

**Article info****Type of article:**

Original research paper

DOI:
<https://doi.org/10.58845/jstt.utt.2026.en.6.4.265-284>
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Email address:

viettb@utc.edu.vn**Received:** 25/12/2025**Received in Revised Form:** 17/03/2026**Accepted:** 24/06/2026

Investigation on damage behavior of concrete based on complex simulations

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Abstract: Concrete is a widely used composite construction material owing to its high compressive strength and long-term durability in engineering applications. This paper presents an investigation into the damage behavior and compressive strength of concrete through numerical simulation approaches, taking into account key micromechanical characteristics of the material. The numerical model is developed with explicit consideration of aggregate shape and distribution, mechanical properties of the cementitious matrix, and the characteristics of the interfacial transition zone between aggregates and mortar. Numerical simulation results are systematically compared with experimental data to assess the accuracy and reliability of the proposed modeling framework. The good agreement between numerical predictions and experimental measurements demonstrates the capability of the model to realistically capture the compressive behavior of concrete. The results provide insight into damage initiation, propagation mechanisms, and stress redistribution under compressive loading. Furthermore, the study elucidates the relationship between microstructural features and macroscopic mechanical responses of concrete. The proposed numerical model demonstrates strong potential for application in structural analysis, design optimization, and performance assessment. Overall, this research contributes to the development of high-performance and sustainable concrete materials for advanced engineering practice.

Keywords: Concrete, compressive strength, damage behavior, numerical simulations.

1. Introduction

Concrete is one of the most widely used construction materials in civil engineering owing to its high compressive strength, durability, and economic efficiency. Nevertheless, its mechanical performance is strongly influenced by its

heterogeneous internal structure, including aggregate morphology, water–cement ratio, and, most critically, the interfacial transition zone (ITZ) between aggregates and cement paste [1, 2]. Numerous experimental investigations have demonstrated that the ITZ exhibits weaker

mechanical properties compared to the bulk cement matrix, leading to stress concentration, early microcracking, and a significant influence on the macroscopic strength and failure modes of concrete [3–7]. While experimental approaches provide valuable insights into these mechanisms, they are often time-consuming, costly, and impractical for extensive parametric studies involving complex microstructural variations.

To overcome these limitations, numerical modeling has become an indispensable tool for investigating the mechanical behavior and fracture processes of concrete. In particular, mesoscale modeling approaches, in which concrete is explicitly represented as a three-phase composite consisting of aggregates, ITZ, and cement paste, have proven effective in capturing damage initiation and crack propagation under compressive loading [5, 8, 9]. In parallel Concurrently, data-driven and artificial intelligence-based methods have recently gained increasing attention due to their efficiency and predictive accuracy in estimating compressive strength and failure characteristics [10, 11]. Despite these advances, physics-based numerical methods remain essential for elucidating the fundamental mechanisms governing fracture and failure in heterogeneous quasi-brittle materials [12].

Among existing numerical techniques, the phase-field method has emerged as a powerful and versatile framework for fracture modeling. By regularizing sharp cracks through a continuous damage-like variable, the phase-field approach enables the simulation of complex crack nucleation, propagation, branching, and merging without the need for predefined crack paths or remeshing procedures [13, 14]. The classical formulation introduced by Miehe et al. [15] has been widely adopted and successfully applied to tensile-dominated fracture problems. However, concrete subjected to compressive loading exhibits a combination of tensile cracking around aggregates, shear localization, and crushing-induced damage, which cannot be adequately

captured by purely tensile-based phase-field formulations.

Consequently, extending phase-field models to account for compression- and shear-related failure mechanisms has become an active and critical research topic [16]. Several enhanced formulations have been proposed to address this challenge. Zhou et al. [17] incorporated frictional effects into a poroelastic phase-field framework to model shear-compression behavior, while Jia et al. [18] developed a compressive–shear damage criterion based on a modified Hoek–Brown failure envelope. More recently, Wang et al. [19] proposed a unified phase-field formulation capable of capturing tensile–shear as well as compressive–shear failure modes. These studies reflect a growing effort to bridge the gap between classical phase-field fracture models and the realistic failure behavior of concrete under complex stress states. This trend is further supported by recent review articles emphasizing the necessity of robust, multi-mechanism formulations for heterogeneous materials [20–22].

