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# Three-Dimensional Modelling of Concrete Mix Structure for Numerical Stiffness Determination

**M. Mahdi[1*], I. Marie[2]**

1. Department of Mechanical Engineering, KFU, KSA
2. Department of Civil Engineering, the Hashemite University, Jordan

Corresponding author: *mofid@kfu.edu.sa*

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## ABSTRACT

A three dimensional (3-D) numerical model with explicit representation of two distinctive phases is used for precise prediction of the stiffness and Poisson's ratio of concrete mixture, CM. Using ANSYS code, a 3-D macro scale numerical finite elements model was developed. The aggregates size, shape and distribution are created randomly using enclosing spheres. The sizes of spheres determine the nominal sizes of stone aggregates. Uniform simplified regular spherical stones aggregates are also considered for comparison purposes. The obtained results are compared with experimental and numerical models ones from the literature. The comparison shows a reliable and reasonable agreement. The results are found to be bounded by the upper and the lower bound of the mixtures rule. The results show a close agreement with Hobbs model as well. Therefore, the finite element model perform well under induced compression loading for predicting the stiffness and the Poisson's ratio of the concrete mix.

## 1. Introduction

Concrete is a complicated heterogeneous and an anisotropic material, therefore, analysis of such material necessitate a numerical model with reasonable representation of its geometry and

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structure. The behaviour of concrete under compression load is an important factor for design purposes. A number of research articles uses artificial neural networks and fuzzy logic to predict the compressive strength of concrete. Bilim et al. [1] carried out an artificial neural networks study to predict the compressive strength of ground granulated blast furnace slag concrete. They constructed an artificial neural networks (ANN) model to predict the compressive strength of ground granulated blast furnace slag concrete using concrete ingredients and age. Sarıdemir [2],[3] developed ANN models for predicting compressive strength of concretes containing metakaolin and silica fume. They employed ANN and fuzzy logic and developed models for predicting compressive strength of mortars. Vakhshouri and Nejadi [4] designed adaptive neuro-fuzzy inference system (ANFIS) models to establish relationship between the compressive strength versus slump flow and mixture proportions. Yaseen et al. [5] proposed a machine learning model namely extreme learning machine (ELM) to predict the compressive strength of foamed concrete. The behaviour of concrete mix (CM) under compression was also presented by its effective Young’s modulus. Li et al. [6] proposed a two-step analytical procedure to evaluate the quantitative influence of the maximum aggregate size and aggregate gradation on the effective Young’s modulus of concrete. They assumed concrete as a sphere of special three-phase composite material, namely aggregates, mortar matrix, and interface transition zone (ITZ). Zhou, Song and Lu [7] presented a full 3-D mesoscale finite element model for concrete. Concrete was considered as a non-homogeneous composite of three main constituent phases namely aggregates, mortar matrix, and ITZ. They adopted a direct approach for meshing the mesoscale structure of concrete. The meshing model included picking a series of random points, creating individual aggregate particles by bounded polyhedrons, and placing the particle into the predefined sample space in a random manner. The placing is subjected to prescribed physical constraints. This meshing code is one type of Delaunay triangulation. It aimed to maximize the minimum angle of all the angles of a triangle in the triangulation, thus largely avoiding skinny or badly shaped triangles. Recently, Mahdi and Marie [8] used two dimensional model to treat the concrete mix as bi-composite subjected to compressive loading. They assumed circular aggregates shape. Thirumalaiselvi et al. [9] generated 2D-mesoscale simulations of concrete using circular aggregate model by idealizing the actual irregular shaped aggregate to circular one in determining some mechanical properties of concrete. The accurate 3-D modelling of a composite material is a promising technique for concrete mechanical properties detection and evaluation. Li et al. [10] presented a finite element simulation of recycled coarse aggregate-filled concrete for compressive strength determination using ANSYS. Tarek I. Zohdi and Peter Wriggers [11] employed numerical simulation for structural response determination. Lie, Nurhuda and Setiawan [12] investigated experimentally the effect of aggregate shape and configuration on the stress-strain relationship of concrete. In particular, the Poisson's ratio of CM was studied by M. Anson and K. Newman [13]. They examined experimentally the relation between the CM proportions and the over-all Poisson's ratio for mortars and concretes. It is found that Poisson's ratio is affected by the method of testing, the mix proportions, the moisture condition and temperature of the specimens.

The current study targeted the role of the stone particles volume and their random arrangement within a volume of concrete as a main factor in affecting the stiffness and Poisson’s ratio of concrete mixture. The main variable considered here is the aggregate volume percentage content in CM. This study focuses on the use of finite elements method (FEM) to reveal the stiffness and Poisons ratio of CM. A Three-Dimensional (3-D) FEM model is developed to predict both the equivalent compressive stiffness and the equivalent Poisson's ratio. The CM is assumed to have two phases, namely the stone aggregates and the mortar. This study uses different approach for modelling and meshing other than that used by [7]. The technique used is a type of numerical simulation which is essential to detect more accurate micro-macro concrete material response. It is the first time that a 3-D FEM modelling of CM has been applied for stiffness and Poisson's ratio determination using irregular aggregates shape rather than spherical one. However, both shapes have been applied for comparison purposes. The success of this work will focus on its application in determining further properties that can minimize experimental work. This study provides a step towards future work for other mechanical properties determination and for the application of more material phases that may be available in heterogeneous composite materials.

