Available online at www.sciencedirect.com
ScienceDirect
Cement and Concrete Research 38 (2008) 396–402
Cement and Concrete Research

# A numerical model for elastic modulus of concrete considering interfacial transition zone

K.M. Lee [a], J.H. Park [b,*]

[a] Department of Civil and Environmental Engineering, Sungkyunkwan University, Cheoncheon-dong, Suwon 440-746, Republic of Korea
[b] Division of Environmental, Civil, and Transportation Engineering, Ajou University, San 5 Woncheon-dong, Suwon 443-749, Republic of Korea

Received 17 October 2006; accepted 19 September 2007

**Abstract**

The effect of interfacial transition zone on mechanical properties of concrete has been found to be significant, thus the interfacial transition zone should be considered in the analysis for better estimation of elastic modulus of concrete. However, it is difficult to estimate elastic modulus of concrete practically using simple models proposed so far. In this study, a numerical concrete model that adopts three-phase model and finite element with material discontinuity was proposed to analyze concrete with complex interface in three dimensions. The validity of the proposed model was verified by comparing the calculated elastic moduli of concrete with those obtained from experiments. The effect of interfacial transition zone on elastic modulus of concrete with either low or high w/c was also investigated. The analysis results suggest that careful selection of characteristics for interfacial transition zone should be made for the accurate estimation of elastic modulus of concrete.


*Keywords:* Concrete; Elastic modulus; Interfacial transition zone; Numerical concrete model

## 1. Introduction

Elastic modulus of concrete, which plays an important role in the analysis and design of concrete structures, has been studied extensively by many researchers. In practice, the elastic modulus of concrete used in the analysis and design has been determined by empirical formula obtained from experimental results. However, the empirical formula is often too simple to differentiate the influence of various parameters, such as cement-to-sand volume ratio, composition of aggregates, and etc., on the elastic modulus of concrete.

Many researches have attempted to estimate the elastic modulus of concrete by both analytical and numerical methods. In the simplest model for the estimation of elastic modulus of concrete, the concrete is assumed to be a two-phase material, which consists of coarse aggregates and mortar matrix. The use of two-phase model provided reasonable estimation for practical purposes, but did not give insightful results. The difference between the real value and the estimated value by two-phase model arose from the fact that the model did not consider interfacial transition zone in concrete at all [1]. This interfacial transition zone, which deeply affects the characteristics of concrete such as strength, permeability, and crack, must be considered in the modeling of concrete to capture more realistic behavior of concrete. Three-phase model, which assumes that concrete is composed of aggregate, mortar matrix, and interfacial transition zone, has been introduced for the estimation of elastic modulus of concrete by other researchers [2–6]. In studies by Hashin et al., Neubauer et al., Ramesh et al., and Garboczi et al., interfacial transition zone was modeled as thin shell surrounding aggregate and the model gave reliable results [3–6]. However, it is difficult to estimate elastic modulus of concrete practically using the three-phase model, since interfacial transition zone is too thin to be modeled precisely by conventional numerical methods.

This paper presents a numerical concrete model, which adopts a three-phase model and finite element with material discontinuity, for the estimation of elastic modulus of concrete. Conventional finite element methods allow only one material

* Corresponding author. Tel.: +82 31 219 2506; fax: +82 31 219 1613.
*E-mail address:* jangho@ajou.ac.kr (J.H. Park).

0008-8846/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.cemconres.2007.09.019

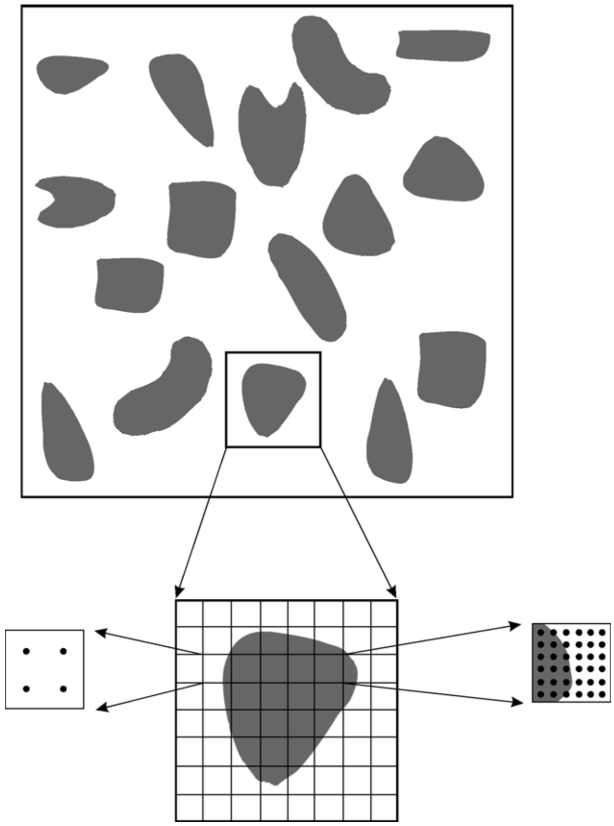

Fig. 1. Modeling of a structure with material discontinuity.