In addition to single-field extensions, alternative modeling strategies have also been explored. Lenarda et al. [23] proposed a dual phase-field formulation employing separate scalar fields to distinguish between tensile- and compression-driven damage mechanisms. Furthermore, cohesive-zone-enhanced phase-field approaches have been developed to improve the description of fracture process zones and nonlinear softening behavior in quasi-brittle materials, thereby combining the advantages of phase-field regularization and cohesive fracture mechanics [24, 25]. These developments indicate a clear shift toward hybrid modeling frameworks capable of capturing multiple interacting failure mechanisms.

Recent comparative studies have further highlighted the importance of carefully selecting phase-field formulations when modeling concrete fracture. In particular, Nguyen et al. [26] demonstrated that the choice of spectral

decomposition and crack density function has a decisive impact on the predicted fracture response of concrete, especially when heterogeneity and size effects are taken into account. Beyond purely physics-based approaches, hybrid strategies combining phase-field modeling with machine learning techniques have also been proposed to significantly reduce computational cost while maintaining predictive accuracy, especially for complex composite configurations [27]. At the same time, advances in micromechanical and homogenization-based modeling have underscored the crucial role of microstructural morphology, interfacial effects, and packing characteristics in governing the effective mechanical behavior of heterogeneous materials such as concrete.

Motivated by these developments, the present study aims to develop a numerical framework based on a coupled tensile–compressive phase-field formulation tailored for mesoscale modeling of concrete. By explicitly accounting for material heterogeneity through the aggregate–ITZ–matrix representation, the proposed model seeks to accurately reproduce key features of concrete behavior under compressive loading, including damage localization, crack interaction, and failure patterns. The predictive capability of the model is assessed through comparison with available experimental results, providing insights into the mechanisms governing compressive fracture and offering a reliable tool for optimizing concrete material design and structural performance.

2. Fundamental

The stress-strain response of concrete is governed by the initiation and propagation of microcracks at the mesoscale level. Peak strength is attained when microcracks develop in the vicinity of aggregates, after which their coalescence leads to the formation of larger cracks, marking the onset of the softening phase in the stress-strain curve. In this study, the compressive strength of concrete is predicted through numerical simulations using the

phase-field method, a widely recognized approach in fracture mechanics modeling, and validated against experimental results. Within this framework, a scalar field variable ranging from 0 to 1 is employed to characterize the transition between the intact and fully fractured states of the material. In highly heterogeneous materials such as concrete, two primary fracture modes are observed: tensile fracture and compressive crushing. These fracture mechanisms are described using two distinct phase-field variables: d_1 represents the tensile damage, while d_2 accounts for compressive damage.

The total energy of the cracked body in accordance with Griffith's theory of brittle fracture can be defined by:

$$E = \int_{\Omega/\Gamma} \psi^e(\varepsilon) d\Omega + \int_{\Gamma_t} g_1 dS + \int_{\Gamma_c} g_2 dS \quad (1)$$

, where ψ^e is the elastic energy density, $\varepsilon = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ and g_1, g_2 are, respectively, the tensile fracture energy and compressive fracture energy.

Within the regularized framework, with the introduction of the crack density function $\gamma_{d_1}(d_1, \nabla d_1)$, $\gamma_{d_2}(d_2, \nabla d_2)$ for tensile damage and compressive damage, respectively, the fracture energy can be approximated as follows:

$$\int_{\Gamma_t} g_1 dS = \int_{\Omega} g_1 \gamma_{d_1}(d_1, \nabla d_1) d\Omega \quad (2)$$

$$\int_{\Gamma_c} g_2 dS = \int_{\Omega} g_2 \gamma_{d_2}(d_2, \nabla d_2) d\Omega \quad (3)$$

where the crack density function can be expressed as:

$$\gamma_{d_1}(d_1, \nabla d_1) = \frac{1}{2l_1} d_1^2 + \frac{l_1}{2} \nabla d_1 \cdot \nabla d_1 \quad (4)$$

$$\gamma_{d_2}(d_2, \nabla d_2) = \frac{1}{2l_2} d_2^2 + \frac{l_2}{2} \nabla d_2 \cdot \nabla d_2 \quad (5)$$

where l_1, l_2 is a model parameter that controls the width of the smooth approximation of the crack.

The phase-field length-scale parameters l_1 and l_2 control the width of the diffusive damage zone and the degree of strain localization in the

regularized formulation. In the present dual-field model, l_1 is associated with tensile cracking, whereas l_2 governs compressive crushing.

Physically, these parameters can be interpreted as effective internal material length scales representing the characteristic size of the fracture process zone (FPZ) at the mesoscale. They are not direct geometric measures of aggregate diameter or the physical thickness of the ITZ, but rather homogenized quantities emerging from microstructural interactions.