## 2. Finite element modelling

The modelling of a concrete mixture depends on its heterogeneous composition. It is beneficial to be generated depending on information provided from the real concrete mix design. Häfner et al. [14] modelled a concrete cube with edge length 10 cm, and aggregate volume of 69%. In the current study, a cube of edge length 15 cm was used as a concrete mix specimen to simulate real concrete cube dimensions under compression. This size of cube is commonly used for compressive strength determination if the greatest nominal aggregate size is 20mm. Figure 1 shows the considered cubic specimen. A normal concrete of average compressive strength of 27 MPa is considered. The concrete mix is composed of stone aggregates and mortar. The stone aggregates have Young's modulus of $45x10^3$ MPa and Poisson's ratio of 0.25 whares the mortar has Young's modulus of 15 $x10^3$ MPa and Poisson's ratio of 0.30. The stiffness of CM can be obtained as the stress (pressure load/area) divided by the axial strain. The stiffness of concrete in the elastic range is defined as the slope of the line drawn from a stress of zero to a 45% of the compressive strength of concrete. The simulated concrete cube is subjected to a small uniaxial pressure, not exceeding 11MPa such that linear stiffness can be obtained. Moreover, the predicted static Poisson's ratio ($\nu$) will remain constant up to a stress not exceeding 50 to 60 % of the ultimate stress [13] .In a realistic concrete mix, the aggregate shape may be considered as angular or rounded. The geometrical shape and the angularity of aggregates are supposed to have a noticeable contribution on the mechanical properties of concrete. Accordingly, two types of aggregates are considered and generated for comparison purposes, namely randomly created irregular shapes and spherical shape. The non-homogeneous structure of CM will result into non-homogeneous displacement solutions at the cubic specimen boundaries. To model an equivalent linear stiffness of CM, coupled degrees of freedom need to be enforced as shown via Figure 2. The boundary conditions of coupled degrees of freedom imply that all boundary nodes should have the same displacement boundary conditions. Therefore, the displacement field will be similar to that of homogenous structure. The CM cube is subjected to loading conditions together with set of boundary conditions such that there is no rigid body motion. The boundary conditions are expressed as

$$u_x(x=0)=u_y(y=0)=u_z(z=0)=0 \quad (1)$$

$$u_x(x=a)\,coupled,\; u_y(y=a)\,coupled,\; u_z(z=a)\,coupled \quad (2)$$

where a equals 15 cm

The loading conditions are

$$P_y(y=a)=Elastic\ pressure=11MPa \quad (3)$$

The applied compressive pressure is small therefore, small strain theory applies.

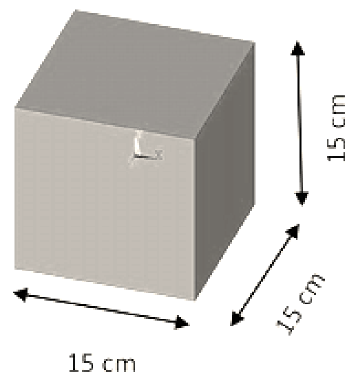



**Fig. 1.** Three-D Model of test specimen.

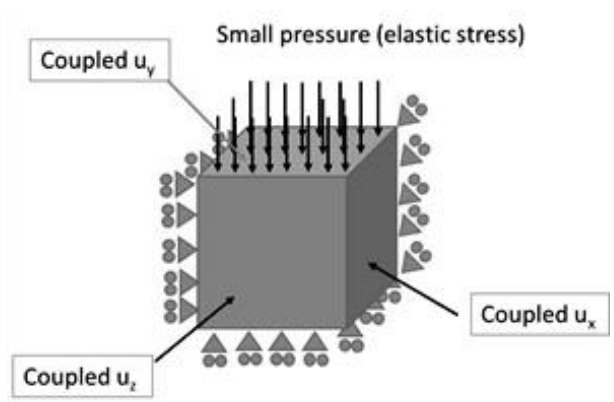
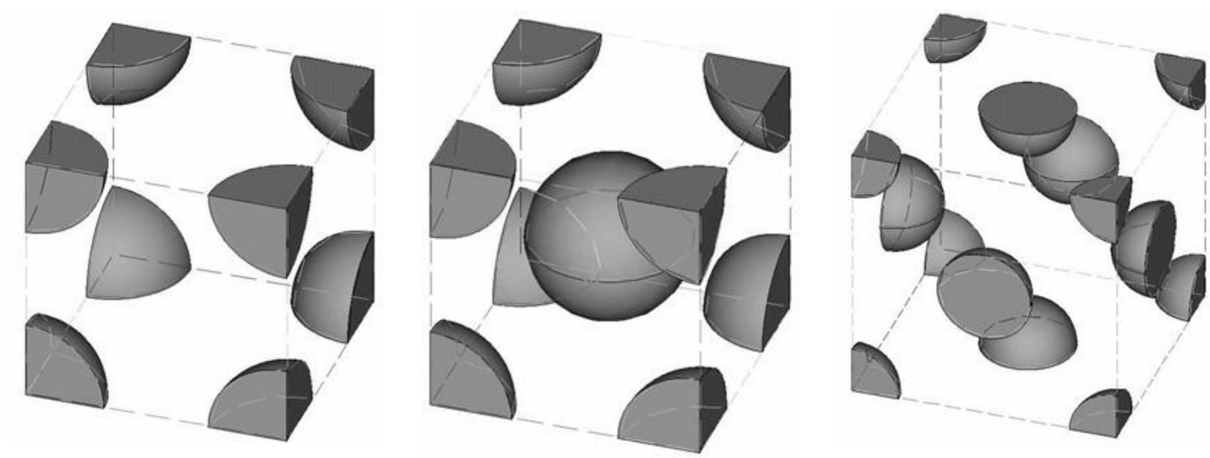



