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A THREE-LAYER BUILT-IN ANALYTICAL MODELING OF CONCRETE

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ABSTRACT

It has been accepted in recent years that concrete can be treated as a three-phase composite, consisting of a cement mortar continuous phase, a coarse aggregate dispersed phase, and interface transition zone (ITZ)– an interphase between cement mortar and coarse aggregates. A large number of experiments have been conducted to investigate the effect of every phase on the mechanical properties of concrete; however, the analytical modeling studies have not been conducted as extensively as experimental studies have. In this paper, a three-layer built-in model was developed by assuming coarse aggregates as spheres and embedding a spherical coarse aggregate coated with an ITZ-like interphase and cement mortar layer with uniform thickness into equivalent concrete media. The preliminary calculation results show that, for the three-phase concrete, each phase has several effective factors for the improvement of the mechanical properties of concrete. For overall evaluations, the effective factors are: 1) reducing the elastic modulus of cement mortar and ITZ-like interphase and increasing the elastic modulus of coarse aggregates, 2) decreasing the coefficient of thermal expansion of each phase, 3) enhancing the tensile strength of cement mortar and reinforcing the deformability of ITZ-like interphase, 4) reducing the volume fraction of cement mortar and increasing the concentration of ITZ-like interphase and coarse aggregates phase, 5) decreasing the maximum grain size of coarse aggregates, and 6) adopting open-graded coarse aggregates. *© 1998 Elsevier Science Ltd*

Introduction

The earliest and simplest model of concrete was based on the assumption that it was a two-phase composite with coarse aggregate dispersed in cement mortar matrix. It is now known that the structure of the cement paste in the vicinity of the coarse aggregates differs from that of bulk cement paste (1,2). The phase in which the presence of the coarse aggregates affects the properties of cement paste is called the interface transition zone (ITZ). Experiments have shown that ITZ has a significant effect on the mechanical properties of concrete, and when the properties of ITZ are changed by taking some measures such as

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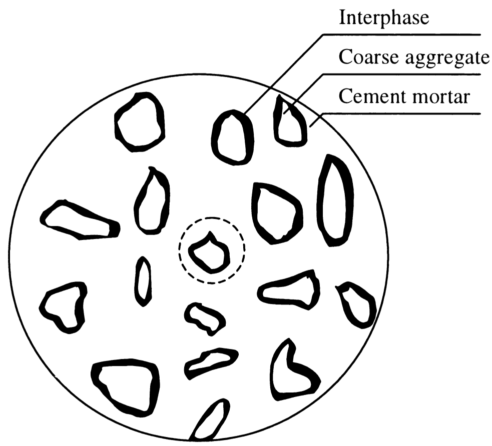


FIG. 1.
Microstructure schematic of three-phase concrete.

refinement by polymer modifications, the mechanical properties of concrete can be improved to a great extent (3–5).

To evaluate the effect of ITZ on the elastic modulus of concrete, Ramesh et al. (6) developed models in which ITZ was represented by a thin film coated on coarse aggregates, forming a three-phase model. To investigate the effect of the ITZ-like film and other phases on the stress-strain field of concrete, Garboczi (7) developed a three-phase model involving the embedding of a spherical coarse aggregate surrounded with a shell of arbitrary thickness into cement mortar matrix; this model can calculate the stress-strain field due to the mismatch of elastic modulus and coefficient of thermal expansion among each phase. However, Garboczi's model has some limitations. It cannot consider the effect of volume fraction of each phase on stress-strain field and the stress-strain field interactions among different coarse aggregates; therefore, it is only suitable for concrete containing very low concentrations of coarse aggregates (as low as 0.01–0.03), (7) and not for the concrete encountered in practice.

In this paper, a three-layer built-in model was developed by assuming a coarse aggregate as a sphere which is coated with an ITZ-like film and surrounded by cement mortar shell, and embedding all of them into a finite equivalent spherical concrete media. For evaluation, the ITZ-like film is not necessarily to be an ITZ alone, but is only to be a parameter of the problem, to be discussed as Garbozci has done. It is the purpose of this paper to present some of the findings by employing the proposed three-layer built-in model.

