



Exploring the Influence of Heterogeneity on Determination of an RVE for Concrete Structures

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Abstract. The mechanical behavior of heterogeneous materials is strongly influenced by its constituents at lower scales. This fact accounts for nonlinearities observed at the macroscale, and consequently, the challenges in formulating constitutive models that provides accurate predictions in a practical application context. Essentially, there are two primary ways to represent a heterogeneous material, either through Phenomenological Models at a Single Scale or Multiscale Models. Multiscale models represent the most robust approach to depicting a heterogeneous material. In these models, the connection between macro and meso-levels is made through the concept of Representative Volume Element (RVE). The RVE is the smallest material sample that can statistically represent the mechanical behavior of the material. However, the appropriate determination of an RVE for quasi-brittle materials remains a subject of study. This paper discusses the determination of RVEs for concrete using normalized graded aggregate curves. For this purpose, numerical simulations were performed using the Finite Element Method, employing constitutive models based on Phase Field theory. Throughout the study, issues related to the RVE' size and the determination of ergodic properties are discussed. The influence of the aggregate gradation curve on the behavior of the RVE and the influence of the aggregate-mortar interface are also examined.

Keywords: Multiscale modeling, Representative Volume Element (RVE), Finite Element Method (FEM).

1 Introduction

The properties of different materials and their applications have always been of interest to engineers and scientists around the world, particularly in the pursuit of innovative ways to enhance human societies and technologies. However, defining these properties and understanding their behavior in practical situations is not as straightforward as it might appear. It requires considerable effort and creativity from researchers to describe and model them accurately. For this reason, one of the primary areas of study in materials science, alongside electrical and thermal characteristics, involves determining the mechanical behavior of materials like concrete, the focus of this work. Concrete is a well-known material used since ancient times, especially in infrastructure and construction projects throughout history. Yet, some of its aspects remain poorly understood, largely due to the nature of its internal structure, which is defined by a mixture of distinct particles with intricate interactions among them. This complexity suggests a tendency toward heterogeneous behavior, as discussed by Schafer et al [1]. Indeed, materials can be categorized based on their structural characteristics. Homogeneous materials, for instance, exhibit uniform properties and composition throughout their volume, ensuring consistent behavior across all units. In contrast, heterogeneous materials have an irregular structure due to their multi-phase composition, which results in varying properties and configurations across different units of the material. However, even materials considered homogeneous can exhibit heterogeneous characteristics at certain observational scales, where isolated internal effects become more pronounced at finer scales, as noted by Gitman [2].

In practical applications, numerical models serve as an indispensable tool in the analysis of structural elements, enabling the simulation of complex behaviors under various load conditions. However, the efficacy of these models is intrinsically linked to the quality of the constitutive models employed. Generally, constitutive models can be categorized into two broad groups: single-scale constitutive models and multiscale models.

Single-scale constitutive models are developed to describe material behavior by assuming homogeneity at the scale of interest. They can provide a robust representation of the material and are computationally efficient, but may fail to capture critical phenomena occurring at smaller scales. On the other hand, multiscale models simultaneously consider multiple observational scales. Thus, they integrate material behavior across different levels, allowing for a

more detailed and accurate depiction of physical phenomena. This feature makes these models particularly suitable for representing heterogeneous materials such as concrete.

In any multiscale modeling, it is essential to define the Representative Volume Element (RVE). The RVE is the smallest unit of a material that still retains properties statistically equivalent to the material as a whole. This enables scientists and engineers to model the behavior of heterogeneous materials by considering all significant microstructural variations within this volume. Correctly defining the size of the RVE is crucial: a volume too small may not capture all the necessary features, while a volume too large may include structural behaviors beyond the material itself. The importance of the RVE has spurred extensive research on its definition and remains a subject of study today.

Another important aspect of multiscale models is the high computational cost due to the detailed simulations of microstructural variations within the Representative Volume Element (RVE), requiring substantial processing power and time. This can hinder their practical application in structural design projects. However, this cost can be mitigated with the aid of machine learning models. By training a machine learning model to represent the RVE, it is possible to predict the complex behavior of materials without performing all the detailed simulations. This model replaces the parallel models that represent the RVE in multiscale simulations, speeding up the process and reducing the computational cost while maintaining accuracy. Training data can be generated from numerical simulations representing the RVE in elementary tests. The success of this approach depends on an appropriate definition of the RVE size and the development of numerical models that employ constitutive models capable of representing each modeled phase and their interactions.