**Fig. 2.** Loading and boundary conditions of cubical specimen.

Although the study is based on random stones aggregates sizes and locations, uniform regular stones aggregates are considered first for comparison purposes. To consider the stiffness of regular uniform stone aggregates (spherical shapes), special mesh shall be developed. ANSYS software is used to create a cubical shape matrix containing aggregates of spherical shape in the finite element model. Typical uniformly distributed spherical stones are shown in Figure 3. Three structures were generated, following crystal lattice forms, for presenting stone spheres locations [15]. They are Simple Cubic (SC), Body Centred Cubic (BCC) and Face Centred Cubic (FCC) structures. The outmost aggregates are partially enclosed inside the cubic cell. The cubic cell of

SC contains one sphere stone whereas BCC and FCC cells contain two and four spheres respectively. For simplicity, the test specimens contain on crystal (cell) structure. The modelling of spherical shapes inside cubical specimen requires Booleans operations supported by ANSYS Parametric Design Language (APDL). The spherical stone aggregates and the mortar are meshed by ANSYS separately to model two materials properties. Three-dimensional elements are used to achieve this. As the aggregates geometry is complex, 3-D Four-noded tetrahedral structural solid elements are employed for mesh generation. Figure 4 shows a local 3-D Four-noded tetrahedral element where I, J, K and L are the local nodes. This element has linear displacement field and constant stress thereafter. Nevertheless, it is ideal for modelling complex shapes with smaller number of nodes. This element type is utilized throughout this study.



Simple Cubic Body Centred Cubic Face Centred Cubic

**Fig. 3.** Typical control volumes with uniformly distributed spherical stones.

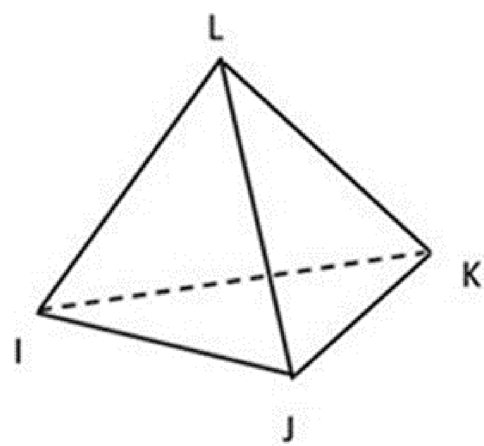
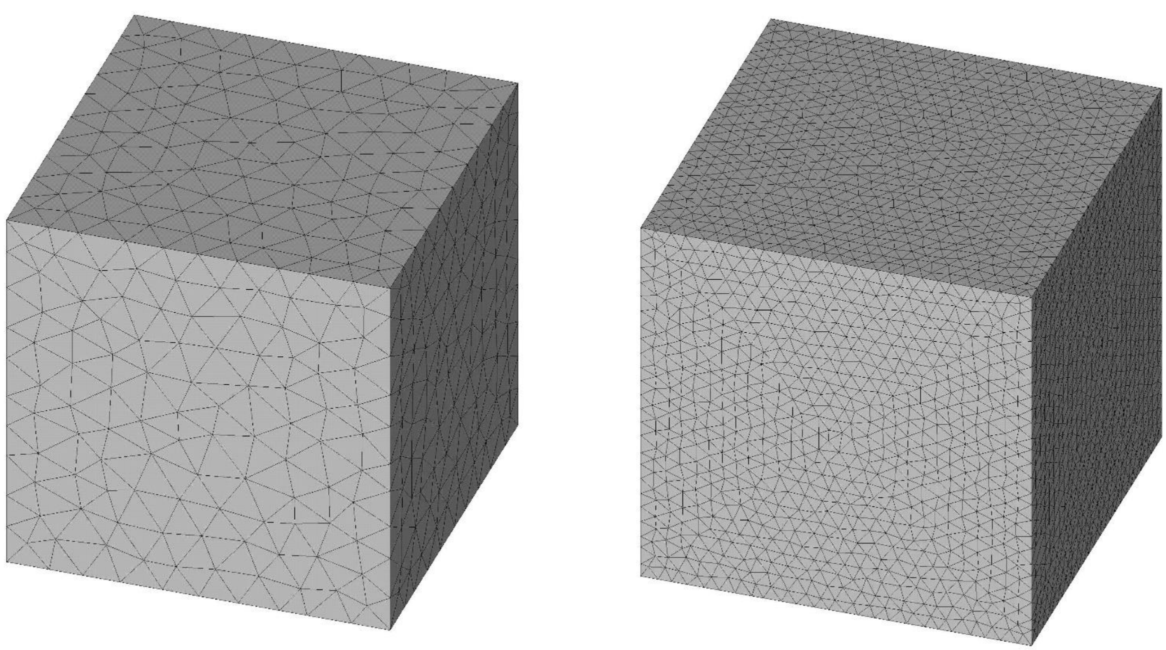