In the adopted mesoscale model, the length scales satisfy $l_i \ll D_{\max}$, where $D_{\max}$ is the maximum aggregate size. This ensures that damage localization remains governed by material heterogeneity and is not artificially smeared across aggregates. Moreover, the selected values are smaller than or comparable to the idealized ITZ thickness used in the model, allowing realistic damage concentration in the weaker interfacial region.

Therefore, l_1 and l_2 should be understood as effective fracture-process-zone parameters that ensure mesh objectivity and physically meaningful localization, rather than direct geometric descriptors of concrete microstructure.

In order to account for the loss of material strength, the phase field d_1, d_2 is incorporated into the elastic energy density using the following expression:

$$\psi(\varepsilon, d_1, d_2) = g(d_1)\psi^+(\varepsilon) + g(d_2)\psi^-(\varepsilon) \quad (6)$$

The elastic energy is decomposed into tensile and compressive parts, $\psi = \psi^+ + \psi^-$. The tensile phase-field d_1 degrades only ψ^+ , whereas the compressive phase-field d_2 degrades only ψ^- . This split ensures a unilateral effect: tensile cracks do not artificially reduce the compressive stiffness upon crack closure, unless compression crushing develops through d_2 .

The degradation function is expressed as:

$$g(d_1) = (1 - d_1)^2 + \xi \quad (7)$$

$$g(d_2) = (1 - d_2)^2 + \xi \quad (8)$$

ξ is a very small number used to avoid loss of stability at the fully broken state.

As a consequence, the total energy in Equation (1) in the regularized framework reads as:

$$\int_{\Omega} \left[((1 - d_1)^2 + \xi)\psi^+(\varepsilon) + ((1 - d_2)^2 + \xi)\psi^-(\varepsilon) + g_1 \left(\frac{d_1^2}{2l_1} + \frac{l_1}{2} |\nabla d_1|^2 \right) + g_2 \left(\frac{d_2^2}{2l_2} + \frac{l_2}{2} |\nabla d_2|^2 \right) \right] d\Omega \quad (9)$$

Applying the principle of maximum dissipation and energy minimization, the strong form of the phase field and the displacement problems can be written respectively as:

For tensile damage:

$$\begin{cases} 2P_1(1 - d_1)H_1 - \frac{g_c}{l_1}(d_1 - l_1^2 \Delta d_1) = 0 & \text{in } \Omega \\ d_1(x) = 1 & \text{on } \Gamma_f \\ \nabla d_1(x) \cdot n = 0 & \text{on } \partial\Omega \end{cases} \quad (10)$$

For compression crushing:

$$\begin{cases} 2P_2(1 - d_2)H_2 - \frac{g_c}{l_2}(d_2 - l_2^2 \Delta d_2) = 0 & \text{in } \Omega \\ d_2(x) = 1 & \text{on } \Gamma_c \\ \nabla d_2(x) \cdot n = 0 & \text{on } \partial\Omega \end{cases} \quad (11)$$

$$P_1 = \begin{cases} 1, & \text{when } \frac{\text{Tr}(\sigma)}{\sigma_{\text{ref}}} > 1 \\ 0, & \text{otherwise} \end{cases} \quad (12)$$

$$P_2 = 1 - P_1 \quad (13)$$

where σ_{ref} denotes the reference stress.

In this study: For tensile damage activation, $\sigma_{\text{ref}} = f_t$, where f_t is the tensile strength of the corresponding material phase. For compression crushing activation, $\sigma_{\text{ref}} = f_c$, where f_c represents the compressive strength of the material phase.

The history strain energy density function is introduced to describe a dependence on history and possible loading-unloading:

$$H_1(x, t) = \max_{\tau \in [0, t]} \left\{ \left((1 - d_1)^2 + \xi \right) \psi^+(x, \tau) \right\} \quad (14)$$

$$H_2(x, t) = \max_{\tau \in [0, t]} \left\{ \left((1 - d_2)^2 + \xi \right) \psi^-(x, \tau) \right\} \quad (15)$$

The displacement field:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, d_1, d_2) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u}(x) = \mathbf{u} & \text{on } \partial\Omega_u \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{F}} & \text{on } \partial\Omega_F \end{cases} \quad (16)$$