In light of the foregoing, this paper discusses the determination of Representative Volume Elements (RVEs) for concrete using normalized graded aggregate curves. For this purpose, numerical simulations were performed using the Finite Element Method, employing constitutive models based on Phase Field theory. Throughout the study, issues related to the size of the RVE and the determination of ergodic properties are discussed. The influence of the aggregate grading curve on the RVE behavior, as well as the influence of the aggregate-mortar interface, are also examined.

2 Theoretical Principles

2.1 RVE Definition

Multiscale methods owe their success to the existence and selection of a Representative Volume Element (RVE) with appropriate dimensions. Trusov and Keller conceptualize the RVE as the minimum material volume that contains a statistically sufficient number of deformation mechanisms [2]. Increasing this volume should not result in changes to the evolution equations for field values that describe these mechanisms. Various authors have proposed different definitions for the RVE, according to Gitman [2]. However, all aim to ensure that the RVE is small in comparison to the structural dimensions at the macroscale, yet large enough to represent the material's microstructure and all the mechanisms responsible for its physical non-linearities. Concerns about the small size of the RVE relative to the problem dimension are to ensure that its representativeness remains independent of the boundary conditions at the macroscale. Moreover, to accurately define the RVE, it is essential to clearly distinguish between the observation scales. Additionally, the RVE should exhibit homogeneous and ergodic properties. It should be noted that the RVE necessarily requires ergodic properties to ensure that its average characteristics are equal to the average characteristics of the entire material when observed at different points. This is crucial because it guarantees that the behavior of the RVE is statistically representative of the behavior of the material as a whole, allowing for accurate and consistent analysis of properties and physical phenomena, regardless of the specific location within the material.

There is no standardized method for determining the size of a Representative Volume Element (RVE). Various methodologies have been developed and implemented to derive quantitative data on the dimensions of RVEs. However, comparing RVE sizes remains challenging due to variations (i) across different stages of loading, (ii) among materials with distinct properties, and (iii) in various testing configurations.

In the quest to determine the size of the representative volume element (RVE), many researchers have attempted to correlate the RVE size with the maximum dimension of inclusions. Specifically, for concrete, Van Mier and van Vliet [3] suggest that the RVE should be approximately 3-5 times the size of the largest inclusion. Meanwhile, Bazant [3] proposed a specific volume for the RVE, denoted as x .

While some studies focus on the correlation between the RVE size and inclusion dimensions, others explore alternative methods to ascertain RVE dimensions [2, 4, 5]. These alternatives consider factors such as the volumetric fraction of inclusions, differences in stiffness between inclusions and the matrix, and the material's particle size distribution. This approach generally involves more sophisticated methodologies and a stronger reliance on statistical analyses.

In our current study, we aim to identify the RVE size by considering the influence of the aggregate particle size distribution. We determined the RVE size by conducting a similarity analysis between stress-strain curves from RVEs of various sizes, as discussed in Section 3.

2.2 Phase-field theory applied to constitutive models.

Phase field models are mathematical/computational approaches that describe the evolution of cracks using continuous field variables to represent the state. Thus, these models capture the gradual transition between intact and damaged phases, allowing for accurate simulation of crack nucleation, propagation, and coalescence without the need for explicit tracking of fracture surfaces.

The formulation of these models is based on the variational approach to Griffith's classical energy balance for brittle fractures. For this purpose, the energy balance of a deformable body Ω with a crack of surface S is formulated variationally as follows [6]:

$$\Pi = \int_{\Omega} \psi(u) \, d\Omega + \int_s G_c \, dS. \quad (1)$$

Where $\psi(u)$ is the elastic strain energy density as a function of displacement, and G_c is the critical energy release rate characterizing the fracture resistance of the material.

