294882,11.219317,177.259574
*USE,Ellipse,6.069804,5.290012,72.299825,85.507400,166.428914
*USE,Ellipse,5.424863,3.727463,52.051362,90.285507,90.360305
*USE,Ellipse,1.788587,1.515241,89.862843,92.969200,129.189008
*USE,Ellipse,8.717630,6.935127,56.330020,31.744581,96.208012
*USE,Ellipse,7.279531,5.480662,90.461323,59.169395,130.215856
*USE,Ellipse,4.925669,4.627047,91.338628,36.170201,29.077261
*USE,Ellipse,6.670120,5.331677,91.399836,74.284831,104.361521
*USE,Ellipse,5.987665,4.916375,80.653710,8.766727,50.569892
*USE,Ellipse,4.301784,3.674996,10.161789,29.738097,54.278842
*USE,Ellipse,4.950498,4.111465,10.149541,6.376148,135.947537
*USE,Ellipse,6.516669,5.302838,30.218608,71.865604,32.234859
*USE,Ellipse,2.411661,1.649097,61.784506,55.493785,161.358300
*USE,Ellipse,2.479309,2.157634,8.485971,70.772717,89.354048
*USE,Ellipse,6.220322,4.647236,42.284842,80.679749,116.167637
*USE,Ellipse,2.126188,1.533166,9.012704,42.124724,55.832974
*USE,Ellipse,5.070309,3.458696,32.069687,60.002740,119.757929
*USE,Ellipse,3.923161,2.860246,39.856241,6.998054,11.201519
*USE,Ellipse,3.342814,2.504197,7.456129,19.550110,13.196167
*USE,Ellipse,3.274058,2.490930,74.959395,16.489124,33.723881
*USE,Ellipse,3.943759,2.934650,94.473613,6.625220,43.127762
*USE,Ellipse,3.888517,2.500527,20.311280,76.454254,4.671072
*USE,Ellipse,3.486448,2.456613,37.128353,15.854762,148.343679
*USE,Ellipse,6.763078,3.441793,31.843625,92.986426,127.753136
*USE,Ellipse,3.524810,1.921549,92.000421,46.017065,38.649113
*USE,Ellipse,5.297464,3.807747,31.411716,27.281663,1.830598
*USE,Ellipse,4.199727,3.613776,62.138653,93.202795,146.206665
*USE,Ellipse,5.861076,3.767871,47.034151,18.086488,30.266645
*USE,Ellipse,4.556385,4.193785,30.313132,82.771604,41.295097
*USE,Ellipse,4.464319,3.036808,41.931793,92.813449,148.538242
*USE,Ellipse,5.927248,3.872145,57.983189,46.940370,154.451736
*USE,Ellipse,5.093815,2.637423,62.204828,62.214182,143.237162
*USE,Ellipse,4.472913,3.316975,67.456547,21.800614,115.259542
*USE,Ellipse,4.771140,2.759138,4.684256,54.244807,66.872412
*USE,Ellipse,4.410275,2.157813,43.315676,35.265633,130.312882
CM,Koerner,AREA
*get,l_max,line,,num,max
```

```
k,,
k,,100
k,,100,100
k,,,100
l,kp(0,0,0),kp(100,0,0)
l,kp(100,0,0),kp(100,100,0)
l,kp(100,100,0),kp(0,100,0)
l,kp(0,100,0),kp(0,0,0)
al,l_max+1,l_max+2,l_max+3,l_max+4
*get,a_max,area,,num,max
asba,a_max,Koerner,,,keep
ET,1,SHELL63
MP,EX,1,89900
MP,PRXY,1,0.18
MP,EX,2,37900
MP,PRXY,2,0.18
R,1,1
esize,1
MSHAPE,1,2D
mat,1
amesh,174
mat,2
cmsel,s,Koerner
amesh,all
cmsel,s,koerner
ESLA,S
cm,korn,elements
esel,inve
cm,matrix,elements
nsel,s,loc,y,100
cm,disp_nodes,nodes
allsel
cm,theelement,elements
FINISH
```

Code for BC`s for calculating Effective Coefficient C11:

```
/SOL
FLST,2,2,3,ORDE,2
FITEM,2,216
FITEM,2,219
/GO
DK,P51X, , , ,1,ALL, , , , , ,
FLST,2,4,3,ORDE,2
FITEM,2,216
FITEM,2,-219
/GO
DK,P51X, , , ,1,UY, , , , , ,
FLST,2,2,3,ORDE,2
FITEM,2,217
FITEM,2,-218
/GO
DK,P51X, ,2, ,1,UX, , , , , ,
/STATUS,SOLU
SOLVE
FINISH
/POST1
```

```
AVPRIN,0,0,
ETABLE, ,S,X
AVPRIN,0,0,
ETABLE, ,S,Y
AVPRIN,0,0,
ETABLE, ,EPTO,X
AVPRIN,0,0,
ETABLE, ,VOLU,
SMULT,sx*vol,SX,VOLU,1,1,
SMULT,sy*vol,SY,VOLU,1,1,
SMULT,ex*vol,EPTOX,VOLU,1,1,
SSUM
```

Code for BC`s for calculating Effective Coefficient C22:

```
/SOL
FLST,2,2,3,ORDE,2
FITEM,2,216
FITEM,2,-217
!*
/GO
DK,P51X, , , ,1,ALL, , , , , ,
FLST,2,4,3,ORDE,2
FITEM,2,216
FITEM,2,-219
!*
/GO
DK,P51X, , , ,1,UX, , , , , ,
FLST,2,2,3,ORDE,2
FITEM,2,218
FITEM,2,-219
!*
/GO
DK,P51X, ,2, ,1,UY, , , , , ,
/STATUS,SOLU
SOLVE
FINISH
/POST1
AVPRIN,0,0,
ETABLE, ,S,X
!*
AVPRIN,0,0,
ETABLE, ,S,Y
!*
AVPRIN,0,0,
ETABLE, ,EPTO,Y
!*
AVPRIN,0,0,
ETABLE, ,VOLU,
!*
SMULT,sx*vol,SX,VOLU,1,1,
SMULT,sy*vol,SY,VOLU,1,1,
SMULT,ey*vol,EPTOY,VOLU,1,1,
SSUM
```

Code for BC`s for calculating Effective Coefficient C66:

```
/SOL
FLST,2,1,3,ORDE,1
FITEM,2,216
!*
/GO
DK,P51X, , , ,1,ALL, , , , , ,
/AUTO, 1
/REP
FLST,2,1,4,ORDE,1
FITEM,2,347
!*
/GO
DL,P51X, ,UX,2
FLST,2,1,4,ORDE,1
FITEM,2,346
!*
/GO
DL,P51X, ,UY,2
FLST,2,1,4,ORDE,1
FITEM,2,348
!*
/GO
DL,P51X, ,UY,-2
FLST,2,1,4,ORDE,1
FITEM,2,345
!*
/GO
DL,P51X, ,UX,-2
/STATUS,SOLU
SOLVE
FINISH
/POST1
AVPRIN,0,0,
ETABLE, ,S,XY
!*
AVPRIN,0,0,
ETABLE, ,EPTO,XY
AVPRIN,0,0,
ETABLE, ,VOLU,
SMULT,sxy*vol,SXY,VOLU,1,1,
SMULT,exy*vol,EPTOXY,VOLU,1,1,
SSUM
```

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