Analytical Model Development

Analytical Model Establishent

Figure 1 shows a schematic of the microstructure of concrete. For the sake of overall evaluations, the interphase is taken as an ITZ-like film but is not necessarily the real ITZ alone. Therefore, the ITZ-like film is called interphase hereafter. Consider a randomly-selected and interphase-coated coarse aggregate and its surrounding cement mortar (shown by the dashed circle in Fig. 1) as a separate body, which is enclosed by equivalent concrete

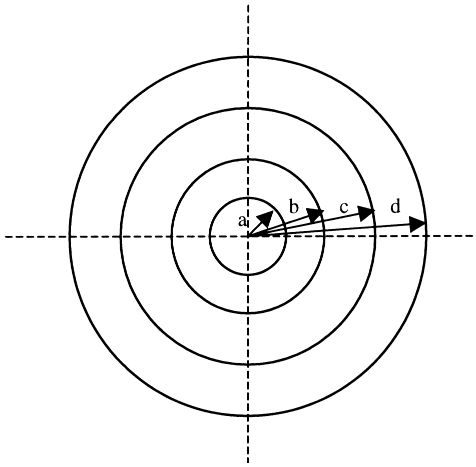


FIG. 2.
Three-layer built-in model.

media formed by other interphase coated coarse aggregates and their corresponding cement mortar matrix. For simplicity, the selected coarse aggregate is assumed as a sphere coated with uniform thickness of interphase and cement mortar layer so that a three-layer sphere in space is formed. In order to consider the stress-strain field effects of other coarse aggregates on this three-layer sphere separate body, a three-layer built-in model is developed by embedding this three-layer sphere into finitely ranged equivalent concrete media as shown in Figure 2. The reason to take the equivalent concrete media as finitely ranged instead of infinite is that this model can consider the stress-strain field induced by both temperature variation and boundary stress, and if the radius of the outer circle in Figure 2 is taken to be infinity, the case for an infinite equivalent concrete media can also be considered.

In Figure 2, a is the radius of the coarse aggregate, b-a the thickness of interphase layer, c-b the thickness of cement mortar layer, d-c the thickness of enclosing equivalent concrete media. For other physical-mechanical parameters, p is the radial boundary stress at $r = d$ applied as external force; p_0 the radial stress at $r = c$; p_1 the radial stress at $r = b$; p_2 the radial stress at $r = a$; r the spherical polar coordinate; and T the temperature variation ($T > 0$ denotes temperature rising and $T < 0$ temperature dropping). E_0, E_1, E_2, E_3, ν_0, ν_1, ν_2, and ν_3 are the elastic modulus and Poisson's ratio of equivalent concrete media, cement mortar, interphase, and coarse aggregate, respectively.

Development of Formulation

In addition to general assumptions for elastic bodies (isotropism, linear elasticity, etc.), assuming continuous contact at the interface of $r = a$, $r = b$, and $r = c$, and taking p and T as uniformly distributed, Figure 2 describes a spherical symmetry problem. By considering boundary conditions and continuous conditions that radial stress and radial displacement are equal at the interface of $r = a$, $r = b$, and $r = c$, the following formulas for p_1, p_2, and p_0 can be developed by applying the theory of elasticity (8):

$$p_1 = A/B \tag{1}$$

$$p_2 = \frac{(\alpha_2 - \alpha_3)T + A_2B_9p_1}{A_3 + A_2B_{10}} \tag{2}$$

$$p_0 = \frac{(\alpha_0 - \alpha_1)T + A_0B_1p + A_1B_4p_1}{A_0B_2 + A_1B_3} \tag{3}$$

where

$$A = (\alpha_1 - \alpha_2)T + \frac{A_1B_5(\alpha_0 - \alpha_1)T + A_0A_1B_5p}{A_0B_2 + A_1B_3} + \frac{(\alpha_2 - \alpha_3)TA_2B_8}{A_3 + A_2B_{10}}$$

$$B = A_2B_7 + A_1B_6 - \frac{{A_1}^2B_4B_5}{A_0B_2 + A_1B_3} - \frac{{A_2}^2B_8B_9}{A_3 + A_2B_{10}}$$

$$A_0 = \frac{1 + \nu_0}{E_0};\ A_1 = \frac{1 + \nu_1}{E_1};\ A_2 = \frac{1 + \nu_2}{E_2};\ A_3 = \frac{1 - 2\nu_3}{E_3}$$

$$B_1 = \frac{0.5+\xi}{1 - m};\ B_2 = \frac{0.5m^{-1} + \xi}{m^{-1} - 1};\ B_3 = \frac{0.5 + \delta}{1 - n};\ B_4 = \frac{0.5 + \delta}{n^{-1} - 1};\ B_5 = \frac{0.5 + \delta}{1 - n}$$

$$B_6 = \frac{0.5n^{-1} + \delta}{n^{-1} - 1};\ B_7 = \frac{0.5\mathrm{k} + \eta}{1 - k};\ B_8 = \frac{0.5 + \eta}{k^{-1} - 1};\ B_9 = \frac{0.5 + \eta}{1 - k};\ B_{10} = \frac{0.5k^{-1} + \eta}{k^{-1} - 1}$$

$$\xi = \frac{1 - 2\nu_0}{1 + \nu_0};\ \delta = \frac{1 - 2\nu_1}{1 + \nu_1};\ \eta = \frac{1 - 2\nu_2}{1 + \nu_2};\ m = \frac{c^3}{d^3};\ n = \frac{b^3}{c^3};\ k = \frac{a^3}{b^3}$$