Minimizing eq.1 is mathematically impossible because of the unknown nature of S . To overcome this impossibility, the regularization of the fracture topology is proposed as a zone of diffuse damage, where the damage of material is represented by a variable, ϕ , which varies from 0 (intact material) to 1 (fully damage). Consequently, the existence of a physical discontinuity in the material is not admitted. This approach results in a model with ability to handle topologically complex fractures, an important ability for representing the degradation of quasi-brittle materials like concrete. This capability was the principal factor for the model's adoption in this study. Accordingly, eq.1 can be approximated as [7, 8].

$$\Pi = \int_{\Omega} \underbrace{(1 - \phi)^2}_{g(\phi)} \psi(u) \, d\Omega + \int_{\Omega} G_c \underbrace{\frac{1}{2l_0} \phi^2 + \frac{l_0}{2} |\nabla \phi|^2}_{\Gamma_c(\phi, \nabla \phi)} \, d\Omega. \quad (2)$$

Where $g(\phi)$ is a continuous degradation function that monotonically degrades the stiffness of the material as the phase-field approaches the crack phase ($\phi = 1$) and $\Gamma_c(\phi, \nabla \phi)$ represents the crack density functional, which enables tracking of the evolving crack surface S . There are several propositions for function $g(\phi)$ [7, 9, 10], in the present work, the proposal by [7] has been adopted. Several crack density functionals have been proposed [11–13], in this work, was adopt the form [7].

It is essential to note that the crack density functional is dependent on the parameter l_0 , which, in turn, is a prescribed length scale parameter that governs the extent of fracture regularization. Some view this parameter as a purely mathematical construct designed to enable the representation of Griffith's fracture as a diffuse continuous zone, such that the phase-field solution should converge to a discrete fracture solution as l_0 approaches zero [6]. Moreover, some argue that l_0 denotes a particular material characteristic that is intimately associated with the critical stress required for the initiation of fractures [14, 15].

Based on eq.1, it is possible to derive the macroscopic equilibrium condition and the evolution equations for the phase field, resulting in an interaction between the displacement field (u) and the phase field (ϕ).

$$\begin{aligned} \sigma_{ij,i}(u, \phi) + b_i &= 0 \\ G_c \left(\frac{\phi}{l_0} - \nabla^2 \phi \right) - 2(1 - \phi)\psi(u) &= 0 \end{aligned} \quad (3)$$

where b_i is the body force term, with the Cauchy stress, σ_{ij} , related to the elastic strain, ε_{ij} , and the fourth-order elasticity (stiffness) tensor, C_{ijkl} , by

$$\sigma_{ij} = \frac{\partial \Pi}{\partial \varepsilon_{ij}} = g(\phi) C_{ijkl} \varepsilon_{kl} \quad (4)$$

The weak formulation of eq. 3 allows for the discretization of (u, ϕ) using a conventional finite element approach, enabling the derivation of the residual and stiffness matrices. This numerical implementation is described in detail in [16].

Note that l_0 was originally introduced (see Eq. 1) as a mathematical construct to transform a discrete crack surface into a smooth continuous gradient, representing a diffused crack. It also indirectly dictates the size of elements in a finite element mesh, as overly large elements can lead to models that fail to capture the dynamics of data evolution accurately, resulting in errors. Thus, the use of phase field models in the modeling of RVEs requires highly refined meshes, especially if the RVEs consider the existence of an ITZ (Interface Transition Zone). Consequently, the computational cost of these models is also significant, which encourages research seeking alternatives for the RVE simulations.

3 Methodology

To achieve the objective of this research, series of simulations were tested to describe a concrete element by means of an RVE through computational methods as the Finite element Method (FEM) in association with Phase-field theory (PF), to validate the RVE existence and concepts used to define it, discussing its difficulties and applications to quasi-brittle materials such as concrete. The steps of the simulations are addressed in more detail as follows.