The Cauchy stress:

$$\begin{aligned} \boldsymbol{\sigma} = & \left((1 - d_1)^2 + \xi \right) \left\{ \lambda \langle \text{tr } \boldsymbol{\varepsilon} \rangle_+ \mathbf{1} + 2\mu \boldsymbol{\varepsilon}^+ \right\} \\ & + \left((1 - d_2)^2 + \xi \right) \left\{ \lambda \langle \text{tr } \boldsymbol{\varepsilon} \rangle_- \mathbf{1} + 2\mu \boldsymbol{\varepsilon}^- \right\} \end{aligned} \quad (17)$$

The matrix form:

$$\mathbf{K}_{d_1} = \int_{\Omega} \left\{ \left(\frac{g_c}{l_1} + 2P_1 H_1 \right) \mathbf{N}_{d_1}^T \mathbf{N}_{d_1} + g_1 l_1 \mathbf{B}_{d_1}^T \mathbf{B}_{d_1} \right\} d\Omega \quad (18)$$

$$\mathbf{F}_{d_1} = \int_{\Omega} 2P_1 \mathbf{N}_{d_1}^T d\Omega \quad (19)$$

$$\mathbf{K}_{d_2} = \int_{\Omega} \left\{ \left(\frac{g_c}{l_2} + 2P_2 H_2 \right) \mathbf{N}_{d_2}^T \mathbf{N}_{d_2} + g_2 l_2 \mathbf{B}_{d_2}^T \mathbf{B}_{d_2} \right\} d\Omega \quad (20)$$

$$\mathbf{F}_{d_2} = \int_{\Omega} 2P_2 \mathbf{N}_{d_2}^T d\Omega \quad (21)$$

$$\begin{aligned} & \mathbf{K}_1(d_{n+1}) \\ & = \int_{\Omega} \mathbf{B}^T \left\{ \left((1 - d_1)^2 + k \right) \left(\lambda \mathbf{R}_n^+ \mathbf{1}^T \mathbf{1} + 2\mu \mathbf{P}_n^+ \right) \right\} \mathbf{B} d\Omega \end{aligned} \quad (22)$$

$$\begin{aligned} & \mathbf{K}_2(d_{n+1}) \\ & = \int_{\Omega} \mathbf{B}^T \left\{ \left((1 - d_2)^2 + k \right) \left(\lambda \mathbf{R}_n^- \mathbf{1}^T \mathbf{1} + 2\mu \mathbf{P}_n^- \right) \right\} \mathbf{B} d\Omega \end{aligned} \quad (23)$$

$$\mathbf{F}_{n+1} = \int_{\Omega} \mathbf{N}^T \mathbf{f} d\Omega + \int_{\partial\Omega_F} \mathbf{N}^T \bar{\mathbf{F}}_{n+1} d\Gamma \quad (24)$$

3. Numerical validation

In this section, the reliability and predictive capability of the proposed numerical model presented in Section 2 (Equations (18)–(24)) are evaluated through compressive simulations of concrete specimens and comparison with experimental results. To achieve a balance between computational efficiency and accuracy, a two-dimensional (2D) concrete specimen with dimensions of 50 x 50 mm is constructed, in which concrete is idealized as a three-phase composite consisting of aggregates, the ITZ, and the cement mortar matrix. The boundary conditions are defined such that the bottom boundary is fully fixed, while

a compressive load is applied to the top boundary under displacement control with a loading rate of $\bar{u} = -0.001$ mm/s.

First, the influence of aggregate morphology on the compressive behavior of concrete is investigated by considering two representative aggregate shapes: circular and elliptical. Subsequently, the numerical model is employed to analyze three different cases corresponding to variations in the mechanical properties of the cement mortar matrix, allowing for an assessment of the model sensitivity to material parameters. Concurrently, experimental compression tests were conducted on standard cubic concrete specimens with dimensions of 150 x 150 x 150 mm, prepared with three different water-to-cement ratios (W/C), to provide experimental data for model validation.

Finally, a comprehensive comparative analysis between the numerical predictions and the experimental results is carried out, focusing on the stress–strain responses, peak compressive strength, and failure patterns of concrete. The main findings and detailed discussions are presented in the subsequent sections.

3.1. Numerical compression model

3.1.1. Numerical compression model with circular aggregates

In the mesoscale numerical model for the case of circular aggregates, the concrete specimen is idealized as a three-phase composite consisting of coarse aggregates, the interfacial transition zone (ITZ), and the cement paste matrix, with corresponding volume fractions of 40%, 10%, and 50%, respectively. The aggregate phase is represented by randomly generated circular particles, which provide a simplified yet commonly adopted geometric idealization in mesoscale studies and serve as a baseline configuration for comparative analysis.