In Eqs. 1–3, letting $p = 0$ and $T \neq 0$, temperature-induced stresses can be obtained; letting $p \neq 0$ and $T = 0$, boundary stress induced stresses can be determined; letting $p \neq 0$ and $T \neq 0$, the overall stresses caused by temperature variation and boundary stress can be obtained. Once p_0, p_1, and p_2 are derived, the stress-strain field, the hydraulic static stress, and the equivalent stress, etc., can be obtained by applying the theory of elasticity (8). Due to space limitation, the formulas are not listed here.

Although the interface stresses p_2, p_1, and p_0 can be calculated by Eqs. 1–3, only the stress at the interface between the interphase and coarse aggregates, p_2, and the stress at the interface between interphase and cement mortar, p_1, are shown in the results due to their significance in causing the damage of interface debonding, coarse aggregates fracture, and cement mortar yielding. For simplicity, the effects of p and T on p_2 and p_1 will be considered independently, and the non-dimensional form of p_2/p and p_1/p and the ratio of p_2/T and p_1/T will be assumed hereafter. The following calculations of p_2/p, p_1/p, p_2/T, and p_1/T are based on the specified parameters E_0, E_1, E_2, E_3, ν_0, ν_1, ν_2, ν_3, α_0, α_1, α_2, α_3, a, b, c, d, and size distribution of coarse aggregates.

Computational Parameters

The value of E_0 for the three-phase concrete was predicted by the first author in a previous work as follows (9):

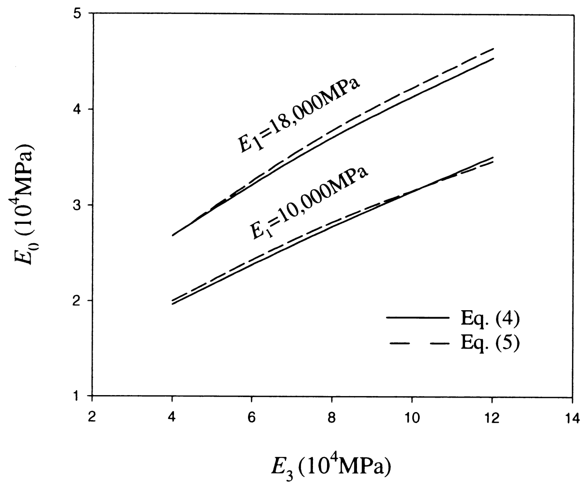


FIG. 3.
Elastic modulus prediction result of concrete.

$$E_0 = 0.265E_1f_1 + \frac{[0.735f_1 + 0.662(f_2 + f_3)]^2 E_1E_2E_3}{0.735f_1E_2E_3 + 0.662(f_2E_1E_3 + f_3E_1E_2)} + \frac{0.338(f_2 + f_3)^2 E_2E_3}{f_2E_3 + f_3E_2} \tag{4}$$

where f_1, f_2, and f_3 are volume fractions of cement mortar, interphase, and coarse aggregates, respectively.

For the specified case of when the three-phase concrete is treated as two-phase concrete, the E_0 value calculated by Eq. 4 agrees with the E_0 value calculated by the following equation, Eq. 5, which was developed by Zhou et al. (10) for the two-phase concrete. Figure 3 plots the calculation results by Eqs. 4 and 5, which show a maximum relative error of 2.36%.

$$E_0 = E_1\left(\frac{E_3}{E_1}\right)^{f_3} \tag{5}$$

For the calculation of α_0, the well-known Schapery's formula is assumed (11):

$$\alpha_0 = \sum_{i=1}^{3} f_iE_i\alpha_i \Big/ \sum_{i=1}^{3} f_iE_i \tag{6}$$

It has been shown that, in realistic concrete, although the thickness of interface transition zone (ITZ) depends on factors such as water/cement ratio, it seems to be independent of the size of inclusions (12). Therefore, it is reasonable to assume the thickness of interphase layer (*b*-*a*) is constant, regardless of the size distribution of coarse aggregates, and the thickness of enclosing cement mortar layer (*c*-*b*) is also constant, regardless of the difference in the size of interphase coated coarse aggregates. Based on these assumptions, the following relationship can be derived:

TABLE 1
Coarse aggregate gradation.