Firstly, to establish the structural models that were used in each experiment, five distinct granulometric curves (A, B, C, D, and E; “A” being the thinnest (starting sieve size: 12.5 mm) and “E” the thickest (starting sieve size: 75 mm)) were defined to characterize concrete’s aggregates. Each of those distributions ascribed grains with different diameter lengths to concrete, simulating a sieve analysis with the aggregates that would be used, for example, sand and gravel, which were scattered in each sieve after a normal distribution curve. For each of them, three experiments were conducted, using the particles to concrete ratios of 0.2, 0.3 and 0.4, to evaluate the impact that would be produced in the RVE’s representation. Furthermore, to measure the RVE sensitivity to variance in size, the experiments were replicated for sample sizes of 2.0, 2.5 and 3.0 times the maximum thickness of the grains in question. In addition, one more experiment was done with interface implementation to granulometric sample “b” for comparison purposes, consisting of tests of interface models with thickness of 5% and 10% of the size of the smallest particle in concrete, modelled with diffuse crack length scales l_0 of 0.05 and 0.1 each.

The experiments consisted of measurements on the behavior of stresses and strains manifested by the sample while subjected to an incremental load, under boundary conditions, which in turn were settled to simulate a compressive test for each sample. The results, produced by a FEM mesh combined with PF, were stored into databases, hence transformed by means of a homogenization process. Finally, those databases were used to generate the stress-strain curves for the RVE’s, seeking to verify what differences in mechanical behavior could be observed from the samples, comparing sets of constitutive curves statistically to quantify their deviation, tendencies and other relevant patterns, while looking for convergences that could lead to a proper RVE model suitable to concrete representation.

4 Results

At first, to evaluate the material heterogeneity pattern and the behavior of the RVE, tests consisting of five concrete samples with 0.3 of particle fraction for each of all five granulometric curves and each of the sample sizes were defined. For every specific set of five samples no feature between them were changed, neither in size, nor in constituents, the only perceived difference was in the displacement of particles inside it. The reason behind this, is to simulate the procedure of taking random units of the same material, trying to tell if those units are leading to equivalent mechanical behaviors, therefore applying directly the concept of RVE. Three graphics with the stress-strain curve for each RVE sample were created, each plot representing one distinct granulometric curve, as displayed in Fig. 1. As expected, based on Gitman [2] analysis, the curves were quite close following a similar path with little difference in slope, insofar they are at the linear-elastic regime, but as soon as the curves reach the hardening regime, minor distortions become clear, getting extrapolated at the softening region, as shown in Fig. 1b.

Nevertheless, when more tests for that exact set were executed and plotted along the former curves, a resemblance started to be formed, as their averages tended to converge at some point (take Fig. 2a as an example). For this reason, we did a total of 15 samples for that set, separating them into groups of 5, 6, 7, 8, . . . , and finally, 15 concrete samples, then proceeded to compare the mean curves and medians for each of those groups. Those statistical parameters didn’t seem to improve significantly the approximation for the constitutive model of concrete beyond 5 samples, so this was used in the other experiments as a reference. In turn, Fig. 2 reveals the mean curves for analogous sets of five samples taken from the same concrete, suggesting that in average, there is a degradation

pattern that could be measured for that material, a convergence in behavior for the first half of the softening regime. With this approach from a statistical point of view, the RVE would be defined with a virtual average element that is not actually part of the material but one that every unit cell is a deviation from.

