How to consider the Interfacial Transition Zones in the finite element modelling of concrete?

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ABSTRACT

Because the ITZs' thickness in concrete surrounding aggregates is tiny, it is difficult to take them into account explicitly in the modelling of concrete. A methodology is suggested to consider the effect of the ITZs on the mechanical behaviour of concrete at the mesoscopic scale. For that, the mechanical ITZ properties have been calculated according to the hydration of cement at various distances of the aggregate boundary. Then, we have defined an effective mixed interphase (EMI) around each aggregate which is formed by the ITZ and a volume fraction of the bulk cement paste. Simulations have been performed to show the influence of this EMI on the tensile failure of concrete. Results have shown that the maximum strength of the specimens depends on the local tensile strength of the ITZs. Stresses were more diffused for the cases without the ITZs and with the ITZs having a lower tensile strength.

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1. Introduction

This study aims to suggest a method to consider the presence of the Interfacial Transition Zone (ITZ) around aggregates in concrete. The ITZs are the thin thicknesses of cement paste around aggregates with different properties than the cement paste which form the matrix of concrete (called the bulk cement paste). The main theory suggests that it is due to the cement grains in contact with the aggregate boundary at the moment of mixing (called the wall effect) which limit the water motion in this area and this water, after hydration of the cement clinkers, results in the formation of the porosity [1,2]. As a high quantity of water is maintained in this area, a high volume of porosity is created. The ITZ thickness (δ_{ITZ}) is between 20 μm and 50 μm and some experimental studies have shown that it corresponds to the mean radius of cement grains [1]. The value of the thickness and the ITZ properties could also depend on the aggregate size [3] and its mineralogic composition [4]. The differences observed in numerical results in comparison with experimental measurements on the mechanical behaviour of concrete are often explained by the fact that the ITZ is not taken into account in the model. Should consideration of the ITZ in modelling be gained?

Standard codes and models used in civil engineering do not take it into account because these models are empirical and the ITZ effects are not of a magnitude relevant to engineering application. Recent numerical models do not allow going down to the fine scale of the ITZ and justify the calculation error by the ITZ effect which cannot be

digitalized. Some attempts have been performed to consider the ITZ in numerical models [5–8] and in analytical models [9–12] to calculate the effective properties of concrete as a heterogeneous material. Garboczi and Berryman [7] and Zheng et al. [12] have suggested a homogenization of aggregates with ITZs which then form a new inclusion in the matrix. The homogenization of aggregate + ITZ is unsatisfactory because it leads to a decrease in the strength of the aggregate and it becomes impossible to check the hypothesis of the brittleness of the ITZ which could be the cause of the concrete failure. For modelling the ITZ properties can be calibrated on experimental observations [4,13,3]. Many authors have suggested some methods to calculate the ITZ properties by considering some empirical assumptions [14–17], but without linking with the effective behaviour of concrete. Bentz and Garboczi [5] were the only ones who suggest a model which determines the ITZ properties according to the hydration of the cement paste, but the link with the mechanical properties was not established.

In this study, the calculation of the effective behaviour of concrete was performed according to the numerical characterization of the ITZ properties. Two parts of this study are the originality of this work: the calculation of the ITZ mechanical properties according to the hydration of cement and the implementation of the ITZs in a finite element (FE) calculation.

Nadeau [16] has calculated the ITZ properties by supposing an evolution of the water-to-cement (w/c) ratio according to the distance from the aggregate boundary [18]. By considering this hypothesis, the ITZ properties were calculated according to the age of the concrete, i.e. the cement hydration. The model of Bernard et al. [19], modified by Grondin et al. [20], was retained for the calculation of the cement hydration. The ITZ around an aggregate was supposedly formed by n layers having the same thickness. In each layer the w/c ratio is different, so

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the volume fraction of the residual clinkers and formed hydrates was calculated in each layer according to the local hydration kinetic. Then, the effective properties of the ITZs were calculated by homogenization [20] by averaging the local properties of each layers. The homogenization of the ITZ layers keeps the initial strength of the aggregate and allows defining a brittle area between the aggregate and the matrix. This homogenization method does not take into account the brittleness within the layers, but the main goal of this study is the consideration of a brittleness area around aggregate to show its effect on the global behaviour of the specimen.

The ITZ thickness is commonly between 20 μm and 50 μm. In a finite element model it is very numerically expensive to represent it explicitly, even less to decompose it in many layers with different properties. For instance, in a 2D representative elementary volume (REV) of concrete with dimensions $50 * 50$ mm^2, if we would represent the ITZ by one finite element with a thickness of 30 μm, we have to mesh the REV by $2.7 \cdot 10^6$ elements. So, in order to take into account the ITZ properties in the calculation with a limitation of the finite elements, we have considered a three-phase material for concrete: aggregates, the bulk paste, and an effective mixed interphase (EMI). The EMI around an aggregate is formed with the ITZ and a part of the bulk cement paste. Its properties are homogenized with the effective properties of ITZs and the bulk cement paste properties according to the volume fractions of ITZs and of the bulk cement paste in EMI. Calculations were performed in the finite element code of calculation Cast3m to assess the damage of concrete with and without ITZs. The damage was obtained by considering a damage model based on the microplane theory [21].