property to be assigned to each element. This makes mesh generation a cumbersome task, especially when composition of materials is complicated and some elements are relatively much small compared with the rest of the elements as seen in concrete. Furthermore, complicated interface may cause that the shape of a finite element loses its convexity and leads to ill-conditioned stiffness matrix. Zohdi [7] introduced a numerical integration method, which can accurately calculate the stiffness of a finite element with material discontinuity in recent years. Applying the numerical integration method to the three-phase model, we analyzed concrete with complex interface using uniform finite elements, and the elastic modulus of concrete was determined accurately using the force–displacement relationship. The proposed numerical concrete model has the advantages of the rapid mesh generation of 3-D concrete model and guaranteed convexity of element. The validity of the proposed numerical concrete model was verified by comparing calculated results with those obtained from the experiment, and the effect of the interfacial transition zone on elastic modulus of concrete was also investigated.

## 2. A numerical model for estimation of elastic modulus of concrete

Finite element method is one of widely used and effective numerical methods for structural analysis involving various materials. In conventional finite element analysis of composite material, the interfacial zone between different materials is ignored and treated as an element boundary to avoid material discontinuity in an element, and the equation for the static problem is represented as follows.

$$[\mathrm{K}]\{\mathrm{u}\} = \{\mathrm{F}\}. \tag{1}$$

In Eq. (1) [K], {u}, and {F} represent stiffness matrix of a structure, nodal displacement vector, and nodal force vector acting on the structure, respectively.

A finite element can be endowed only with a single material property to avoid material discontinuity within the element. Hence, it becomes very difficult to generate proper mesh when the interface between materials is complicated as concrete in three dimensions. Furthermore, complex interface may cause the finite element to lose its convexity and lead to ill-conditioned stiffness matrix [8]. To overcome these shortcomings, this study adopts the numerical integration method which accurately calculates the stiffness matrix of a finite element with material discontinuity.

Fig. 1 shows two dimensional uniform mesh of a solid consisting of two different materials, and each element is composed of one or two materials. The conventional numerical integration generally used in finite element method is suited for an element consisting of a single material, but the conventional numerical integration is not for an element composed of two or more materials. Adopting the numerical integration method which accurately calculates the stiffness of finite elements with material discontinuity, the concrete composed of various materials can be conveniently modeled using the uniform finite element mesh and the elastic modulus of concrete was estimated based on the more realistic model. The main concept of the numerical integration for an element with material discontinuity is as follows [7].

To simplify the problem, let us consider a scalar discontinuous function $F(\varsigma)$ in Fig. 2, which has a jump at $\varsigma=\delta$. This

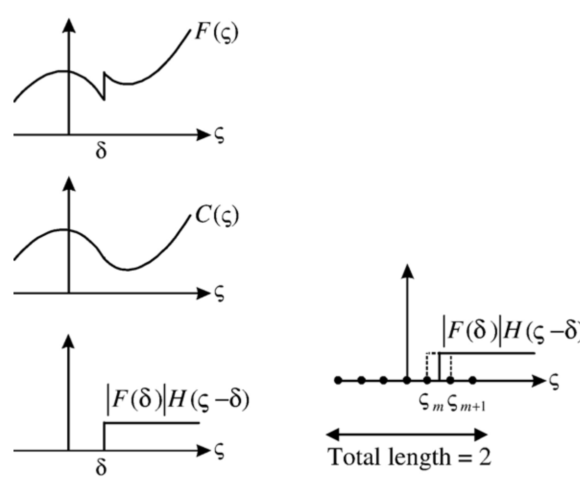


Fig. 2. Separation and integration of a discontinuous function.

discontinuous function can be expressed as the sum of a continuous function $C(\varsigma)$ and a step function $|F(\delta)|H(\varsigma-\delta)$.

$$F(\varsigma) = C(\varsigma) + |F(\delta)|H(\varsigma-\delta) \tag{2}$$

where, $\varsigma$ is the local coordinate system and $|F(\delta)|$ is a jump at $\varsigma=\delta$ ($|F(\delta)|=F(\delta)_+ - F(\delta)_-$). The integration of the discontinuous function $F(\varsigma)$ over an element leads to Eq. (3)

$$\int_{-1}^{1} F(\varsigma)d\varsigma = \int_{-1}^{1} \{C(\varsigma) + |F(\delta)|H(\varsigma-\delta)\}d\varsigma. \tag{3}$$