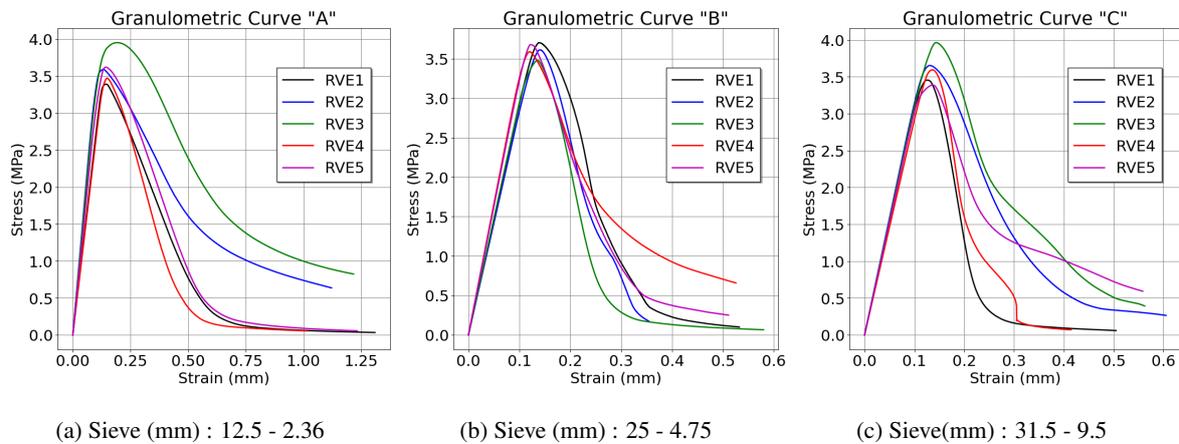


Figure 1. Stress-strain curves for 5 RVE tests in different granulometric constitutions

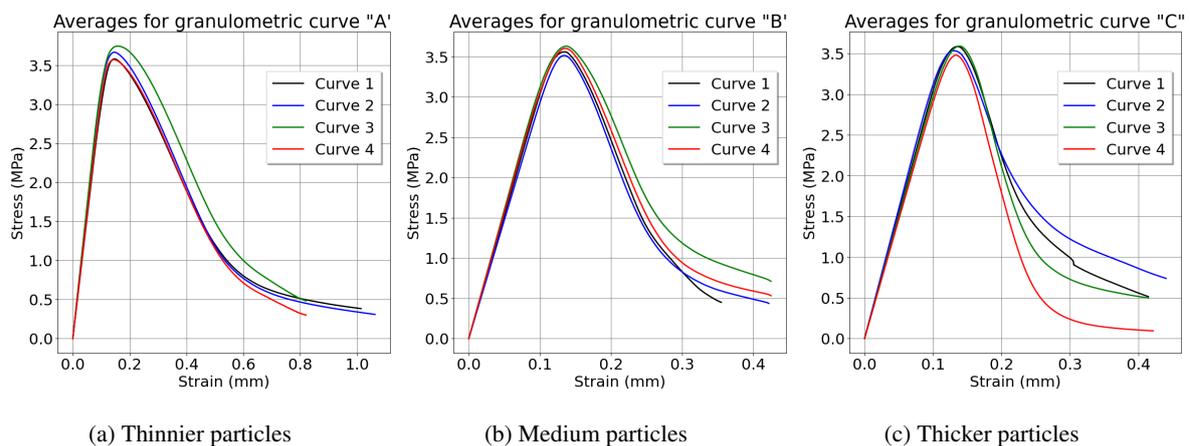
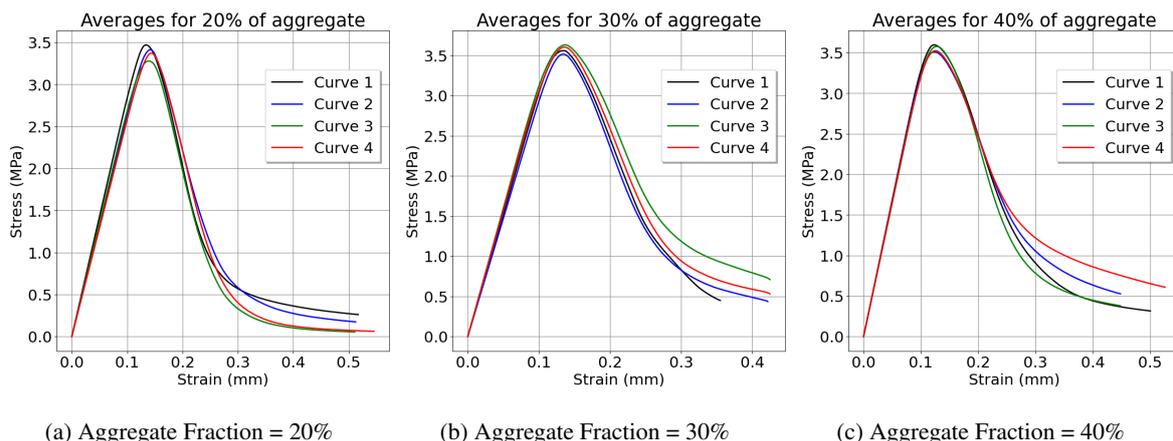