**Fig. 4.** A Three-Dimensional Four-noded Tetrahedral Solid Element.

The random stone aggregate shapes and sizes are presented by combined solid elements. The shapes of stone aggregates rely on the size of FEM elements, and therefore the mesh size. Two different typical FEM meshes are demonstrated in Figure 5. To generate sharp stone aggregates, a coarse mesh of 7674 elements and 1635 nodes is utilized as it is shown by Figure 5-a. Figure 5-

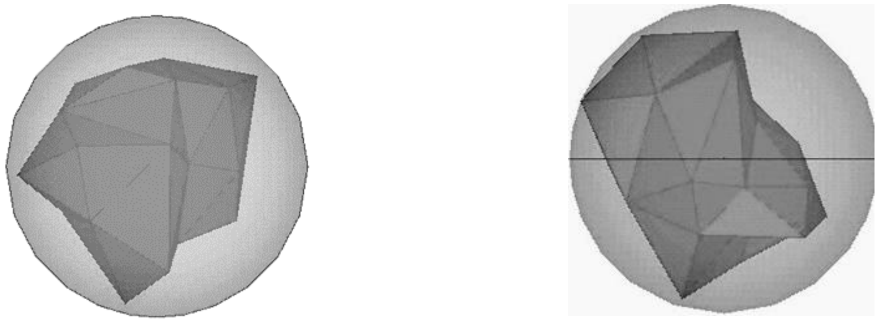
b, on the other hand, presents a finer mesh that consists of 63595 elements and 11928 nodes. This shall be considered when smooth stone aggregates are required.

The generation of random stone aggregates starts with uniform elements such as in Figures 5-a, b. The locations of elemental nodes are altered slightly keeping the elements' Jacobian positive. This is done by calling an external developed FORTRAN code. The call is performed using /SYS command of APDL. Initially all generated FEM elements have mortar properties. The stone aggregates are generated by altering the properties of some selected elements. The selection of stone aggregates is done by generating random spheres. Therefore, the random stone aggregates are assumed as random spheres. To generate random stone aggregates, random spheres are generated within the control volume by calling an external FORTRAN code. The generated spheres enclose the stone aggregates. Thus, the selected spheres should enclose all elemental nodes. Therefore, elements with partially included nodes will be omitted. Thus, the stone elements should have all of their nodes within the sphere volume. The spheres are generated such that no overlapping exists between them. Thus, each sphere diameter is considered as the maximum nominal size of a stone aggregate. Figure 6 demonstrates a typical sphere that encloses a typical stone aggregate. The cube specimen will have a number of spheres that reflect the maximum number of stone aggregates. Figure 7 illustrates the generated spheres and the associated stone aggregates. The spheres are located randomly. Some of the spheres are included completely within the cube structure whereas some are included partially. The partially included spheres will present partially involved stone aggregates within cubic specimen. ANSYS APDL is used to change the properties of the enclosed mortar aggregates to those of stone aggregates using MPCHG command.



(a) Coarse mesh, 7674 elements, 1635 nodes. (b) Fine mesh, 63595 elements, 11928 nodes.