The aggregate particle sizes follow a prescribed gradation curve, with a maximum diameter of $D_{\max} = 12$ mm and a minimum diameter

of $D_{\min} = 4 \text{ mm}$, ensuring a representative size distribution for conventional concrete. A random sequential adsorption (RSA) algorithm is employed to generate a non-overlapping aggregate distribution, thereby preventing artificial clustering and maintaining statistical uniformity of the mesoscale structure within the computational domain [5, 8].

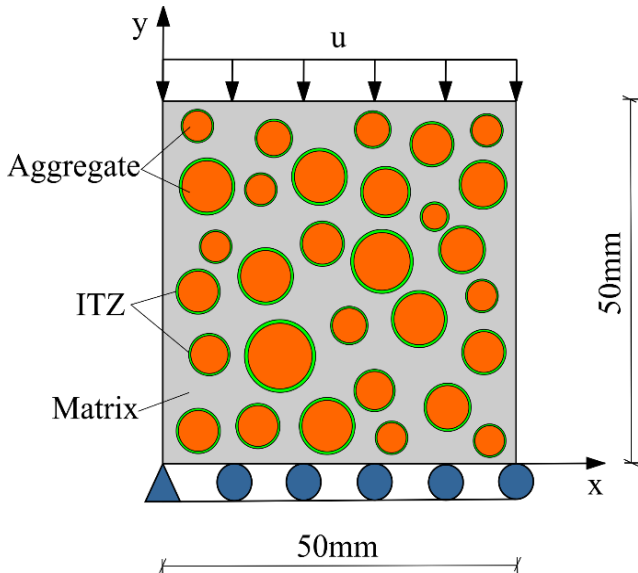


Fig. 1. Circular aggregate particles and boundary conditions

A two-dimensional (2D) square specimen with dimensions of 50 x 50 mm was constructed, as shown previously in Fig. 1. The bottom boundary is fully restrained, while a compressive load is applied to the top boundary under displacement control with a constant loading rate of $\dot{u} = -0.001 \text{ mm/s}$. This boundary condition setup enables stable evaluation of the post-peak response, which is essential for analyzing strain-softening behavior and damage evolution under compressive loading.

The finite element mesh consists of approximately 80,000 triangular elements, with significant refinement along aggregate boundaries and within ITZ regions to accurately resolve steep strain gradients (Fig. 2). The characteristic length scale of the phase-field model is set to $l_0 = 0.25 \text{ mm}$, and the element size in critical regions satisfies the requirement $h < l_0 / 2$ to ensure proper

resolution of the diffusive crack zone. A staggered solution scheme is adopted to avoid spurious localization, in which the displacement and phase-field variables are solved sequentially at each load increment using a Newton–Raphson iterative procedure with a convergence tolerance of 1.0×10^{-8} .

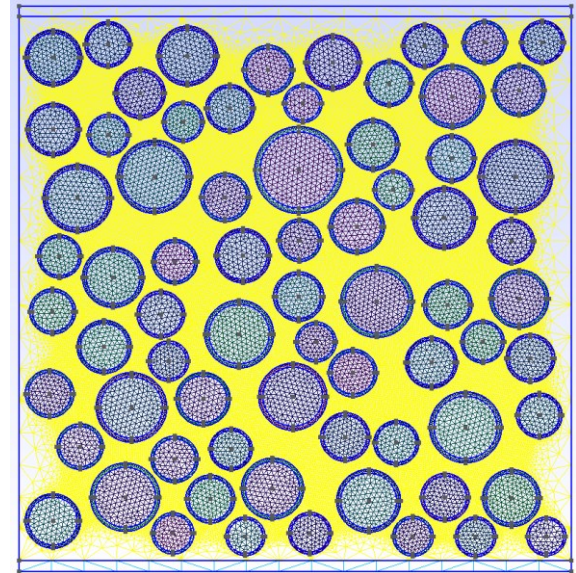


Fig. 2. Triangular finite element mesh, incorporating circular aggregate particles

To realistically reproduce concrete behavior, the aggregate phase is assumed to remain undamaged during loading due to its significantly higher stiffness and strength compared to the surrounding matrix. Its tensile fracture energy is set to 10 times that of the cement paste matrix, consistent with mesoscale studies reported in [5, 8]. For the cement paste and ITZ phases, three different material parameter sets were assigned to simulate the influence of varying mix proportions. These variations correspond to the experimental mixtures with water–cement ratios of 0.50, 0.45, and 0.40. The elastic modulus of the cement paste is adjusted accordingly, and the ITZ modulus is taken as 50% of the corresponding cement paste stiffness, as shown previously in Table 1.