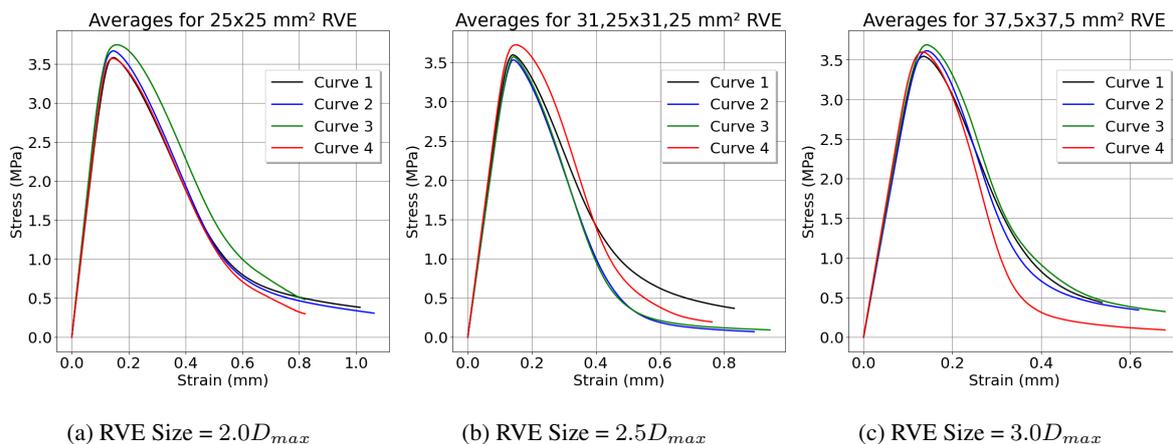
Figure 2. Mean stress-strain curves for sets of 5 samples each

This approach was performed for other concrete samples with particle fractions of 0.2 and 0.4 as well. The results to the granulometric curves “A” and “B”, which had a larger range between intermediary and thinner particles were more uniform overall along the simulations compared to the results obtained to curve “C” with a prevalence of intermediate to thicker grains that presented good approximations until it reached the softening region. Beside that, granulometric curves “D” and “E” did not display a satisfactory outcome, with the unit cell abruptly breaking before the end of the linear elastic-regime, even at higher RVE dimensions as ten times the largest grain of the aggregate. Those two curves had the thickest grains, making it difficult to get a more gradual distribution of microcracks and stress inside the element without a interface to control that. From the increase in the aggregate fractions the peak resistance was also augmented while the total deformations were reduced in the process as can be inferred from Fig. 3, comparing Fig. 3a with Fig. 3b.

From observations concerning the unit cell dimensions, increasing the size of the RVE seemed to reduce distance between constitutive curves until around half of the softening region, after that, softening behavior estimation becomes uncertain, with better results for the larger and smaller samples than for the medium sample. Those results were presented at Fig. 4 representing the stress-strain curves for granulometric curve “A” consisting of concrete with 30% of particles. It suggests that simultaneously with the increase of the sample sizes the material also becomes more fragile and a significant loss of ductility and stability in mechanical behavior for much larger dimensions at the softening region of the curve are expected, presenting less strain, more oscillations like sudden slope changes as the experiment advances. This proclivity to brittleness as the size increases, probably are extrapolated due to the absence of an interfacial zone responsive to microcracks formation, so the softening process doesn’t happen as gradually as it should, leading to abruptly failures.

Figure 3. Effect of aggregate fraction for constitutive curve "B" ($50 \times 50 \text{ mm}^2$ sized RVE)

Finally, the last experiment in this research was focused on the implementation of an interface region around the sample particles of granulometric curve "B" considering 30% of aggregate in the concrete to compare the results with the experiments without this interface (Fig. 3b). Therefore, interface models as described at Section 3 were tested leading to the outcome displayed at Fig. 5. When it comes to ductility, the samples that had an interface were remarkably ductile compared to those which do not, apart from the fact that the former has more than 25% reduction in its peak resistance compared to the latter. The model produced by the 10% sized interface with l_{ϕ} of 0.05 was preferred for this study, especially for the equilibrium in its results compared to the other models.