**Fig. 5.** 3-D Four-noded tetrahedral solid elements and typical 3-D meshes.



Top view of sphere Front view of sphere

**Fig. 6.** A sphere enclosing stone aggregate.

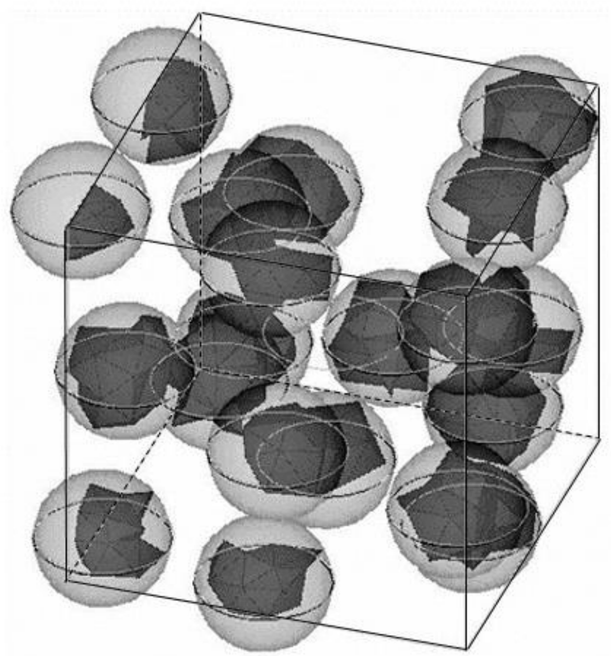
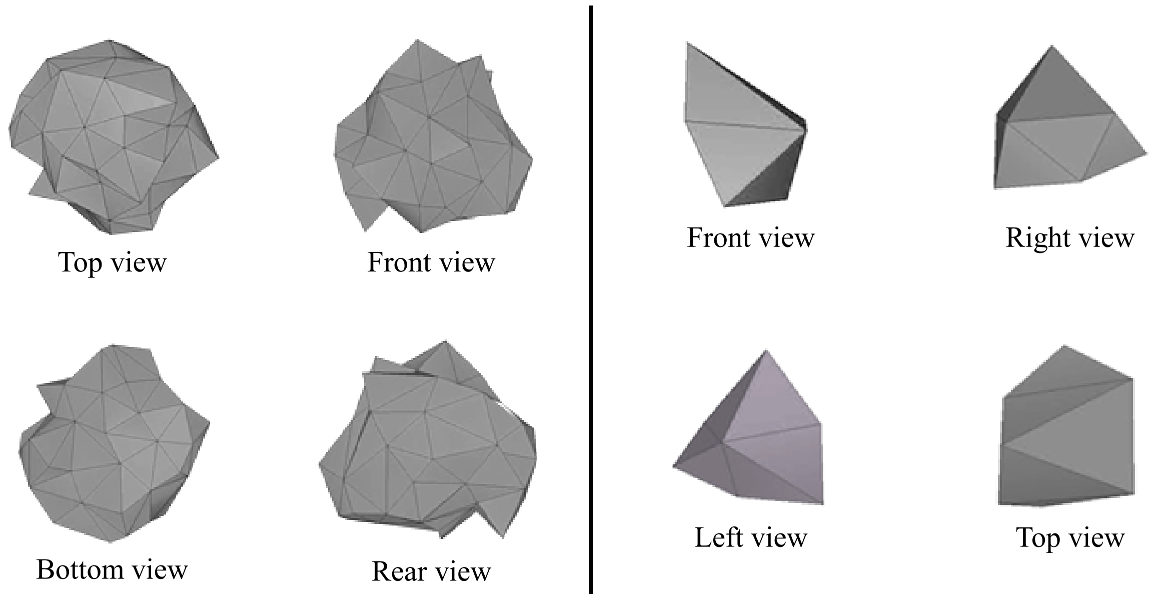


**Fig. 7.** A typical generated random spheres of 20mm radii along with associated stone aggregates inside a cube.

Figure 8 shows typical 3-D views of irregular coarse stones aggregates that are imbedded in the concrete matrix. Figure 8-a shows the aggregate obtained by applying a fine mesh of 63595 elements and 11928 nodes. Figure 8-b, on the other hand, illustrates aggregate shape obtained by the use of coarse mesh of 7674 elements and 1635 nodes.

Using the fine mesh of Figure 5-b, results in fine aggregates shapes as demonstrated by Figure 9. It should be noted that a finer mesh requires considerable amount of CPU memory and processing time. Therefore, this study uses the fine mesh of Figure 5-b. Thus, the maximum numbers of elements and nodes are limited to 63595 and 11928 respectively.




(a) A fine mesh aggregate (b) A coarse mesh aggregate

**Fig. 8.** Typical irregular stone geometry views using fine and coarse meshes.

## 3. Results and discussion

This study implements two dimensionless variables, namely the stiffness ratio and the volume ratio. The stiffness ratio is defined as the ratio of CM stiffness to that of the stone aggregate one. The volume ratio (fraction) is the ratio of the total volume of stone aggregates to that of CM. Thus the volume ratio= stone aggregates' volume/$0.15^3$. The current study results are compared with associated ones of the rue of mixture [15] and those of Hobbs model [16]. The rule of mixture presents upper and lower limits. An upper limit of the elastic modulus (stiffness) of the bi-composite material ($E_{CM}$) is calculated in terms of the elastic moduli of the mortar matrix ($E_{MM}$) and that of the aggregates ($E_A$) phases by:

$$E_{CM} = E_{MM}V_{MM} + E_A V_A \tag{4}$$

where $V_{MM}$ and $V_A$ are the volume ratio (fraction) of the mortar matrix and the aggregates respectively. Eq.4 presents linear function of volume fraction. An expression of the lower bound of the elastic modulus is given by:

$$E_{CM} = \frac{E_{MM}E_A}{\left(E_A V_{MM} + E_{MM} V_A\right)} \tag{5}$$

Eq.5 reflects a curve function. Using the model of Hobbs, the bi-phase system concrete stiffness is achieved by:

$$E_{CM} = E_{MM}\left[\frac{\left(1-V_A\right)E_{MM} + \left(1+V_A\right)E_A}{\left(1+V_A\right)E_{MM} + \left(1-V_A\right)E_A}\right] \tag{6}$$