Applying the Gauss quadrature integration to the equation, each term in Eq. (3) can be approximated as follows.

$$\int_{-1}^{1} C(\varsigma)d\varsigma \cong \sum_{i=1}^{N} C(\varsigma_i)w_i \tag{4}$$

$$\begin{aligned}\int_{-1}^{1} |F(\delta)|H(\varsigma-\delta)d\varsigma &\cong \sum_{i=1}^{N} |F(\delta)|H(\varsigma_i-\delta)w_i \\ &= |F(\delta)|\sum_{i=1}^{m} 0\cdot w_i + |F(\delta)|\sum_{i=m+1}^{N} 1\cdot w_i\end{aligned} \tag{5}$$

where, $N$ is the number of quadrature points, $w_i$ is the weight of the quadrature point, and $\varsigma_i$ is the location of the quadrature point. The error occurring in the integration of the discontinuous function in an element is estimated by the following relations [7].

$$\begin{aligned}\text{error} &= \left|\int_{-1}^{1} F(\varsigma)d\varsigma - \left\{\sum_{i=1}^{N} (C(\varsigma_i) + |F(\delta)|H(\varsigma_i-\delta))w_i\right\}\right| \\ &= |F(\delta)|\left|(1-\delta) - \sum_{i=m+1}^{N} w_i\right| \\ &\le |F(\delta)|\left|\sum_{i=m}^{N} w_i - \sum_{i=m+1}^{N} w_i\right| \\ &\le |F(\delta)|\cdot \max|w_i| \cdot \max|\varsigma_i - \varsigma_{i+1}|.\end{aligned} \tag{6}$$

The maximum error arisen from the Gauss quadrature integration for the discontinuous function is governed by the largest quadrature weight, $w_i$, and the largest distance between two neighboring Gauss points, $\varsigma_i - \varsigma_{i+1}$. Therefore, the maximum weight, $\max|w_i| \approx 1.93N^{-0.759}$, and the maximum distance between two neighboring points, $\max|\varsigma_i - \varsigma_{i+1}| \approx 2.6N^{-1.02}$, in the Gauss quadrature integration lead to the following error bound

$$\text{error} \le \max|w_i| \cdot \max|\varsigma_i - \varsigma_{i+1}| \approx 5.07N^{-1.82}. \tag{7}$$

This concept can be extended to the calculation of stiffness matrix. The error bound for the calculation of stiffness matrix of a three-dimensional element with discontinuity is estimated and presented in Table 1 [7]. The results show that the stiffness matrix of an element with material discontinuity can be calculated with enough precision using an adequate number of quadrature points.

It is very difficult to model concrete of three dimensions using the conventional finite element method because complex mesh generation is required. Moreover, the interfacial transition zone, which affects the characteristics of concrete such as strength, permeability, and crack, must be included in the modeling of concrete for more realistic analysis. By adopting the numerical integration method which allows the use of finite elements with material discontinuity, the concrete composed of various materials can be modeled with uniform finite elements including the interfacial transition zone more conveniently, and the elastic modulus of concrete was calculated more accurately. Coarse aggregates are randomly placed in the modeling of concrete to capture more realistic behavior of concrete. To maximize the efficiency in the calculation of stiffness matrix, a small number of quadrature points were used in ordinary elements, and a large number of quadrature points were used for the elements with discontinuity.

Table 1
Error bounds of the proposed integration method

| Gauss rule | Error bound $\left(\frac{[5.07N^{-1.82}]^3}{8}\right)$ |
|---|---|
| 2×2×2 | 0.370 |
| 3×3×3 | 0.040 |
| 5×5×5 | 0.0025 |
| 7×7×7 | 0.0004 |
| 9×9×9 | 0.0001 |

## 3. Estimation of elastic modulus of concrete by a proposed numerical model

### *3.1. Elastic moduli for models with various numbers of inclusions*

To study the effects of the number of inclusions on the elastic modulus of concrete and verify the validity of the proposed numerical concrete model, five models with the five different numbers of inclusions are analyzed. Concrete was first assumed to be of the two-phase material composed of aggregates and mortar in order to compare the calculated results with the values obtained by the conventional methods. Concrete is modeled using 12×12×12 uniform solid elements and the effect of shear deformation is neglected since the effect of shear deformation on the elastic modulus would be minute under uniaxial loading. The following mechanical properties are used for the analysis: elastic modulus $E_a=70$ GPa, Poisson's ratio $\nu_a=0.2$ for aggregates, elastic modulus $E_m=30$ GPa, Poisson's ratio $\nu_m=0.2$ for mortar. Volume fraction of aggregates is set to 23%. Coarse aggregates are randomly placed in the modeling of concrete. The random disposition of coarse aggregates can describe more realistically the spatial distribution of coarse aggregates in concrete and produces the realistic variations on properties and behaviors of concrete, although it becomes more difficult as the volume fraction of aggregates increases.

