Comparison Between Biphasic and Triphasic Model for Predicting the Elastic Modulus of Concrete

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Abstract. The concrete is a composite material which, on the scale of the microstructure, can be considered as consisting of three phases: the matrix, the inclusions and the interface transition zone. The latter has features that reduce the properties of concrete and therefore limits its performance. Thus, with such complex structures, this zone is the weakest zone of the composite. The evaluation of the effective behavior of composite using predictive models requires a consideration of this zone. In this context an approach based on the model of double inclusion and on the Mori Tanaka theory to predict the elastic modulus of concrete are used. This approach will be compared with some analytical biphasic model such as Reuss model, Voigt model, the Voigt and Reuss combined models and Hashin and Shtrikman (HSS) models. Many experimental results are considered in the confrontation. So the model developed predicts very satisfactorily the elastic modulus of the concrete unlike other models in which a discrepancy in the results is demonstrated in the majority of cases.

1 Introduction

Many studies have shown that the concrete is not a simple biphasic composite material consisting of inclusions randomly dispersed in a matrix, but it contains a third phase. This phase is a thin layer of cement surrounding the inclusions [1-3]. It is typically more porous than the rest of the matrix. It is called the interface transition zone (ITZ). It is, rather, due to the wall effect initiated by the aggregate surface in which there is a limit in the cement grains arrangement compared to the rest of the matrix. Its thickness varies between 10 - 50 µm [4-6]. This zone is dependent on the size and the degree of roughness of the aggregates. It also depends on the size of the largest cement particle and the W / C ratio [1-3]. The ITZ, with complex structures, is the lowest region in composite, when exposed to external loads. [7] This limits the performance of the material in a significant way. It appears that any model of the concrete should be considered as triphasic material. In fact, since the Voigt work in 1889 many theoretical works were done in the 1960 and many numerical works in 1980, and that made the modeling discipline an active one. This article focuses primarily on the development of a triphasic model for predicting concrete elastic modulus. The second part is devoted to a brief presentation of some biphasic models such as Voigt model, Reuss model, Voigt and Reuss combined models and the limits of Hashin and Shtrikman. Finally a comparative confrontation will be represented between the predicted effective elastic modulus resulting from different approaches and the experimental results obtained by Z.Sun [8] and the results of lightweight concretes tested by K.Yang [9]

2 Modeling

2.1 Elastic Modulus prediction

The chosen analytical calculation is derived from the equivalent inclusion method [10] and from Mori Tanaka theory [11]. This calculation predicts the elastic modulus $E_c$ of heterogeneous composite from $V_t$ volume required to loading fig.1.

This composite consists of spherical inclusions which are aggregates $G = \sum_{i=1}^{n} G_i$ with volume $V_g$ and elastic modulus $E_g$ surrounded by layers of interfacial transition zone $ZIT = \sum_{i=1}^{n} zit$ which are considered in turn as the second type of inclusion with volume $V_{iz}$ and elastic modulus $E_{iz}$ all embedded in a cement paste with $V_m$ and elastic modulus $E_m$.

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Fig. 1. The stress field $\sigma^e$ on a heterogeneous composite

If the composite $V_t$ were uniform throughout its volume the stress field developed inside $V_t$ and the associated strain field would be uniform under the influence of $\sigma^e$; these fields would be $\sigma^e$ and $\epsilon^e$. However, because the material is heterogeneous, the stress fields and resulting strains are not uniform.

By applying the equivalent inclusion method, the heterogeneous composite is simulated to a homogeneous composite with stiffness $E_w$ and distributing (eigenstrains) $\langle \epsilon^g \rangle$ in $G$ and $\langle \epsilon^*_{itz} \rangle$ in ITZ are introduced so that the equivalent homogeneous composite is subjected to the same stress fields and strains that are resulting from solid heterogeneous. Disturbances in the whole stress applied $\sigma^e$ are due to these inclusions they can be simulated by $\langle \sigma_m \rangle$, $\langle \sigma_g \rangle$ and $\langle \sigma_{itz} \rangle$ for the matrix, the aggregates and the ITZ.