Grain size of coarse aggretates (mm)	40 ~ 30	30 ~ 20	20 ~ 10	10 ~ 5
No. 1: percent content	25	25	25	25
No. 2: percent content	50	40	5	5

$$b = a + \frac{f_2}{3f_3\sum_{i=1}^{N-1}\frac{k_i}{r_i}} \tag{7}$$

$$c = b + \frac{f_1}{3(f_2 + f_3)\sum_{i=1}^{N-1}\frac{k_1}{\rho_1}} \tag{8}$$

where r_i (i = 1, 2, . . . , N − 1) is the average grain size of No. i sieve and No. (i + 1) sieve for coarse aggregates; $\rho_i = r_i + (b\text{-}a)$; $k_i = s_{i+1}/S$, in which s_{i+1} is the residue of coarse aggregates on No. (i + 1) sieve, with S the percent content of coarse aggregates among total aggregates.

In practice, concrete and polymer-modified concrete involve a large variety of cement types, aggregate types, and polymer types, which will inevitably influence the physical-mechanical parameters of the cement mortar phases, coarse aggregate phases, and interphases. In order to reflect this situation, the parameters adopted in the following calculations should cover a reasonably large range. By referring to (3–5, 11), the following physical-mechanical parameters are assumed: E_1 = 20,000 MPa (range 10,000 ~ 30,000 MPa), E_2 = 5,000 MPa (range 1,000 ~ 30,000 MPa), E_3 = 50,000 MPa (range 5,000 ~ 100,000 MPa), $\alpha_1 = 3 \times 10^{-5}$/°C (range 1 ~ 6 × 10^{-5}/°C), $\alpha_2 = 5 \times 10^{-5}$/°C (range 1 ~ 10 × 10^{-5}/°C), $\alpha_3 = 0.8 \times 10^{-5}$/°C (range 0.5 ~ 1.0 × 10^{-5}/°C), $\nu_0 = \nu_1 = \nu_2 = \nu_3 = 0.3$, $f_1 = 0.5$ (range 0.3 ~ 0.7), $f_2 = 0.1$ (range 0.01 ~ 0.2), and $f_3 = 0.4$ (range 0.3 ~ 0.7). Coarse aggregate gradation is shown in Table 1.

Results and Discussions

It is known that large interface stresses, p_2, at the interface of coarse aggregate and interphase layer, $r = a$, and p_1, at the interface between interphase layer and cement mortar, $r = b$, are likely to result in the damage of interface debonding, coarse aggregate fracture, and cement mortar yielding. Therefore, in the results and discussions that follow, the positive result suggests p_2 and/or p_1 decrease; the negative result, on the other hand, means p_2 and/or p_1 increase.

For considering the stress-strain field interactions between different coarse aggregates, Figures 4 and 5 show boundary-stress-induced stresses and temperature-induced stress variations with the thickness of surrounding equivalent concrete media, d, respectively, where p_2 is the interface radial stress at $r = a$, p_1 is the interface radial stress at $r = b$, p is the boundary stress at $r = d$, and T is the temperature variation. Thus p_2/p and p_1/p in Figure 4 represent the interface stresses due to unit boundary stress, while p_2/T and p_1/T in Figure

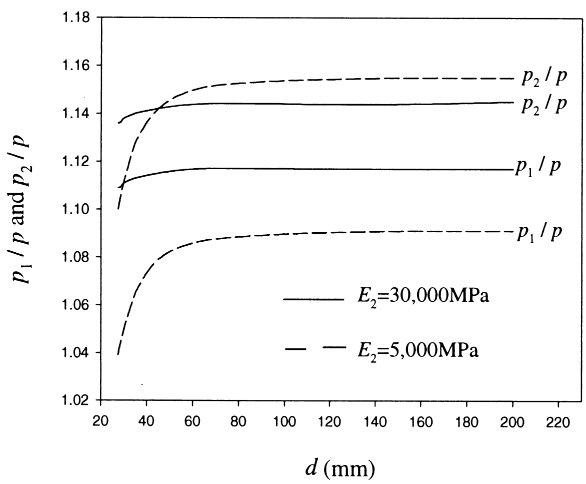


FIG. 4.
Effect of d on boundary-stress-induced interface stresses.