One hundred analyses were performed for each model with the different numbers of aggregates to test the convergence in the averaged value of elastic modulus of concrete. Fig. 3 shows the calculated values of elastic modulus for the model with eight aggregates. Elastic moduli of concrete estimated by the analysis show variations, and the cumulated average value for the elastic

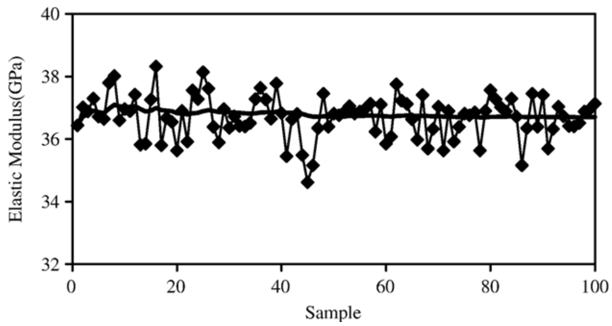


Fig. 3. Elastic modulus of each sample.

modulus converges to 36.7 GPa after seventy runs by the weak law of large numbers. Averaged elastic moduli of the concrete consisted of various numbers of inclusions with fixed volume fraction of aggregate (23%) are presented in Fig. 4. The averaged elastic modulus of the model with one large aggregate is greater than the others with greater number of aggregates. The results also show that the difference in the averaged elastic moduli due to the varying number of aggregates is reduced when a sufficient number of aggregates are considered in the analysis.

The average elastic moduli obtained from the analysis were compared with the values obtained by Christensen–Lo's model (three-phase composite sphere model, see the Appendix) [9,10] to verify the effectiveness of the proposed numerical concrete model. The values calculated by the proposed numerical concrete model agree well with the values by Christensen–Lo's model, as shown in Table 2, although the proposed model provides greater values than the Christensen–Lo's model as the elastic modulus of inclusions increases.

### 3.2. Comparison with experimental results

To verify the proposed numerical concrete model and investigate the effect of interfacial transition zone, the elastic moduli of concrete calculated by the proposed numerical concrete model were compared with those obtained by the experiments. It is reported that the thickness of the interfacial transition zone is around 50 μm in normal strength concrete [7], and the elastic modulus of the interfacial transition zone is about 30–50% of the elastic modulus of mortar [11]. Bentz et al. [12] and Ramesh et al. [5] estimated the elastic modulus of concrete assuming that the volume fraction of interfacial transition zone is 10%. In this study, the elastic moduli of concrete were calculated within the range of 30–70% in ratio of elastic modulus of the interfacial transition zone over elastic modulus of concrete and 1–7% in volume fraction of interfacial transition zone.

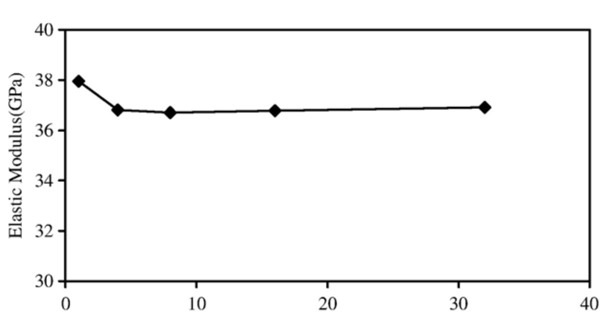


Fig. 4. Averaged elastic modulus for models with various numbers of inclusions.

Table 2
Comparison of elastic modulus without consideration of interfacial transition zone (unit: GPa)

| Elastic modulus of inclusions | Proposed method | Christensen–Lo model |
|---|---|---|
| 50 | 34.05 | 33.66 |
| 70 | 36.91 | 36.10 |
| 90 | 39.18 | 37.84 |
| 150 | 44.34 | 41.00 |

The mix proportions of concrete used in experiments are shown in Table 3. Mechanical properties of the aggregates and the mortar, water–cement ratio (w/c), and volume fraction of aggregates are presented in Table 5. The elastic moduli of the aggregates and the mortar were not obtained from static test, but from dynamic test (impact echo test). Dynamic elastic modulus was used for better estimation, since static elastic modulus has large variation in the measurement due to using secant elastic modulus in static test.

For the analysis, concrete is assumed to be the three-phase material which is composed of coarse aggregates, mortar, and interfacial transition zone. Four three-dimensional analysis models with randomly placed aggregates were analyzed as shown in Fig. 5, and Table 4 presents the size, the number, and the volume fraction of aggregates for each model.