By applying the theory of Mori and Takana and the equivalent inclusion method, developed total stresses in the aggregates and the ITZ may be written as follows:

$$\sigma^e + \langle \sigma_g \rangle = E_m [E_m^{-1} (\sigma^e + \langle \sigma_m \rangle) + \langle \Delta \gamma_g \rangle - \langle \epsilon^g \rangle] = E_m [E_m^{-1} (\sigma^e + \langle \sigma_m \rangle) + \langle \Delta \gamma_g \rangle]$$  \hspace{1cm} (1)

$$\sigma^e + \langle \sigma_{itz} \rangle = E_m [E_m^{-1} (\sigma^e + \langle \sigma_m \rangle) + \langle \Delta \gamma_{itz} \rangle - \langle \epsilon^*_{itz} \rangle] = E_m [E_m^{-1} (\sigma^e + \langle \sigma_m \rangle) + \langle \Delta \gamma_{itz} \rangle]$$  \hspace{1cm} (2)

Where $\langle \Delta \gamma_g \rangle$ is the average disturbance strain caused by the eigenstrain $\langle \epsilon^g \rangle$ in a single and related to $\langle \epsilon^g \rangle$ by:

$$\langle \Delta \gamma_i \rangle = S_i \langle \epsilon^i \rangle \text{ with } (i = g \text{ or } itz)$$ \hspace{1cm} (3)

Where $(S)$ is the Eshelby tensor for a single inclusion independent of the aggregate mechanical properties [12] it depends only on Poisson's ratio of the matrix $(\nu)$ and the geometry of the inclusion.

The averages disturbance stress in each phase i.e. $\langle \sigma_m \rangle$, $\langle \sigma_g \rangle$, and $\langle \sigma_{itz} \rangle$ are obtained by solving the equation (1), (2) and equation (3)

$$\langle \sigma_g \rangle = \langle \sigma_m \rangle + E_m (S_g - 1) (\epsilon^g)$$  \hspace{1cm} (4)

$$\langle \sigma_{itz} \rangle = \langle \sigma_m \rangle + E_m (S_{itz} - 1) (\epsilon^*_{itz})$$  \hspace{1cm} (5)

Where $I$ is a unit tensor, to maintain the equilibrium, the sum of averages disturbance stresses must be zero. Thus for a volume proportion we have seen:

$$V_g \langle \sigma_g \rangle + V_{itz} \langle \sigma_{itz} \rangle + V_m (\sigma_m) = 0$$ \hspace{1cm} (6)

By replacing each term by its equation, we obtain the average disturbance stress in the matrix $\langle \sigma_m \rangle$

$$\langle \sigma_m \rangle = -E_m/V_t [V_g (S_g - 1) (\epsilon^g) + V_{itz} (S_{itz} - 1) (\epsilon^*_{itz})]$$ \hspace{1cm} (7)

Use equation (4) and (5) we obtain the average disturbance strain in the aggregates and in ITZ

$$\langle \sigma_g \rangle = E_m [(1 - V_g/V_t) (S_g - 1) (\epsilon^g) - (V_{itz}/V_t) (S_{itz} - 1) (\epsilon^*_{itz})]$$ \hspace{1cm} (8)

$$\langle \sigma_{itz} \rangle = -E_m [(1 - V_{itz}/V_t) (S_{itz} - 1) (\epsilon^*_{itz}) + -(V_g/V_t) (S_g - 1) (\epsilon^g)]$$ \hspace{1cm} (9)

Substituting equation (8), (9) and (10) in equation (1) and (2) we can write

$$\langle \epsilon^g \rangle = (C_1 + A_1 B^{-1} C) (B_1 - A_1 AB^{-1})^{-1} \sigma^e = D_1 \sigma^e$$ \hspace{1cm} (10)

$$\langle \epsilon^*_{itz} \rangle = [B^{-1} C + B^{-1} A (C_1 + A_1 B^{-1} C) (B_1 - A_1 AB^{-1})^{-1}] \sigma^e = \sigma^e$$ \hspace{1cm} (11)

The average elastic strain $\langle \Delta \gamma_m \rangle$ of the disturbance in the matrix $m$ is given as

$$\langle \Delta \gamma_m \rangle = E_m^{-1} \langle \sigma_m \rangle$$ \hspace{1cm} (12)
Equations (1) and (2) indicate that the average elastic strain $\langle \Delta \gamma g \rangle$ and $\langle \Delta \gamma zit \rangle$ are given by

\[
\langle \Delta \gamma g \rangle = E^{-1}_m (\sigma_m) + \langle \Delta \gamma g \rangle
\]

(13)

\[
\langle \Delta \gamma zit \rangle = E^{-1}_m (\sigma_m) + \langle \Delta \gamma zit \rangle
\]

(14)

From equations (12), (13) and (14)