Figure 4. Effect of different sample sizes in mechanical behavior of the RVE (D_{max} : maximum size of aggregates)

5 Discussion

Results obtained from computational simulations have brought interesting margin for discussion, and expansion of previous studies about the nature of the RVE in quasi-brittle materials. The results demonstrate that concrete properties can be well represented through multiscale modelling, as even without the consideration of an interfacial transition zone separating aggregate particles from the cement matrix, the mechanical behavior of concrete and its implications remained virtually the same along the linear-elastic path and for most of the hardening path, throughout the various samples analyzed, as corroborated by other studies on the matter. Those conclusions were reached similarly by Gitman [2] in her study of quasi-brittle materials, although she used a variety of very small grains compared to those used in concrete production, those that the present research tried to regard. Gitman [2] concluded that an RVE could not exist for a sample that had initiated the softening process, as observed in Fig. 1, in which the constitutive curves for each sample acted in relatively uncertain ways, however through the approach of comparing the average stress-strain curves for different sets of concrete samples (Fig. 2), a certain convergence for softening behavior was demonstrated, hinting at the possibility for the existence of a concrete RVE. As the mechanical response of a material subjected to softening is defined by degradation through microcracks, further

studies in phase-field theory could improve this representation to the point, where those differences in behavior are minimal, and then an RVE would be properly defined.

The implementation of an interface in the simulations led to substantial effects on the mechanical behavior of concrete, turning it in a much more ductile material, increasing its deformations by a large margin, while reducing significantly its peak resistance. In contrast, the samples without one demonstrated a tendency to brittleness with the increase of sample size. Moreover, for larger grains the constitutive model cannot even represent the degradation of concrete at the softening regime properly, because of the inherently fragility of the model, insensitive to microcracks formation. This result demonstrates the importance of the interface to make realistic predictions about concrete structural behavior in practical situations.