The values of elastic modulus calculated by the proposed numerical concrete model were compared to the ones measured in the experiments in Table 5. The elastic moduli of concrete calculated by the proposed numerical concrete model are greater than the ones measured in the experiments for all cases when interfacial transition zone is neglected. The results show that the elastic modulus of concrete decreases as the volume fraction of interfacial transition zone increases or the assumed elastic modulus of interfacial transition zone is reduced. In addition, the elastic modulus of concrete is more influenced by the volume fraction of interfacial transition zone than the elastic modulus of interfacial transition zone. However, the size effect of aggregates on the elastic modulus is not pronounced precisely in the present investigation. The results indicate that the characteristics of interfacial transition zone, although its volume fraction is relatively small, play an important role in the

Table 3
Mix proportion of concrete models used in experiments (unit: kg/m$^3$)

| Mix type | Cement | Silica fume | Water | Coarse aggregate | Fine aggregate | HRWR (%) | S/a (%) | W/B |
|---|---|---|---|---|---|---|---|---|
| C1 | 400 | – | 200 | 988.3 | 702.2 | 0 | 42 | 0.50 |
| C2 | 475 | 25 | 165 | 1040.2 | 680.4 | 1.5 | 40 | 0.33 |

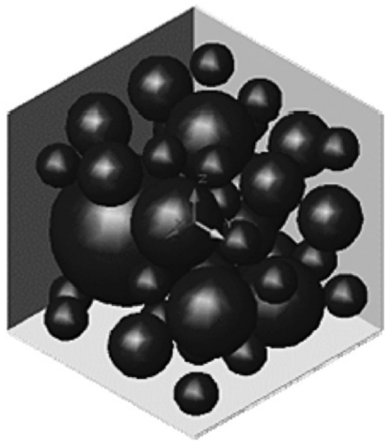

Fig. 5. Concrete model with four types of aggregates.

concrete properties. Therefore, the interfacial transition zone should not be ignored in the analysis.

The elastic moduli of concrete estimated for the normal strength model (C1) show close agreement when the volume fraction of interface and the ratio of elastic modulus of interface to elastic modulus of mortar are assumed to be 6%, 50%, respectively. The elastic modulus for high strength model (C2) shows good agreement around 1% of volume fraction and 70% of elasticity modulus. The volume fraction of interfacial transition zone is closely related to the water–cement ratio. Since the interfacial transition zone is caused by water cumulated around the surface of coarse aggregates, the thickness of interfacial transition zone increases with the water–cement ratio resulting in a higher volume fraction of interfacial transition zone in concrete. The analysis results from the low and high w/c concrete reasonably predict the volume of interfacial transition zone in the concrete with different w/c ratios.

The interfacial properties were estimated by the inverse method, associated with the four-phase composite sphere model (see the Appendix), proposed by Hashin and Monteiro [3] to calibrate the proposed numerical concrete model. The elastic moduli of concrete were also calculated by the proposed numerical concrete model using the interfacial properties obtained from four-phase composite sphere model. For the normal strength concrete model (C1) the difference between the values estimated by two models was less than 0.8%, while for the high strength concrete model (C2) the difference was less than 0.2%, as shown in Table 6. Consequently, the agreement between the values calculated by the proposed numerical concrete model and the values by four-phase composite sphere model is satisfactory.

Table 4
Size, number, and volume fraction of aggregates for numerical models

| Model | Type | Aggregates | A | B | C | D | Sum |
|---|---|---|---|---|---|---|---|
| C1 | I | Radius (mm) | 28.17 | 17.11 | 12.33 | 9.04 | – |
| | | Number of aggregates | 1 | 6 | 11 | 22 | 40 |
| | | Volume fraction (%) | 25.0 | 33.7 | 23.1 | 18.2 | 100 |
| | II | Radius (mm) | 29.52 | 17.11 | 12.33 | 8.37 | – |
| | | Number of aggregates | 1 | 6 | 11 | 22 | 40 |
| | | Volume fraction (%) | 28.8 | 33.7 | 23.1 | 14.4 | 100 |
| C2 | I | Radius (mm) | 28.68 | 17.43 | 12.56 | 9.07 | – |
| | | Number of aggregates | 1 | 6 | 11 | 22 | 40 |
| | | Volume fraction (%) | 25.2 | 34.0 | 23.2 | 17.6 | 100 |
| | II | Radius (mm) | 29.78 | 17.43 | 12.56 | 8.52 | – |
| | | Number of aggregates | 1 | 6 | 11 | 22 | 40 |
| | | Volume fraction (%) | 28.3 | 34.0 | 23.2 | 14.5 | 100 |