Where $\gamma_0$ is the applied strain, the total average strain $\langle \Delta \gamma t \rangle$ of composite is given as

\[
\langle \Delta \gamma t \rangle = \gamma_0 + \nu (\langle \Delta \gamma g \rangle + \nu \langle \Delta \gamma zit \rangle + \nu_m (\Delta \gamma m))
\]

(15)

The average elastic moduli tensor of composite $E^{-1}_c$ is given by

\[
E_c = (E^{-1}_m + \nu D + \nu zit D_t)^{-1}
\]

(16)

With :

\[
A = [(S_g - I)(E_m(1 - \nu_g/\nu_t) + E_g \nu_g/\nu_t) - S_g E_g]
\]

(17)

\[
A_1 = [(S_{itz} - I)(E_m(1 - \nu_{itz}/\nu_t) + E_{itz} \nu_{itz}/\nu_t) - S_{itz} E_{itz}]
\]

(18)

\[
B = (S_{itz} - I)(E_m - E_g) \nu_{itz}/\nu_t
\]

(19)

\[
B_1 = (S_g - I)(E_m - E_g) \nu_g/\nu_t
\]

(20)

\[
C = 1 - E_g/E_m
\]

(21)

\[
C_1 = 1 - E_{itz}/E_m
\]

(22)

3 Theoretical Models

The macroscopic characteristics of heterogeneous composite result from combination of those constituent. Many micromechanics models of prevision of this elastic behavior exist in literature. Among these models were the Reuss model (R), the Voigt model (V), Reuss / Voigt combined model (RV), Voigt/ Reuss combined model (VR) and Hashin & Shtrikman model [13-16]. These models can be applied for concrete in the validation of triphasic model developed in the first section.

4 Comparisons of analytical models with experimental results

In the confrontation several experimental results are used. In a first place the results obtained by Z.Sun and al [17] on rigid aggregate concretes Table 1 are used. Then the results on the lightweight concretes Table 2 are used K.Yang [18].

In the works of Z.Sun three matrices were used where the ratio W/C was 0.35, 0.5 and 0.6. Only one type of aggregates is introduced in the matrices with varying percentages between 0.476 and 0.70.

<table>
<thead>
<tr>
<th>Designation</th>
<th>W/C</th>
<th>$E_m$(GPa) 7 Days</th>
<th>$E_m$(GPa) 28 Days</th>
<th>$E_g$(GPa)</th>
<th>$V_m$(%)</th>
<th>$V_g$(%)</th>
</tr>
</thead>
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<tr>
<td>2m</td>
<td>0.5</td>
<td>15.3</td>
<td>17.04</td>
<td>62.7</td>
<td>52.4</td>
<td>47.6</td>
</tr>
<tr>
<td>3c</td>
<td>0.5</td>
<td>15.3</td>
<td>17.04</td>
<td>62.7</td>
<td>35.2</td>
<td>64.8</td>
</tr>
<tr>
<td>4c</td>
<td>0.5</td>
<td>15.3</td>
<td>17.04</td>
<td>62.7</td>
<td>32.5</td>
<td>67.5</td>
</tr>
<tr>
<td>5m</td>
<td>0.5</td>
<td>15.3</td>
<td>17.04</td>
<td>62.7</td>
<td>35.2</td>
<td>64.8</td>
</tr>
<tr>
<td>7m</td>
<td>0.35</td>
<td>23.11</td>
<td>24.35</td>
<td>62.7</td>
<td>47.3</td>
<td>52.7</td>
</tr>
<tr>
<td>8m</td>
<td>0.35</td>
<td>23.11</td>
<td>24.35</td>
<td>62.7</td>
<td>41.8</td>
<td>58.2</td>
</tr>
<tr>
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<td>24.35</td>
<td>62.7</td>
<td>35.3</td>
<td>64.7</td>
</tr>
<tr>
<td>11m</td>
<td>0.6</td>
<td>11.72</td>
<td>13.54</td>
<td>62.7</td>
<td>55.2</td>
<td>44.8</td>
</tr>
</tbody>
</table>
In the works of K.Yang, three matrices were used. The $W/C$ ratio was 0.446, 0.35 and 0.29. In each matrix four types of lightweight aggregates are introduced with varying volumes, 0.125, 0.25, 0.375 and 0.45.