5 describe the interface stresses due to unit temperature change. It is found from Figure 4 that, with the increase of d values, interface stresses change substantially when d adopts relatively small values such as $d < 60$ mm. This means when a relatively small number of coarse aggregates are included, the effects of the stress-strain field of these nearby particles on the target particle are very strong; when d takes relatively large values such as $d > 60$ mm, a relatively large number of coarse aggregates are included and the stress-strain field effect of those distant particles on the target particle are relatively small and negligible, resulting in interface stresses nearly independent of d values. Figure 5 shows that, with the increase of d values, interface stresses also change significantly when d is within some range such as $d <$

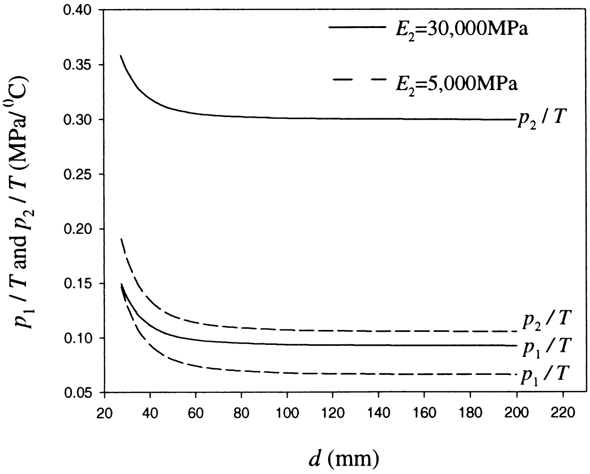


FIG. 5.
Effect of d on temperature-induced interface stresses.

100 mm and is nearly constant when d is comparatively large such as $d > 100$ mm, which supports the results obtained in Figure 4. Therefore, the three-layer built-in model in Figure 2 can take into account the interactions between stress-strain fields of different particles as expected. To mitigate the effect of d on calculation results of interface stresses, $d = 100$ mm is assumed in the following calculations.

Figure 6a, b, and c show the effects of grain size and grain size distribution of coarse aggregates on boundary-stress-induced interface stresses (Fig. 6a) and temperature-induced interface stresses (Fig. 6b and c). It is seen from Figures 6a–c that, with the increase of grain size of coarse aggregates, a, interface stresses increase significantly except for p_2 / T when interphase is harder than cement mortar ($E_2 = 30{,}000$ MPa $> E_1 = 20{,}000$ MPa) (Fig. 6b). This is rarely encountered; therefore, reducing maximum grain size of coarse aggregates is recommended. Grain size distribution of coarse aggregates also has some effects on interface stresses. Reducing size scatter of coarse aggregates has positive effects (Fig. 6c size distribution of No. 2), which means open-graded coarse aggregates are better than that of densely graded coarse aggregates. Certainly there are many factors affecting the mechanical properties and workability of concrete; thus, the determination of the gradation of coarse aggregates should be based on overall considerations. To analyze interface stresses of concrete in unfavorable conditions, the maximum radius of coarse aggregate of $a = 20$ mm and grain size distribution of No. 1 is assumed in the following calculations.

Figure 7 shows temperature-induced interface stress variations, with volume fractions of each phase. It is found from Figure 7 that, with the increase of volume fraction of soft interphase ($E_2 = 5{,}000$ MPa $< E_1 = 20{,}000$ MPa and $E_3 = 50{,}000$ MPa), interface stresses decrease almost linearly. With the increase of volume fraction of cement mortar, f_1, (thus the decrease of volume fraction of coarse aggregates, f_3), interface stresses increase when $f_2 < 0.15$. Therefore, increasing volume fraction of soft interphase within a certain range or reducing the volume fraction of cement mortar has positive effects on reducing thermal stresses.

Figure 8 shows interface thermal stress variations with elastic modulus of coarse aggregates and cement mortar. It is seen from Figure 8 that, with the increase of elastic modulus of coarse aggregates, E_3, thermal stresses decrease except when very soft coarse aggregates and hard cement mortar ($E_3 < 20$ GPa and $E_1 > 30$ GPa) are incorporated; with the increase of elastic modulus of cement mortar, E_1, thermal stresses also increase. Therefore, selecting hard coarse aggregates and soft cement mortar are suggested for the reduction of thermal stresses.

Figure 9a and b show interface thermal stress variations with coefficients of thermal expansion (CTE) of each phase. It is found from Figure 9a that, in the case of soft interphase employed ($E_2 = 5{,}000$ MPa, $E_1 = 20{,}000$ MPa, and $E_3 = 50{,}000$ MPa), with the increase of its CTE, α_2, thermal stresses may turn from compressive stresses into tensile stresses when temperature drops ($T < 0$) except for that very expansive cement mortar ($\alpha_1 = 6\times10^{\times5}$/°C) is incorporated. As tensile thermal stresses can result in interface debonding, reducing the CTE of interphase has a positive effect on mitigating temperature-induced damage when temperature drops. It can also be seen from Figure 9a and b that reducing the CTE of cement mortar, α_1, or coarse aggregate, α_3, can decrease absolute values of thermal stresses, and thus is beneficial.