Table 5
Comparison of calculated elastic modulus and experimental results

| Model | Volume fraction of interface (%) | Elastic modulus of interface ($E_i/E_m$) | Analysis result (GPa) | | Experimental result (GPa) |
|---|---|---|---|---|---|
| | | | Type I | Type II | |
| C1 w/c = 0.50 $E_m$ = 33.7 Gpa $E_a$ = 58.8 Gpa $V_a$ = 37.4% Aggregate type: granite | 0 | – | 41.24 | 41.31 | 39.70 |
| | 1 | 30% | 40.97 | 41.00 | |
| | | 50% | 40.95 | 41.01 | |
| | | 70% | 41.06 | 40.95 | |
| | 4 | 30% | 40.02 | 39.98 | |
| | | 50% | 40.22 | 40.23 | |
| | | 70% | 40.46 | 40.51 | |
| | 5 | 30% | 39.62 | 39.75 | |
| | | 50% | 39.92 | 39.97 | |
| | | 70% | 40.35 | 40.41 | |
| | 6 | 30% | 39.16 | 39.30 | |
| | | 50% | 39.58 | 39.78 | |
| | | 70% | 39.97 | 40.19 | |
| | 7 | 30% | 39.01 | 38.97 | |
| | | 50% | 39.51 | 39.42 | |
| | | 70% | 39.82 | 39.80 | |
| C2 w/c = 0.33 $E_m$ = 37.6 Gpa $E_a$ = 58.8 Gpa $V_a$ = 39.2% Aggregate type: granite | 0 | – | 44.48 | 44.55 | 44.30 |
| | 1 | 30% | 44.17 | 44.14 | |
| | | 50% | 44.27 | 44.22 | |
| | | 70% | 44.31 | 44.34 | |
| | 2 | 30% | 43.86 | 43.84 | |
| | | 50% | 43.96 | 44.00 | |
| | | 70% | 44.10 | 44.16 | |
| | 3 | 30% | 43.44 | 43.52 | |
| | | 50% | 43.67 | 43.67 | |
| | | 70% | 43.90 | 43.98 | |
| | 4 | 30% | 43.08 | 43.13 | |
| | | 50% | 43.39 | 43.43 | |
| | | 70% | 43.68 | 43.96 | |
| | 7 | 30% | 42.01 | 42.05 | |
| | | 50% | 42.53 | 42.54 | |
| | | 70% | 43.04 | 43.07 | |

Table 6
Comparison of elastic modulus with consideration of interfacial transition zone (unit: GPa)

| Model | Volume fraction of interface (%) | Elastic modulus of interface (GPa) | Poisson's ratio of interface | Analysis result (GPa) | | Four-phase composite sphere model (GPa) |
|---|---|---|---|---|---|---|
| | | | | Type I | Type II | |
| C1 | 5 | 17.52 | 0.231 | 39.92 | 40.01 | 39.70 |
| | 5.5 | 18.47 | 0.231 | 39.84 | 39.97 | |
| | 6 | 19.24 | 0.231 | 39.69 | 39.84 | |
| C2 | 1 | 20.34 | 0.228 | 44.28 | 44.26 | 44.30 |
| | 1.25 | 22.18 | 0.228 | 44.25 | 44.32 | |
| | 1.5 | 24.06 | 0.228 | 44.26 | 44.25 | |
| | 1.75 | 25.67 | 0.228 | 44.22 | 44.30 | |

It is shown by the comparison of the results that the proposed numerical concrete model can be effectively used for the estimation of the elastic modulus of concrete considering the size effect of aggregates. However, some discrepancies are inevitable because of the assumptions used in the numerical modeling and various errors in experiments. In addition, careful selection of characteristics for interfacial transition zone must be made for accurate estimation of elastic modulus of concrete.

## 4. Conclusion

A numerical concrete model has been proposed for the better estimation of elastic modulus of concrete. The proposed numerical concrete model adopts three-phase model and effective numerical integration method which allows material discontinuity in a finite element. The proposed numerical concrete model has the advantages such as the rapid mesh generation of three-dimensional concrete models with uniform finite elements and the elimination of element distortion. The proposed numerical concrete model was verified by comparing calculated results with experimental results. The estimations of elastic modulus of concrete calculated by the proposed numerical concrete model are in good agreement with the experimental results. With the verified model, effects of interfacial transition zone, which affects the characteristics of concrete, are studied. The analysis shows that the elastic modulus of concrete may be more influenced by the volume of interfacial transition zone than elastic modulus of interfacial transition zone. It is also confirmed that the elastic modulus of concrete is more affected by interfacial transition zone when the water–cement ratio is large.

The number of analyses can exert influence to some degree on the averaged elastic modulus of concrete. When the small number of analyses is performed, the averaged value may be far from the true value. Therefore, the sufficient number of analyses needed in order to get the converged averaged value by the weak law of large numbers. The size effect of coarse aggregates on the elastic modulus is not very pronounced in the present investigation. Since the present study is based on the limited number of cases, more general conclusions may not be appropriate at the present time. Nevertheless, the proposed numerical concrete model provide a powerful tool for the estimation of elastic modulus of concrete, and the analysis results reported herein help the understanding of effect of interfacial transition zone on the elastic modulus of concrete.