### Table 2. Experimental characteristic concretes tested by K.Yang

<table>
<thead>
<tr>
<th>Volume of aggregates $V_a$</th>
<th>Designation</th>
<th>0%</th>
<th>12.5%</th>
<th>25%</th>
<th>37.5%</th>
<th>45%</th>
</tr>
</thead>
<tbody>
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<td>28588</td>
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<td>33183</td>
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<tr>
<td></td>
<td>M10</td>
<td>35397</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4.1 Results and discussion

From the relationships of the various analytical models mentioned above, the elastic modulus of concrete shown in Tables 2, 3 are calculated. In order to have a clearer representation, the results obtained designated (Ecal) they are compared to the experimental results designated (Eexp) for each table separately. In Figure 2, the result of Z.Sun are compared with theoretical result in Fig.2.
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<table>
<thead>
<tr>
<th>Designation</th>
<th>Young’s modulus E (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Volume of aggregates</td>
</tr>
<tr>
<td></td>
<td>0%</td>
</tr>
<tr>
<td>M8</td>
<td>28588</td>
</tr>
<tr>
<td>M9</td>
<td>33183</td>
</tr>
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<td>M10</td>
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</tr>
</tbody>
</table>

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Fig.2. Comparison of Young’s modulus between the experimental results of Z. Sun and predictions of different models

Regarding to the Z. Sun data, observed in Figure 2, it is clear that there is a wide depression for the majority of the models. The differences between experimental and theoretical result according to volume of aggregate Vg are shown in Fig.3.

Fig.3. Differences on Young’s modulus between predictions and experimental results

The highest disparities are recorded for Voigt model. A value of 63% is obtained in a ratio E_g/E_m=4.63. These differences drop when this ratio decreases, where for a ratio of E_g/E_m=2.57 the gap drops to 12%. The Voigt/Reuss combined model are less accurate. But the Reuss/Voigt combined model and HS inf bounds are more precisely.

In Fig.4, the K.Yang experimental results are compared to the results of the different models. Depending on volume of the aggregates Vg Fig.5 shows the disparities obtained.
The figure 4 and 5 show that the results of all models are distant oneself from experimental results when the contrast in stiffness between the two phases increases. For the ratio $E_g/E_m=0.12$ a maximum 59% of disparities appears with the Reus model the differences between predictions and experimental results are also increase with the volume of aggregates. The rest of the models give lower disparities.

To test the validity of the triphasic model, the experimental results will be compared with those obtained by the last one. However, the application of this model requires knowing of elastic modulus and volume of the interface transition zone. Due to its complex structure, it is difficult to determine these local properties with existing measurement techniques [19, 20]. It is often assumed that the elastic modulus of ITZ as a fraction of the elastic modulus of bulk cement paste [21-22]. Equation (23):

$$E_{ZTI} = \alpha E_m$$  

Where $\alpha$ is between 0.2 and 0.8. Therefore, $E_{ZTI}$ can be easily calculated since we know $E_m$.

Concerning the volume of the ITZ in the present study he’s a fraction from the volumes of the aggregates $V_g$. For $V_g$ below to 60% $V_{ITZ}=0.3V_g$ and for $V_g$ higher than 60% $V_{ITZ}=0.5V_g$.

In Fig 6 the experimental results for Z. Sun are compared to elastic modulus predicted by the triphasic model developed in the previous section.
The results obtained by the model are very similar to all experimental results of Z. Sun in which the maximum disparity is 7%.

Fig.7 represented a confrontation between the experimental results of K. Yang and those predicted by triphasic model.

Generally, there is a good correlation between the triphasic model and the experimental results. With these results the maximum disparities is 8.65%. However; it should be noted that the standard disparities between experience / modeling, increases with the quality of the matrix. According to the observations of K. Yang, on very rigid concrete rupture occurs abruptly, and the measured results are more dispersed than those for less rigid concrete. Also, larger differences appear for concrete low volume ratios of aggregate. According to the author for these aggregates segregation fractions were observed which influenced the experimental measurements of stiffness concrete.

5 Conclusions

The results obtained by the predictive approaches illustrated in Figures 2 and 3 shows that the biphasic models are not appropriate for predicting elastic modulus. For all concretes tested there is a wide disparity between the predictions provided by the different approaches and experimental results he was observed. In particular, when the ratio between the stiffness of the two phases becomes large and the volume of the aggregates exceeds 40%.
For all existing data no method seems to provide accurate predictions to 100%. However, the analysis in the previous section shows that the triphasic model can be used to predict the elastic modulus in rigid aggregates concrete and lightweight concrete. Good accord was found between the model results and experimental results whatever the parameter analysis. Furthermore, the interpretation of experimental results using this model highlights the importance of taking into account the ITZ as the third phase and its influence on the global concrete behavior.

References