It has been known that interface transition zone (ITZ) in ordinary concrete is porous and thus has low elastic modulus. To reflect this situation, addressing the effect of soft interphase on mechanical properties by the present analytical model is interesting. By overall evaluation of Figures 4–9, it is found that, in many cases, adopting soft interphase can reduce interface

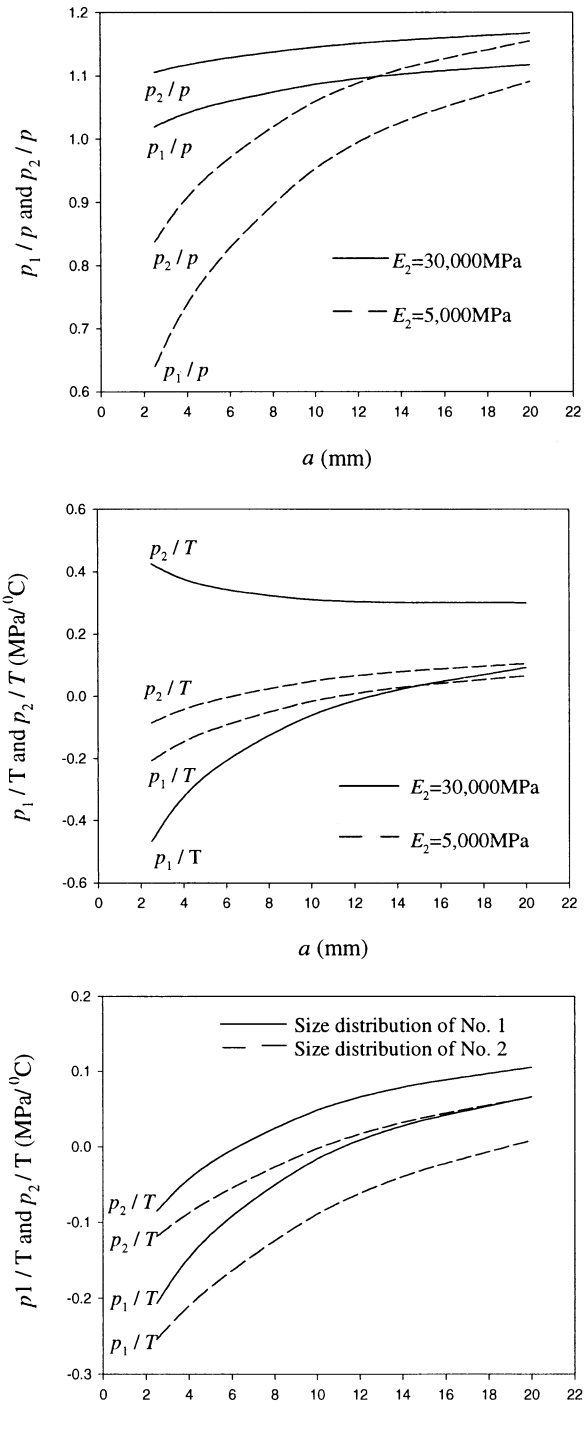


FIG. 6.

Effect of grain size and size distribution of coarse aggregate on interface stresses.

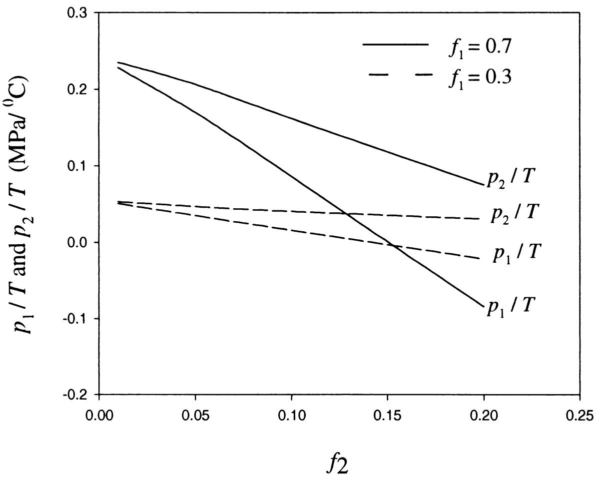


FIG. 7.
Effect of volume fraction on interface stresses.

