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A unit cell based three-phase approach for the mechanical characterization of quasi-brittle cementitious composites

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ABSTRACT

A simple two-dimensional Unit cell (UC) with three different mesoscopic phases may be geometrically modeled as a combination of two concentric circles or squares embedded in a square. In this paper, a two-dimensional three-phase UC with a similar design is developed and utilized for modeling the full deformation and failure response of cement based quasi-brittle cementitious composites under compression. It was identified from the numerical investigation that the three-phase design greatly improved the prediction capability of the UC in suitably capturing the material nonlinearity observed experimentally.

1. Introducing the three-phase UC approach

There are mainly three types of material models seen in the literature, namely macro, meso and micro models as defined by Wittmann [1]. Macroscopic models are used to model the mechanical response of the material, where it is sufficient to assume that the structure of the material is homogeneous. In mesoscopic models, the focus is on the different phases of the material constituting its mesostructure. Modeling of different phases helps us to identify the details of failure in the material and to relate the failure mechanisms to the macroscopic mechanical response. Whereas in microscopic approach, the microstructure of the material is analyzed at the level of molecular interactions of the constituent elements and these interaction details are used to predict the mechanical properties of the material.

For the purpose of characterizing the mechanical response of cementitious composites with several mesoscopic phases as in the case of Plain Concrete (PC), the macroscopic response may be predicted from the independent deformation and fracture properties of its mesoscopic phases. This will help in identifying the influence of the properties of the independent phases in the overall constitutive behavior of the material. In the specific case of cement based materials that are considered in the present paper, such as PC, Glass Fiber Reinforced Cement Composite (GFRC), Polymer Fiber Reinforced Cement Composite (PFRC) and Mixed Fiber Reinforced Cement Composite (MFRC), it may be observed that the mesostructure consists of a plain or a fiber reinforced matrix phase based on cement, an aggregate phase, and an Interfacial Transition Zone (ITZ) phase between the other two phases. In similar cases, most researchers follow a common approach of modeling each and every phase present in the material to exactly replicate the mesostructure, thereby making a highly resource sensitive and complex numerical model.

A better and effective alternate approach is to visualize a simple model, using the concept of Representative Volume Element (RVE) introduced in Hill [2]. In this approach, the visualization of a repeating unit of the material mesostructure is an initial step in minimizing the complexity of the meso-model. The UC concept employed in the present study is more attractive due to its simple definition that it may be of any size when compared to that of a known RVE, and may not contain sufficient number of inclusions similar to that which is physically present in the material mesostructure. It is conceptually a representation of the total volume fractions of some of the distinct phases in the material mesostructure. In the initial design of the UC, Pettermann and Suresh [3], Gupta and Venkatesh [4], and Ghouse et al. [5] assumed the presence of only two distinct phases in their UC models. In their two-phase UC model for normal strength concrete, Ghouse et al. [5] considered only the matrix phase and the aggregate phase. Here the first phase represents the total volume fraction of a continuum that has the overall properties of all the constituents of the mesostructure taken together, excluding the coarse aggregate phase. The second phase represents the total volume fraction of coarse aggregates present in the concrete mix. Hassan et al. [6]

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observed that this simple UC was not sufficient to capture the full mechanical behavior of the material, while dealing with the two-phase UC approach for the mechanical characterization of PFRC. In this paper, the deficiencies identified in the two-phase UC approach are addressed by defining another UC with a three-phase concept consisting of matrix, aggregate and ITZ phases.

Sluis [7] reported that the effectiveness of prediction of a UC is dependent on its size and the type of boundary conditions that are applied on its boundaries. Researchers like Huet [8], Amieur et al. [9], Ostoja-Starzewski [10] and Pecullan et al. [11] also have investigated the convergence of prediction results with respect to the increasing UC size and the type of boundary conditions assigned. There are mainly three types of Boundary Conditions (BC) that are used in connection with the UC approach namely (a) Static (b) Dynamic and (c) Periodic Boundary Conditions (PBC). While the static BC enforces a uniform displacement on the boundaries of the UC, the dynamic BC enforces a constant stress [12]. The PBC is a type of BC applied on the parallel edges of the UC so that deformation can occur without affecting the parallelism of the edges to prevent any discontinuities in the material macrostructure as illustrated by Pettermann and Suresh [3].

To understand the PBC, consider the domain Ω_{UC} defined by the UC boundary shown in Fig. 1 where PBC defined by Eq. (1) is applied between its vertical edges Γ_{ij} and Γ_{kl}:

$$\boldsymbol{y}\left(s^{ij}\right)-\boldsymbol{r}^{i}=\boldsymbol{y}\left(s^{kl}\right)-\boldsymbol{r}^{l} \tag{1}$$

where $\boldsymbol{r}^i$ is the position vector of the node i and $\boldsymbol{r}^l$ is the position vector of the node l with respect to which the boundary is tracked, $\boldsymbol{y}(s^{ij})$ is the position vector of the point A on the boundary $i-j$ at a distance s^{ij} from node i and $\boldsymbol{y}(s^{kl})$ is that of point A' on boundary $k-l$ at a distance s^{kl} from node l. Typically, $s^{ij}=s^{kl}$ for the implementation of PBC.