This study considers the stone aggregates as (1) perfect uniformly distributed spheres and (2) irregular stone aggregates enclosed by perfect random spheres. Initially the stones are assumed as perfectly uniformly distributed spheres. The distribution and the locations of spheres are similar to those of unit cubic cells [15]. Therefore, the cube of CM will be similar to a crystal unit containing SC, BCC and FCC structures. The stiffness is computed for SC, BCC and FCC structures. The results are illustrated by Figure 10. The stiffness ratio can be approximated by continuous cubic functions of volume ratio for SC, BCC and FCC structures. It is noticed that the SC structure shows higher stiffness ratio when compared with those of BC and FCC structures. The stiffness of SC, BCC and FCC stones are bounded by the lower and upper limits of the mixture rule [15]. In contrast to uniform stones results, the random stone aggregates show scattered behaviour. Figure 11 indicates the scattered data for random stone structures. Figure 11 demonstrates wide range of volume ratios and stiffness ratios The stiffness results of stone aggregates are also compared with those of Hobbs [16]. It is found that there is close agreements between the scattered data results and those of associated Hobbs model. The scattered results are slightly larger than the corresponding results of Hobbs. The value of the modulus of elasticity is affected by the volumetric proportions of aggregate due to its two- phase nature of concrete. Aggregate has a greater modulus of elasticity than cement paste. Therefore, the modulus of elasticity of concrete of a given compressive strength will increase for higher content of aggregate.

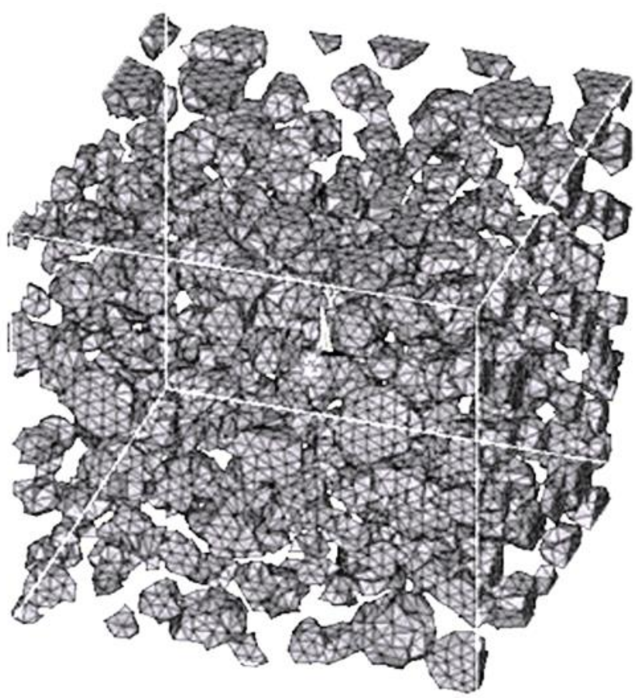


**Fig. 9.** Fine representation of stones geometries within the cubical specimen.

The uniformly distributed spherical stones of FCC and FBC structures show close stiffness results to those of the random aggregate model as shown by Figure 12. The uniform spherical aggregates model of SC has shown the highest deviation from the random aggregate model. The lower and the upper bounds of the rule of mixture bound all results. The results indicate that it is the volume ratio of stone aggregates that affect the CM stiffness. The stone aggregate size has a minor effect on the CM stiffness if the volume ratio is kept the same.