In addition to elastic modulus variation, tensile and compressive fracture energies (g_1, g_2) were calibrated to ensure consistency with the experimentally observed peak strengths. The ratio

$g_2 / g_1 = 200$ was chosen based on previous phase-field studies indicating that compressive fracture processes typically require significantly higher energy than tensile fracture processes [17–20]. A parametric sensitivity study was performed to assess the impact of varying ITZ modulus and fracture energy parameters on the peak stress, crack distribution, and softening behavior. The results demonstrate that reductions in ITZ stiffness lead to earlier crack initiation and increased damage localization, while higher tensile fracture

energy results in smoother post-peak softening curves.

Fig. 3 illustrates the simulated crack patterns at successive displacement levels of $u = -(0.095-0.130)$ mm, showing gradual microcrack development followed by coalescence into a dominant shear band. As expected, the initiation of damage predominantly occurs around the ITZ before propagating into the matrix region, consistent with known mesoscale fracture characteristics of concrete.

Table 1. Main material parameters and phase-field numerical model parameters

	Elastic modulus (GPa)	Poisson	Compressive strength (MPa)	Tensile strength (MPa)	Tensile fracture energy (g_1)	Compressive fracture energy (g_2)	g_2 / g_1
Aggregate	60	0.23	-	-	1.4E-5	2.8E-3	200
Matrix1	32	0.20	45	3.354	1.2E-6	2.4E-4	200
Matrix2	36		55	3.708	1.4E-6	2.8E-4	
Matrix3	40		65	4.025	1.6E-6	3.2E-4	
ITZ1	16	0.20	22.5	1.677	6E-7	1.2E-4	200
ITZ2	18		27.5	1.854	7E-7	1.4E-4	
ITZ3	20		32.5	2.013	8E-7	1.6E-4	

Note: A single type of aggregate was used across all experimental and numerical cases. To maintain model consistency, the aggregate's fracture energy parameters (g_1) and (g_2) are set to 10 times those of the reference cement paste matrix (Matrix2). Since the aggregate is assumed to be undamaged, these parameters do not affect the damage evolution but are provided for completeness.