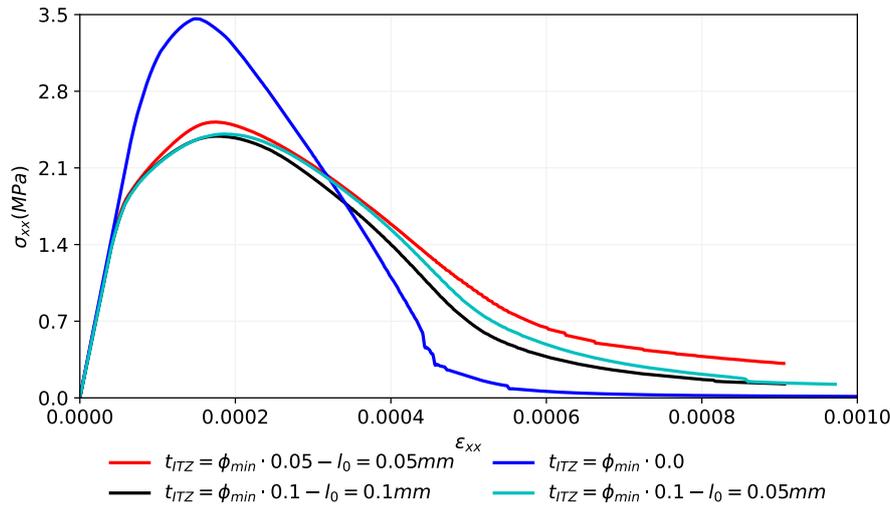


Figure 5. Effect of an interface in the mechanical behavior of the RVE

6 Conclusion

To define an RVE to a quasi-brittle material like concrete can be quite challenging, especially because of its natural heterogeneous internal structure, that lacks particle periodicity along its volume; and its complex degradation mechanism derived from particle interactions. From the simulations performed, in one hand, it was observed that the existence of the RVE for concrete at softening regime is promising, as demonstrated by the granulometric curves “A”, “B” and “C”, while for more granular concretes the softening impact could not be represented satisfactorily in an RVE, possibly due to the lack of an interface model. In the other hand, with the increase of RVE sizes, the similarities along constitutive curves reach an optimal result, which tends to be overturned for much larger dimensions. For further studies, shear test results could bring a light to the discussion on the matter of a Representative Volume Element for concrete, complementing the conclusions presented by this research. According to the findings discussed previously, the impact of the interface in the simulations are substantial, enhancing its ductility, especially in the softening regime, while the peak resistance is decreased, however additional experiments with more samples and other granulometric curves should be made, by the virtue of a better overall analysis of behavior of the interfacial RVE, including those for curves “D” and “E” that couldn’t be represented in this study. Ultimately, Phase-field concepts are promising and further developments in this direction can be fundamental for more effective constitutive models in material engineering and structural analysis in the future.

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References

- [1] J.P.Schaffer. *The Science and Design of Engineering Materials*. McGraw-Hill, Chicago, 2001.
- [2] I. M. Gitman. *Representative Volumes and Multi-scale Modelling of Quasi-brittle Materials*. Inna M. Gitman, 2006.
- [3] Z. P. Bazant and D. Novak. Stochastic models for deformation and failure of quasibrittle structures: recent advances and new directions. *Computational modelling of concrete structures*, pp. 583–598, 2003.
- [4] I. Gitman, H. Askes, and L. Sluys. Representative volume: Existence and size determination. *Engineering fracture mechanics*, vol. 74, n. 16, pp. 2518–2534, 2007.
- [5] C. Pélissou, J. Baccou, Y. Monerie, and F. Perales. Determination of the size of the representative volume element for random quasi-brittle composites. *International Journal of Solids and Structures*, vol. 46, n. 14-15, pp. 2842–2855, 2009.
- [6] H. Tran and H. Chew. Cohesive zone interpretations of phase-field fracture models. *Journal of Applied Mechanics*, vol. 89, n. 12, pp. 121005, 2022.
- [7] B. Bourdin, G. A. Francfort, and J.-J. Marigo. Numerical experiments in revisited brittle fracture. *Journal of the Mechanics and Physics of Solids*, vol. 48, n. 4, pp. 797–826, 2000.
- [8] B. Bourdin and A. Chambolle. Implementation of an adaptive finite-element approximation of the mumford-shah functional. *Numerische Mathematik*, vol. 85, pp. 609–646, 2000.
- [9] C. Kuhn, A. Schlüter, and R. Müller. On degradation functions in phase field fracture models. *Computational Materials Science*, vol. 108, pp. 374–384, 2015.
- [10] A. Karma, D. A. Kessler, and H. Levine. Phase-field model of mode iii dynamic fracture. *Physical Review Letters*, vol. 87, n. 4, pp. 045501, 2001.
- [11] M. J. Borden, T. J. Hughes, C. M. Landis, and C. V. Verhoosel. A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework. *Computer Methods in Applied Mechanics and Engineering*, vol. 273, pp. 100–118, 2014.
- [12] J. M. Sargado, E. Keilegavlen, I. Berre, and J. M. Nordbotten. High-accuracy phase-field models for brittle fracture based on a new family of degradation functions. *Journal of the Mechanics and Physics of Solids*, vol. 111, pp. 458–489, 2018.
- [13] A. Khodadadian, N. Noii, M. Parvizi, M. Abbaszadeh, T. Wick, and C. Heitzinger. A bayesian estimation method for variational phase-field fracture problems. *Computational Mechanics*, vol. 66, pp. 827–849, 2020.
- [14] T. T. Nguyen, J. Yvonnet, M. Bornert, C. Chateau, K. Sab, R. Romani, and R. Le Roy. On the choice of parameters in the phase field method for simulating crack initiation with experimental validation. *International Journal of Fracture*, vol. 197, pp. 213–226, 2016.
- [15] E. Tanné, T. Li, B. Bourdin, J.-J. Marigo, and C. Maurini. Crack nucleation in variational phase-field models of brittle fracture. *Journal of the Mechanics and Physics of Solids*, vol. 110, pp. 80–99, 2018.
- [16] H. M. Leao. A critical study on phase-field modelling of fracture. *Federal University of Minas Gerais (UFMG)*, vol. , 2021.