## Acknowledgments

This work is a part of a research project supported by the Korea Ministry of Construction and Transportation (MOCT) through the Korea Bridge Design and Engineering Research Center at Seoul National University. The authors wish to express their gratitude for the financial support.

The authors also wish to acknowledge Prof. P. J. M. Monteiro and Prof. T. I. Zohdi in UC at Berkeley for helpful discussions.

## Appendix A

For the convenience, the formulae for three-phase composite sphere model and four-phase composite sphere model are collected here.

*Three-phase composite sphere model*

The effective bulk modulus $K_c$ is obtained by

$$K_c = K_m + \frac{V_a(K_a - K_m)}{1 + (1 - V_a)[(K_a - K_m)/(K_m + 4G_m/3)]}. \tag{A1}$$

The effective shear modulus $G_c$ is the solution to the following quadratic equation

$$a(G_c/G_m)^2 + 2b(G_c/G_m) + c = 0 \tag{A2}$$

with the coefficients given by

$$\begin{aligned} a = {} & 8(G_a/G_m - 1)(4 - 5v_m)\eta_1 V_a^{10/3} \\ & - 2[63(G_a/G_m - 1)\eta_2 + 2\eta_1\eta_2]V_a^{7/3} \\ & + 252(G_a/G_m - 1)\eta_2 V_a^{5/3} \\ & - 50(G_a/G_m - 1)\left(7 - 12v_m + 8v_m^2\right)\eta_2 V_a \\ & + 4(7 - 10v_m)\eta_2\eta_3 \end{aligned} \tag{A3}$$

$$\begin{aligned} b = {} & -2(G_a/G_m - 1)(1 - 5v_m)\eta_1 V_a^{10/3} \\ & + 2[63(G_a/G_m - 1)\eta_2 + 2\eta_1\eta_3]V_a^{7/3} \\ & - 252(G_a/G_m - 1)\eta_2 V_a^{5/3} \\ & + 75(G_a/G_m - 1)(3 - v_m)\eta_2 v_m V_a \\ & + \frac{3}{2}(15v_m - 7)\eta_2\eta_3 \end{aligned} \tag{A4}$$

$$\begin{aligned} c = {} & 4(G_a/G_m - 1)(5v_m - 7)\eta_1 V_a^{10/3} \\ & - 2[63(G_a/G_m - 1)\eta_2 + 2\eta_1\eta_3]V_a^{7/3} \\ & + 252(G_a/G_m - 1)\eta_2 V_a^{5/3} \\ & + 25(G_a/G_m - 1)\left(v_m^2 - 7\right)\eta_2 V_a - (7 + 5v_m)\eta_2\eta_3 \end{aligned} \tag{A5}$$

$$\begin{aligned} \eta_1 = {} & (49 - 50v_a v_m)(G_a/G_m - 1) \\ & + 35(G_a/G_m)(v_a - 2v_m) + 35(2v_a - v_m) \end{aligned} \tag{A6}$$

$$\eta_2 = 5v_a(G_a/G_m - 8) + 7(G_a/G_m + 4) \tag{A7}$$

$$\eta_3 = (G_a/G_m)(8 - 10v_m) + (7 - 5v_m). \tag{A8}$$

*Four-phase composite sphere model*

The effective bulk modulus $K_c$ is obtained by

$$K_c = K_m + \frac{(V_a + V_i)}{1/(K_e - K_m) + (1 - V_a - V_i)/(K_m + 4G_m/3)}, \tag{A9}$$

$$\text{where } K_e = K_i + \frac{\overline{V}_a(K_a - K_i)}{1 + \left(1 - \overline{V}_a\right)[(K_a - K_i)/(K_i + 4G_i/3)]}, \tag{A10}$$

$$\overline{V}_a = V_a/(V_a + V_m). \tag{A11}$$

The effective shear modulus $G_c$ is the solution to the following equation

$$4d_{12}^{(3)}(G_c/G_m)^2 + \left(d_{23}^{(3)} - 2d_{13}^{(3)} - 2d_{14}^{(3)} + 3d_{24}^{(3)}\right)(G_c/G_m) - d_{34}^{(3)} = 0 \tag{A12}$$

with the coefficients given by

$$d_{ij}^{(3)} = P_{1i}^{(3)}P_{2j}^{(3)} - P_{1j}^{(3)}P_{2i}^{(3)} \tag{A13}$$

$$\mathbf{P}^{(n)} = \mathbf{P}^{(n-1)}\mathbf{S}^{(n)} \tag{A14}$$

$$\mathbf{P}^{(1)} = \begin{bmatrix} 1-2v_a & 1-2v_a & 1-2v_a & 1-2v_a \\ -6v_a & -7+4v_a & 3v_a & -7-2v_a \end{bmatrix} \tag{A15}$$