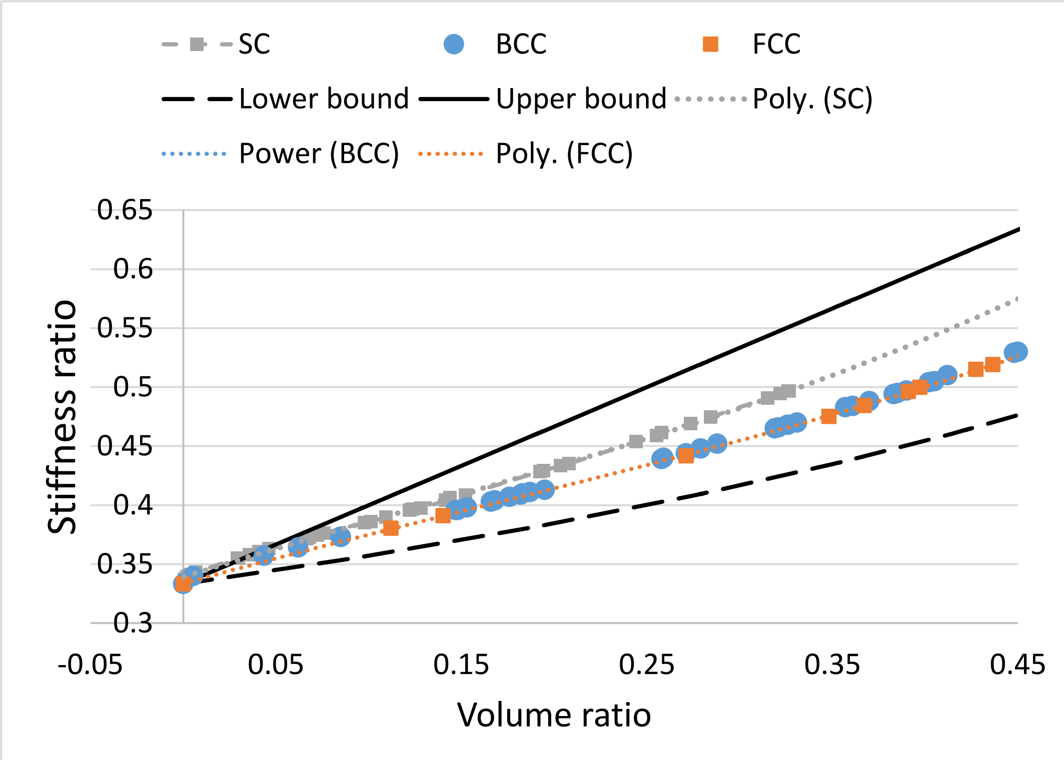



**Fig. 10.** Stiffness ratio of regular uniform spherical stones and the rule of mixture limits.

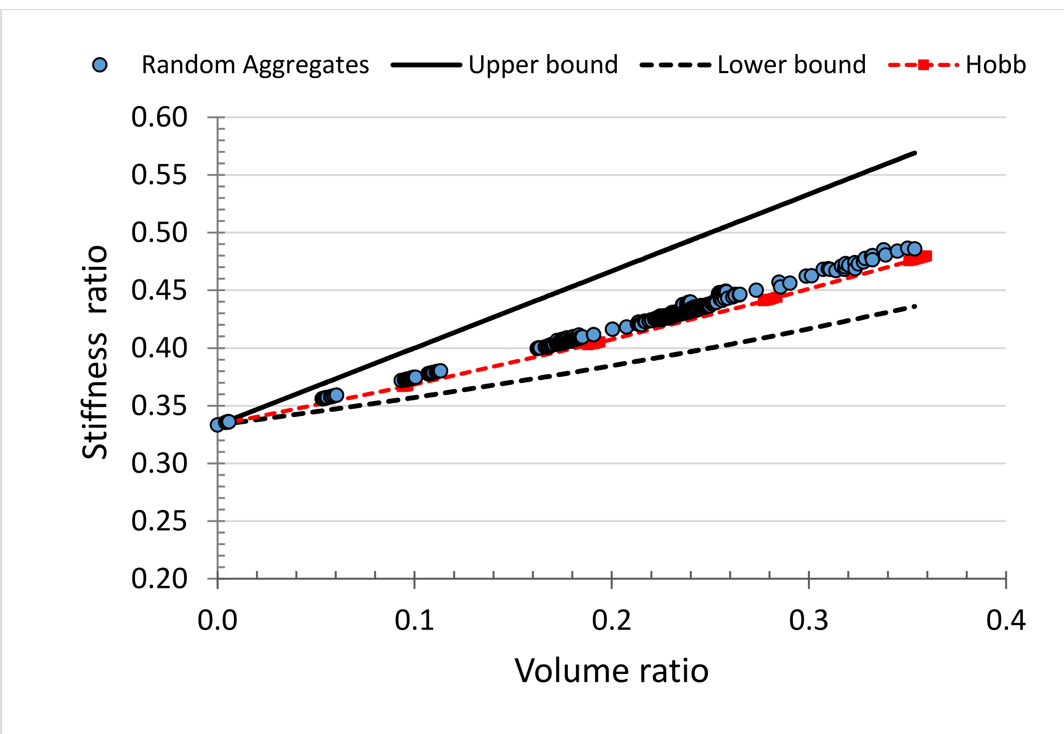



**Fig. 11.** Stiffness ratio of random stone aggregates compared with Hobbs model.

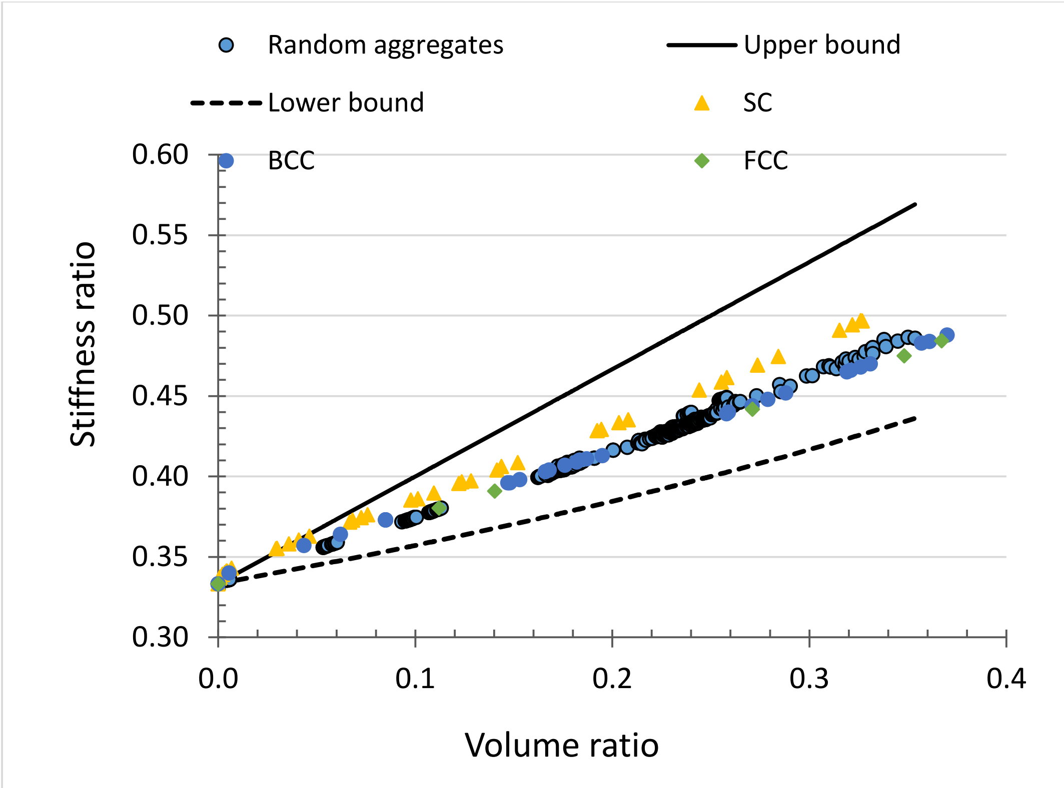



**Fig. 12.** Stiffness of uniform spherical stones aggregates versus those of random stones aggregates

Finally, the Poisson's ratio of CM is considered. Figure 13 shows a graph of Poisson's ratio against the volume ratio of aggregates in the CM mixture. There is random scattering in Poisson's ratio. The minimum magnitudes are slightly less than 0.25 which is Poisson's ratio of stone aggregates. The maximum magnitude of Poisson's ratio is less than 0.3. The relationship between Poisson's ratio and volume ratio cannot be represented as simple smooth function. It appears that the static Poisson's ratio of concretes is affected mainly by the volume fraction of aggregate as it has been approved experimentally by many researchers [13,17]. There is a decrease in Poisson's ratio with the increase of aggregates volume. The trend of the results shows an agreement with the experimental results obtained by Anson and Newman [13]. The upper bound for composite materials expression for Poison's ratio of CM is used for comparison with the current results. Anson and Newman [13] used such expression for the dynamic Poisson's ratio. The upper bound is expressed by $\nu_{CM}$ such that

$$\nu_{CM} = \nu_A V_A + \nu_{MM} V_{MM} \quad (7)$$

where $\nu_A$, $\nu_{MM}$, $V_A$ and $V_{MM}$ are the Poisson's ratios and volume fractions of the aggregate and mortar respectively. The upper bound exhibits linear function of volume fraction which is larger than those of scattered results.