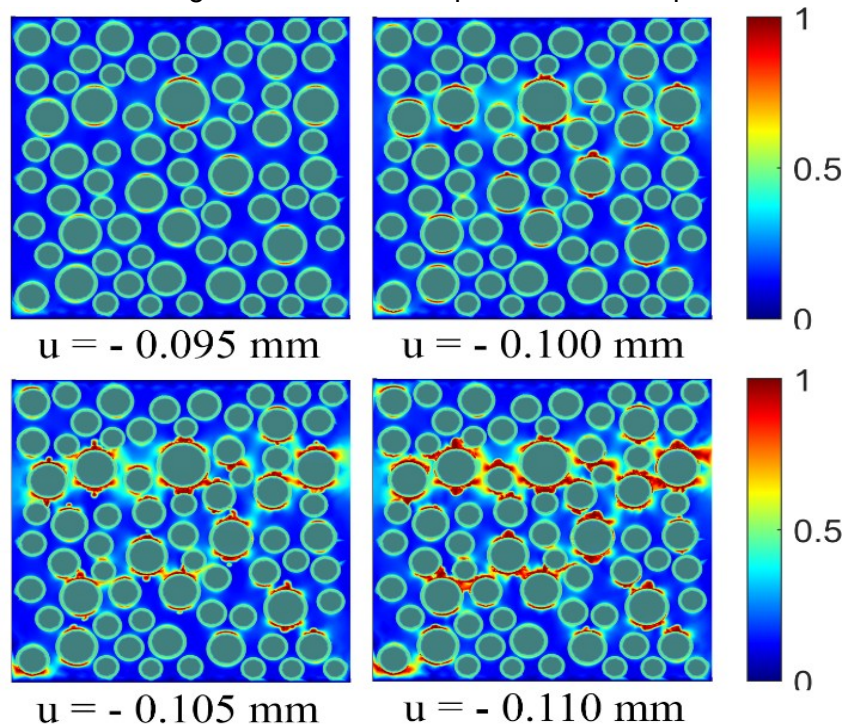


Fig. 3. Crack pattern with circular aggregate

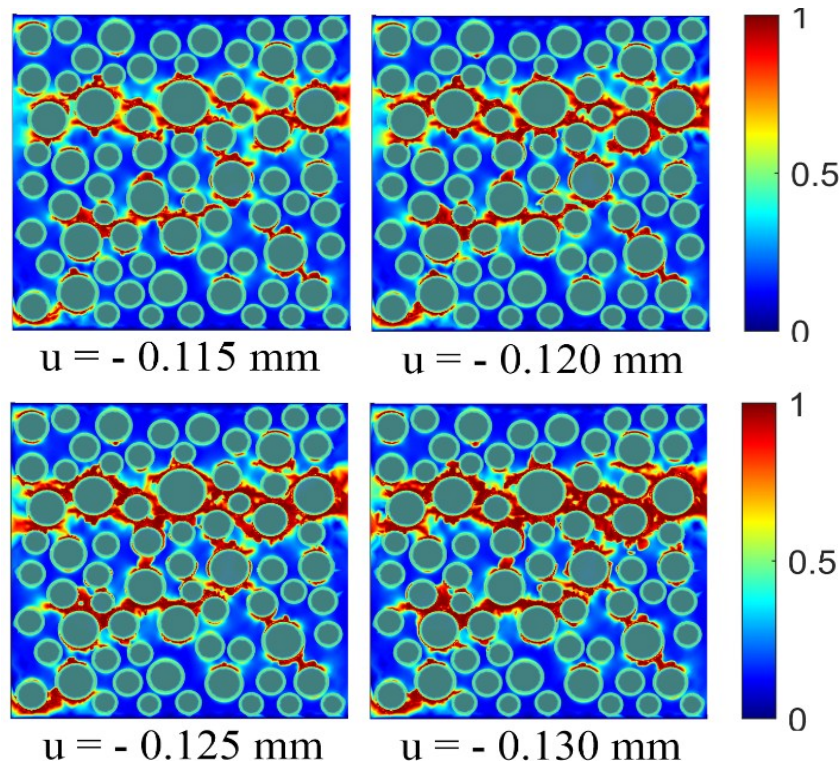


Fig. 3. (continued)

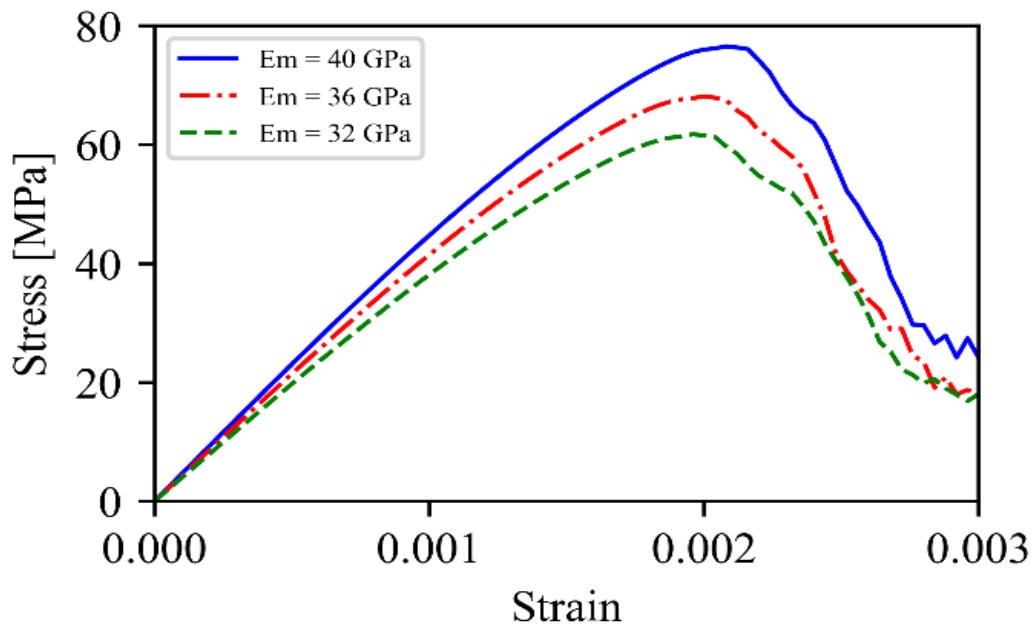


Fig. 4. Stress – strain curve with circular aggregate

Fig. 4 presents the simulated stress–strain responses for the three models. The predicted peak stresses and post-peak softening behavior successfully replicate the trends observed in laboratory tests, confirming the model's capability in capturing both tensile-induced microcracking and compressive crushing mechanisms. The peak stress values for the three cases are 62.24 MPa,