stresses and thus has beneficial effects. To verify further this result and put forward the requirements for the physical-mechanical properties of each phase, one should conduct stress-strain field rather than only interface stresses investigations. Figure 10a and b show overall radial stress ϵ_r, tangential stress ϵ_t, radial strain σ_r, and tangential strain σ_t, in each phase when soft interphas is used and $T = -1°C$, and $p = 1$ MPa are applied. It can be seen from Figure 10a that, when soft interphase is introduced, the stress concentration is in a tangential direction that occurs at the interface of $r = b$ on the side of cement mortar, while the strain concentration is in a radial direction that occurs at the interface of $r = a$ on the side of soft interphase shown in Figure 10b. Therefore, to develop the beneficial effect of soft

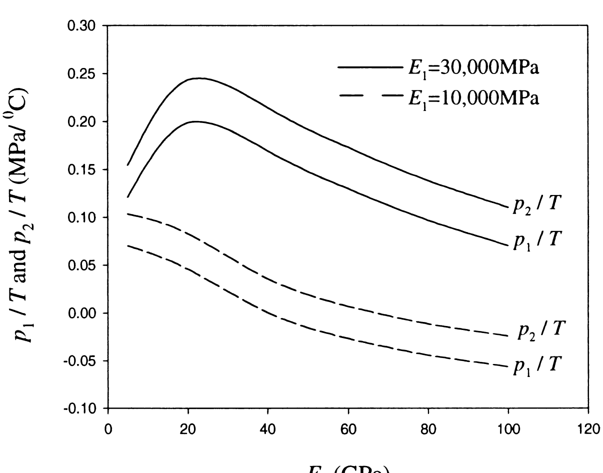


FIG. 8.
Effect of elastic modulus on interface stresses.

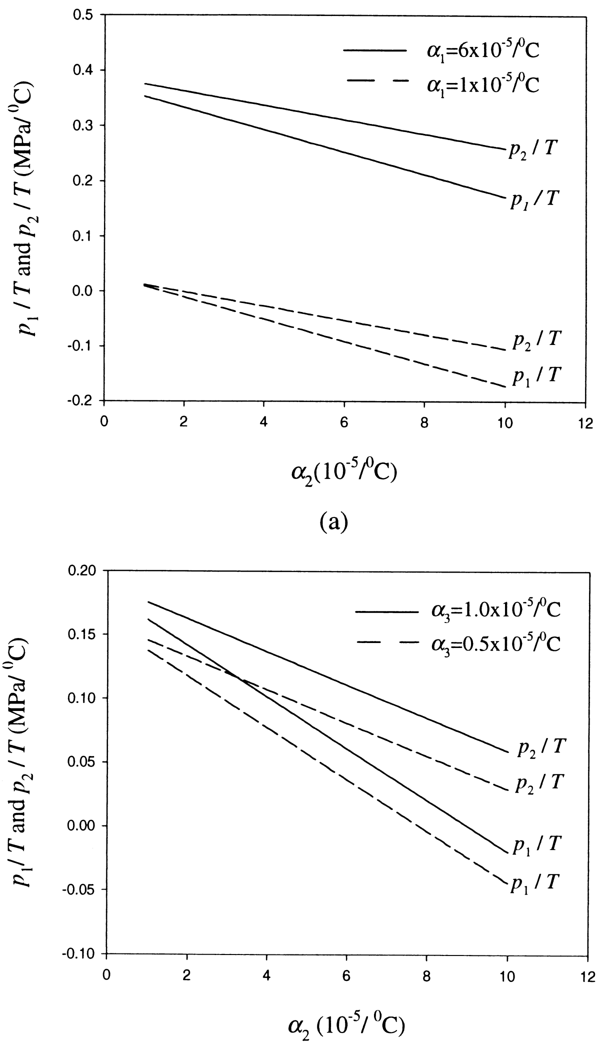
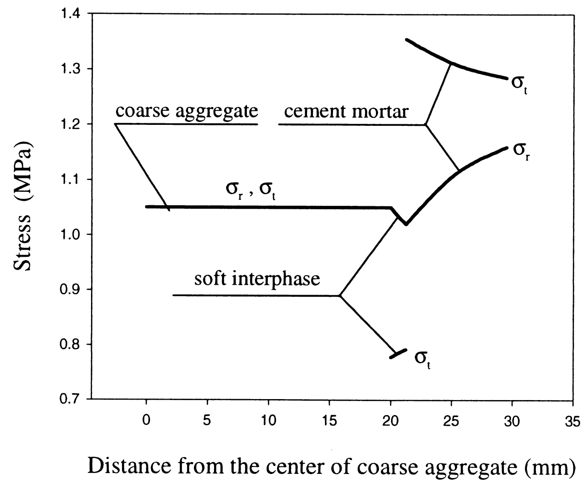