First of all, the algorithm of the model is presented in detail. Second of all, a statistical study is shown in order to define the relevant method to take into account the ITZ properties in the modelling of concrete. Then, the calculation results are analysed for concrete under a tensile load.

2. Digital representation of the EMI in a FE modelling

The ITZs surrounding aggregates in concrete could be modelled by an interfacial law in a FE code [22], but we loss the information about the evolution of the properties into the ITZs. Without taking into account the effect of the aggregate size and its mineralogic properties, Nadeau [16] has suggested a model to calculate the volume fraction of cement f_{citz} through the ITZ at the first contact of cement and aggregates before added water:

$$f_{citz}(r) = f_{cb}\left[1 + a_c\left(\frac{r - r_a - \delta_{ITZ}}{\delta_{ITZ}}\right)^2\right] \tag{1}$$

where f_{cb} represents the volume fraction of cement in the bulk paste.

The ITZ could be divided in n-layers of thickness equal to $\delta_{ITZ}/(r - r_a)$ and the elastic modulus of the n-layers is calculated according to simple relations linking the elastic moduli of cementitious materials to the w/c ratio. Then, the effective elastic modulus of the ITZ can be obtained by averaging the n-layers.

For a detailed modelling of the ITZ influence on the behaviour of concrete, ideally we could represent explicitly each n-layers. But it is easy to notice that a FE modelling is impossible to realize because it needs a too high number of elements due to a high ratio between the specimen volume size and the element size required to represent a layer. Another method could be the modelling of one aggregate in a volume which allows representing all layers. But it is not representative of concrete and it leads to a high approximation of the results.

For a regular FE grid and for a volume size to aggregate size ratio equal to 4 [23], an aggregate maximum size of 12.5 mm leads to a volume size in 2D of 50×50 mm^2. For instance, even if the ITZ is represented by only one layer of 50 μm, the finite elements have to be equal to minimum 50×50 μm and the total number of elements in the volume is of order $1 \cdot 10^3 \times 1 \cdot 10^3$. So, for the ITZ divided in n-layers the

number of finite elements increases substantially. To limit the number of elements, we have considered interphases (EMI) surrounding aggregates containing the ITZ and a volume fraction of the bulk cement paste. The choice of this fraction depends on the interphase thickness:

$$\delta_{fb} = \delta_{int} - \delta_{ITZ}. \tag{2}$$

In this study the concrete volume was formed by composite circles (in 2D) with different diameters according to the aggregate size distribution equal to $\varnothing_{agg} + 2\delta_{int}$ and a matrix formed by the rest of the bulk cement paste. The generation of the volume was made with the algorithm developed by Mounajed [24] (cited in [23]) and modified to consider the interphase surrounding aggregates (Fig. 1).

The distribution algorithm generates randomly candidate positions of the inclusion gravity centres in the area defined by the REV. At this step, an inclusion i is formed by an aggregate surrounding by an EMI. In 2D the unit volume of an inclusion of type i is calculated as follows:

$$VS_i = \pi(R_i^{agg} + \delta_{int})^2. \tag{3}$$

The unit volume of an aggregate is obtained by:

$$VG_i = \pi(R_i^{agg})^2 \tag{4}$$

Some tests are made to validate these positions. A first test consists to check if this position concerns an element of Digital Concrete type. We calculate the distance between the element gravity centre and that of the inclusion. If this distance is higher than the element average size, this element will have the properties of the inclusion.

A second test checks that two inclusions do not overlap. The distance between an existing inclusion gravity centre, of radius $R1$, and a candidate inclusion, of radius $R2$, has to be higher to a value d_{min} defined as:

$$d_{min} = \left(\frac{R_1 + R_2}{2}\right). \tag{5}$$

After the model has validated the inclusions' position, they are affected by characteristic materials defined by the user. Before the inclusions' generation, all the elements were defined by the material parameters of the matrix (the bulk cement paste). Then the model tests if the position of an element gravity centre is in an aggregate, respectively EMI, influence radius. By taking R^{agg} for the aggregate radius, respectively $(R_i^{agg} + \delta_{int})$ for the inclusion, and d_{inf} the distance between an element gravity centre and that of the inclusion, the element takes:

- the aggregate properties if $d_{inf} \leq R^{agg}$,
- the EMI properties if $R^{agg} < d_{inf} \leq R_i^{agg} + \delta_{int}$,
- the matrix properties if $d_{inf} > R_i^{agg} + \delta_{int}$.

In order to take into account local properties of the ITZ a homogenization of the n-layers' properties seems necessary. First of all, the relevant number of layers has to be defined to obtain an optimal result. Zheng et al. [12] have suggested a number of layers over 70 but their method was applied to the calculation of the effective properties averaging the modulus of aggregate, the bulk cement paste and the ITZ layers. Here, the homogenization does not consider aggregates. The Voigt's bound was used to calculate the effective modulus of the EMI:

$$X^{hom} = \sum_{k=1}^{n+1} f^k X^k \tag{6}$$

with f^k the volume fraction of the layer k ($k = [1,n]$ for the ITZ and $k = n + 1$ for the bulk cement paste) with the elastic properties X^k. The individual properties of each layer were calculated with the model developed by Grondin et al. [20] and modified to take into account the evolution of the properties with the distance from the aggregate surface.