Terada et al. [13] considered constant stress, uniform displacement and PBC as boundary conditions in their UC investigations to report that when the case of PBC was considered, a relatively smaller UC was found to be sufficient to predict the apparent elastic properties effectively, for a general heterogeneous material with no geometrical periodicity. This in other words states that a UC of a relatively smaller size would meet the requirements of an RVE of the material when it is assigned with PBC. Miehe and Koch [14], Gupta and Venkatesh [15], and Ghouse et al. [5] also reported the implementation of PBC in their respective UCs. Hassan et al. [6] considered different sizes of two-phase UCs assigned with PBC to determine the minimum required size for modeling the full deformation and failure response of the material and identified that the UC size considered by Ghouse et al. [5] was not sufficient enough to model the full deformation and failure response of the material in comparison with experimental observations.

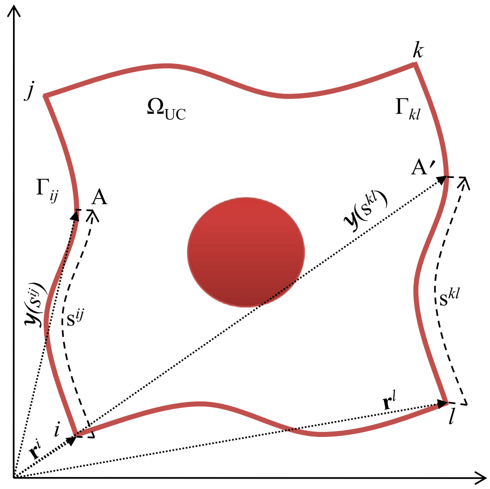

Fig. 1. UC boundary with PBC applied.

The presence of ITZ phase in cement-based composites is one of the factors that affect the overall mechanical behavior of the material in addition to the contribution from the presence of other phases mentioned previously. Initially, Farran [16] reported the presence of ITZ phase in the form of a *transition aureole*. A number of reports can be seen in the literature regarding the properties of this phase being observed as weaker than that of the matrix and as exhibiting a gradient in the properties throughout its thickness. Hadley [17] used a Scanning Electron Microscopy (SEM) technique to describe the ITZ as consisting of a duplex film formed between the aggregate surface and that of the hardened cement paste. The thickness of ITZ was defined by Grandet and Ollivier [18] using an X-ray diffraction technique. Scrivener et al. [19] conducted experiments on real concrete specimens using Backscattered Electron Microscopy (BEM) and computerized image processing to study the microstructure of the ITZ. He concluded that the thickness of ITZ might vary from 30 to 50 µm. Using a nano indentation based technique called Raman Micro Spectroscopy (RMS), Machovic et al. [20] identified that the ITZ phase present between polyethylene fiber and cement matrix has a thickness of 40 µm and its mechanical properties varied across its thickness, based on the variation in the concentration of its constituents namely Calcium Silicate Hydrate (CSH) and Calcium Hydroxide (CH). He also identified that its elastic modulus was in the range of 5–10 GPa in the first 5–10 µm near to the fiber surface and as he moved away from the fiber, the elastic property increased to a value same as that of the matrix. Bentz et al. [21] reported that the composition of cement paste is highly porous in nature with lesser percentage of CSH gel and higher concentration of CH in it. Hashin and Monteiro [22] reported an inverse method to determine the ITZ properties between the aggregate and cement paste, from a three-phase composite model based on experimental investigations. He estimated the average thickness of ITZ as 25 µm and its elastic modulus as 50% of that of the bulk cement paste.

Nilsen and Monteiro [23] suggested that materials like cement composites may be numerically modeled with sufficient details by considering the presence of a third ITZ phase. We can see several lattice or continuum based models in the literature that consider ITZ as a separate phase. Neubauer et al. [24] reported a three-phase mathematical model for modeling the elastic properties of mortar in which the ITZ was modeled as a separate phase with constant properties, without considering the gradient seen throughout its thickness. The thickness of the phase was taken as 20 µm and elastic modulus was taken as 30–50% of that of the matrix. Arslan et al. [25] reported a lattice based model in which he considered ITZ as a linearly elastic phase with perfectly brittle behavior, post-peak. Lilliu and Van [26] reported a 3D lattice model in which the ITZ phase was assigned a tensile strength of 25% of that of the matrix. Ghouse et al. [5] analyzed different variations of a two-phase UC designed for modeling the deformation and failure of normal strength concrete in tension as well as compression and concluded that the UC approach could predict the compressive strength of the material in reasonable limits. However, the results from the two-phase model did not predict any non-linearity in the pre- and post-peak regimes and the experimental correlation of the predicted results was not good. They then considered the presence of a third phase in the UC with ITZ properties and reported that the presence of ITZ layer did not improve the prediction of pre-peak non-linearity in the stress–strain response.

Subsequent to the review of the above-mentioned observations in the literature, the two-phase UC used in Hassan et al. [6] was redefined in this study with a third ITZ phase in addition to the