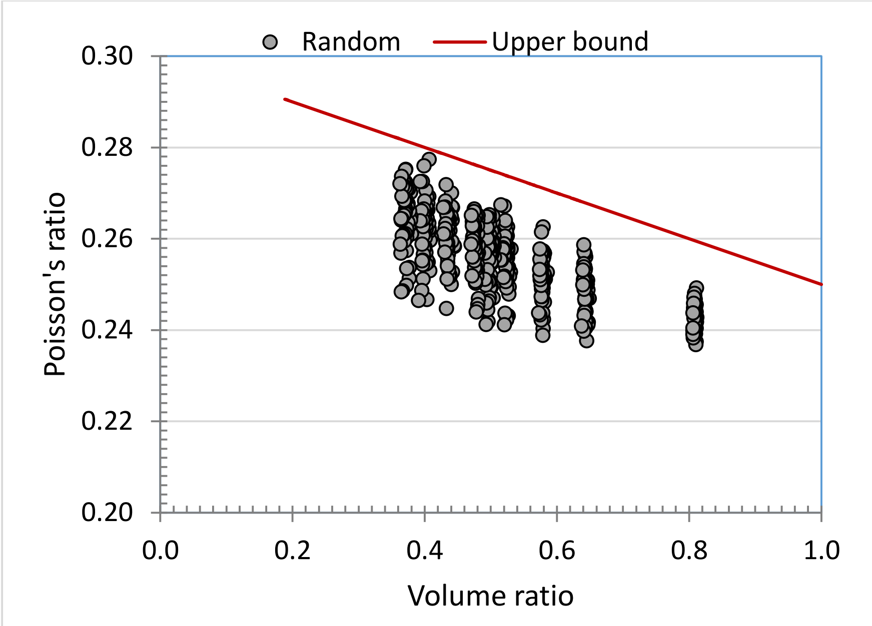



**Fig. 13.** Poisson's ratios versus volume ratio of random stone aggregates.

## 4. Conclusion

A bi-phase 3-D numerical model is established using ANSYS code to predict the mechanical properties of concrete composite namely Young's modulus and Poisson's ratio. It is found that the stiffness of CM is mainly a function of the volume ratio of stone aggregates regardless of its randomness and sizes. As the uniform spherical stones of SC, BCC and FCC are concerned, the SC shows higher stiffness ratio when compared with BBC and FCC structure. The stiffness of BCC and FCC stones are close to those of random irregular aggregate model. Comparatively, the SC aggregates model has shown the highest deviation from the random model results. The predicted stiffness values are bounded by the lower and upper limits of the mixture rule and showed almost acceptable agreements with that obtained by Hobbs model. CM Poisson's ratio can be bounded by the upper bound of the rule of mixtures. CM Poisson's ratio shows complex scattered magnitudes. The experimental work is considered time consuming and expensive, therefore, advances in computer modelling may eventually reduce it to a minimum.

## 5. Further work

This study provides clear vision of a 3-D modelling of normal strength concrete containing aggregates randomly generated. Added to this it provides insight on the effect of volume ratio of aggregates on the stiffness and the Poisson's ratio of concrete. However, more accurate modelling is required to include gradation of aggregates and the effect of interfacial transition zone on concrete mechanical properties.

## Acknowledgment

The ANSYS code is used for all calculations.

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