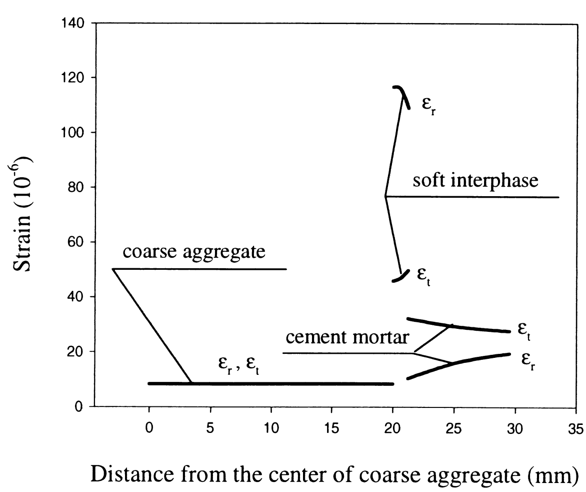
FIG. 9.
Effect of coefficient of thermal expansion on interface stresses.

interphase, increasing the strength of cement mortar and the deformability of interphase are necessary to meet the needs of stress-strain concentrations. Ordinary ITZ lacks strain ability, while polymer is much flexible; hence, adopting polymer- modified concrete or directly introducing polymer film in between coarse aggregate and cement mortar would be expected to improve the mechanical properties of concrete.

As an example, the theoretical prediction in Figure 10 is qualitatively supported by a preliminary experimental study on cement-asphalt emulsion composite (CAEC) (13). The CAEC was a three-phase cement-based composite material with coarse aggregates as dispersed phase, asphalt as an interphase or cushion layer in between coarse aggregates and



(a) Stress distribution



(b) Strain distribution

FIG. 10.
Stress-strain distribution in each phase of concrete.

cement mortar, and cement mortar as continuous phase or matrix. This three-phase microstructure of CAEC was formed by dispersing asphalt-emulsion-coated coarse aggregates into cement mortar matrix. Tests on fatigue, strength, rigidity, toughness, and stress-strain relationship were conducted. Based on the test results, it was concluded that the introduction of the flexible asphalt layer in between coarse aggregate and cement mortar made the resulting CAEC posess the characteristics and advantages of both asphalt and cement and have long fatigue life, high toughness, proper rigidity, etc.

According to Figure 10, the stress-strain distributions require that the interphase have high strain ability to satisfy the strain concentration, and the matrix have high strength to meet the needs of stress concentration. Because of the high deformability of asphalt and the high strength of cement mortar, the stress concentration that occurred in the cement mortar matrix and the strain concentration that appeared at the asphalt interphase can be compensated. As a result, the fatigue characteristics and the toughness of CAEC were significantly improved compared with unmodified ordinary cement concrete. Although the comparison between the test results of CAEC and the theoretical predictions in the current paper is qualitative, the trends shown by test results and theoretical predictions are consistent.

Conclusion

In recent years, concrete has been treated as a three-phase composite material in some literature. Experimental studies and mechanical modeling have been conducted to evaluate the effect of every phase on the mechanical behavior of the three-phase concrete. To complement the three-phase mechanical modeling recently developed by Garboczi, a three-phase built-in model is proposed in this paper. Despite the possible gap between the proposed model and real concrete, it would give valuable insight into the real problem. The preliminary calculation results show that the proposed model can consider the stress-strain field interactions between different coarse aggregates and the volume fractions of each phase as expected and it is suitable for the evaluation of the three-phase concrete. Based on the calculation results, the following conclusions are obtained:

1. The cement mortar phase has significant effects on the mechanical properties of concrete. Increasing its strength, reducing its elastic modulus, decreasing its coefficient of thermal expansion, and reducing its volume fraction are recommended in the design of concrete. Because some of the requirements for the constituents of cement mortar are contradictory (such as that reinforcing strength requires more cement, whereas reducing elastic modulus requires less cement), the design of proper cement mortar should be based on balanced considerations.
2. Reducing the elastic modulus, enhancing the deformability, increasing the volume fraction within a certain range, and decreasing the coefficient of thermal expansion are preferred for interphase. In practice, adopting polymer-modified concrete or directly coating the coarse aggregate surface with polymer emulsion would meet the needs of interphase just mentioned and thus would lead to positive results.
3. In practice, coarse aggregate phase is one of the most important design variables. It is shown in this paper that increasing the elastic modulus, enhancing volume fraction, reducing the coefficient of thermal expansion, decreasing the maximum grain size, and adopting open-graded coarse aggregates have positive results.
4. Although the theoretical analysis by the present model is qualitatively supported by a preliminary experimental study on cement-asphalt emulsion composite, further and systematic experimental studies are needed in order for the proposed model to be applicable in practice.

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