$$\mathbf{S}^{(n)} = \begin{bmatrix} -2(5-v_n) & 24\overline{V}_{n-1}^{-2/3} & 2v_n & -14\overline{V}_{n-1} \\ 3(1+v_n) & -24\overline{V}_{n-1}^{-2/3} & 7+2v_n & -21\overline{V}_{n-1} \\ -(5-4v_n)\overline{G}_{n-1} & 6\overline{G}_{n-1}\overline{V}_{n-1}^{-2/3} & -4v_n\overline{G}_{n-1} & 14\overline{V}_{n-1}\overline{G}_{n-1} \\ -(3-6v_n)\overline{G}_{n-1} & -6\overline{G}_{n-1}\overline{V}_{n-1}^{-2/3} & -(7-4v_n)\overline{G}_{n-1} & 21\overline{V}_{n-1}\overline{G}_{n-1} \end{bmatrix} \times \begin{bmatrix} 14 & 14 & 14 & 14 \\ 6v_n & 7-4v_n & -3v_n & 7+2v_n \\ 9\overline{V}_{n-1}^{5/3} & -6\overline{V}_{n-1}^{5/3} & -36\overline{V}_{n-1}^{5/3} & 24\overline{V}_{n-1}^{5/3} \\ 5-4v_n & 2-4v_n & -2(5-v_n) & 2(1+v_n) \end{bmatrix} \tag{A16}$$

$$\overline{G}_{n-1} = G_{n-1}/G_n (\text{phase 1: aggregate, phase 2: interface, phase 3: matrix, phase 4: composite})$$

$$\overline{V}_{n-1} = \sum_{i=1}^{n-1} V_i \Big/ \sum_{i=1}^{n} V_i.$$

Here

| | |
|---|---|
| $K$ | bulk modulus; |
| $G$ | shear modulus; |
| $V$ | volumetric percentage; |
| $v$ | Poisson's ratio; |
| $a$ | aggregate; |
| $m$ | matrix (mortar); |
| $i$ | interface; |
| $c$ | composite (concrete). |

## References


[1] A.U. Nilsen, P.J.M. Monteiro, Concrete: a three phase material, Cem. Concr. Res. 23 (1993) 147–151.

[2] J.C. Nadeau, A multiscale model for effective moduli of concrete incorporating ITZ water–cement ratio gradients, aggregate size distributions and entrapped voids, Cem. Concr. Res. 33 (2003) 103–113.

[3] H. Hashin, P.J.M. Monteiro, An inverse method to determine the elastic properties of the interphase between the aggregate and the cement paste, Cem. Concr. Res. 32 (2002) 1291–1300.

[4] C.M. Neubauer, H.M. Jennings, E.J. Garboczi, A three-phase model of the elastic and shrinkage properties of mortars, Adv. Cem. Based Mater. 4 (1996) 6–20.

[5] G. Ramesh, E.D. Sotelino, W.F. Chen, Effect of transition zone on elastic moduli of concrete materials, Cem. Concr. Res. 26 (1996) 611–622.

[6] E.J. Garboczi, Stress, displacement, and expansive cracking around a single spherical aggregate under different expansive conditions, Cem. Concr. Res. 27 (1997) 495–500.

[7] T.I. Zohdi, P. Wriggers, Computational micro-macro material testing, Comput. Methods Eng. 8 (2) (2001) 131–228.

[8] R.D. Cook, D.S. Malkus, M.E. Plesha, Concepts and Applications of Finite Element Analysis, John Wiley & Sons. Inc., 2002

[9] R.M. Christensen, K.H. Lo, Solutions for effective shear properties in three phase sphere and cylinder models, J. Mech. Phys. Solids 27 (1979) 315–330.

[10] A.C. Wijeyewickrema, S. Leungvichcharoen, Prediction of interface properties of a three-phase composite using three-phase and four-phase composite models, 16th ASCE Engineering Mechanics Conference, 2003.

[11] M.P. Lutz, P.J.M. Monteiro, R.W. Zimmerman, Inhomogeneous interfacial transition zone model for the bulk modulus of mortar, Cem. Concr. Res. 27 (1997) 1113–1122.

[12] D.P. Bentz, J.T.G. Hwang, C. Hagwood, E.J. Garboczi, K.A. Snyder, N. Buenfeld, K.L. Scrivener, Interfacial zone percolation in concrete: effects of interfacial zone thickness and aggregate shape, Mater. Res. Soc. 370 (1995) 437–442.