68.61 MPa, and 77.06 MPa, respectively.

3.1.2. Sensitivity analysis of the fracture energy ratio g_2 / g_1

In order to justify the selection of the fracture energy ratio $g_2 / g_1 = 200$ and to assess its robustness, a parametric sensitivity analysis was conducted. While previous phase-field studies

have reported that compressive crushing requires significantly higher energy dissipation than tensile fracture [17–20], the quantitative influence of this ratio on the predicted compressive response of concrete must be clarified. Simulations were performed for several representative values of the ratio g_2/g_1 , namely 50, 100, 200, and 300, while keeping all other material and numerical parameters unchanged. Fig. 5 illustrates the influence of the fracture energy ratio g_2/g_1 on the simulated compressive stress–strain responses of concrete, highlighting its effect on peak compressive strength and post-peak softening behavior. The corresponding peak compressive strengths obtained from the simulations are 51.76 MPa, 60.18 MPa, 68.61 MPa, and 72.73 MPa, respectively. The results indicate that when the ratio is relatively low (e.g., $g_2/g_1 = 50$), premature compressive crushing occurs, leading to an underestimation of the peak compressive strength (51.76 MPa) and a more diffused damage distribution. Increasing the ratio to $g_2/g_1 = 100$ improves the predicted peak stress (60.18 MPa); however, noticeable over-localization of compressive damage is still observed. For $g_2/g_1 = 200$, the simulated peak strength reaches 68.61 MPa, showing the best agreement with experimental results (deviation < 2%), and the predicted failure mode is characterized by a realistic inclined shear band consistent with experimental observations. Further increasing the ratio to $g_2/g_1 = 300$ results in a slightly higher peak stress (72.73 MPa) with only minor changes in the overall stress–strain response, indicating that the model response becomes relatively insensitive beyond a threshold value.

These findings demonstrate that the ratio g_2/g_1 is not an arbitrary parameter but a physically motivated quantity controlling the balance between tensile microcracking and compressive crushing mechanisms. Although the exact value is not

mathematically unique, a stable and physically consistent response is obtained within a reasonable range (approximately 150–250). The selected value $g_2/g_1 = 200$ therefore represents a robust calibration that ensures realistic strength prediction, appropriate damage localization, and consistency with experimental evidence.

3.1.3. Numerical compression model with elliptical aggregates

For the case of elliptical aggregates, the mesoscale numerical model is constructed following the same three-phase framework, boundary conditions, loading protocol, and numerical settings adopted in the circular-aggregate configuration to ensure direct comparability. The only modification concerns the geometric representation of the aggregate phase.

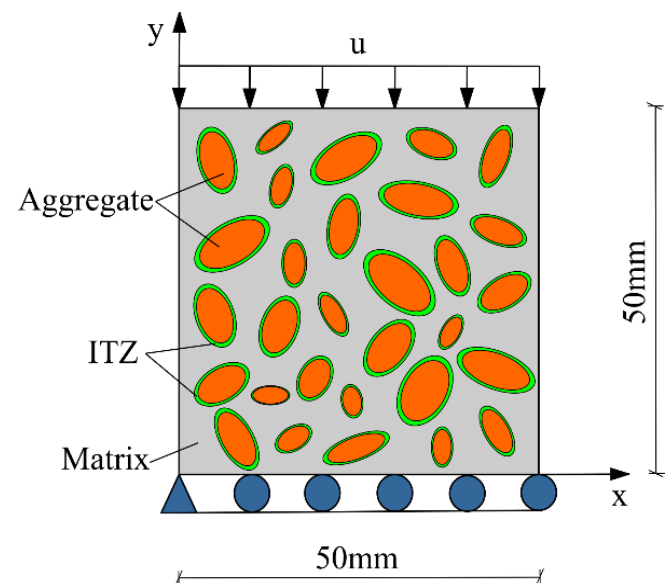


Fig. 6. Elliptical aggregate particles and boundary conditions

Aggregates are modeled as randomly generated elliptical particles with a fixed minor-to-major axis ratio of 0.5, reflecting the inherent geometric anisotropy of natural coarse aggregates (Fig. 6). The particle size distribution follows the same prescribed gradation curve, and a random sequential adsorption (RSA) algorithm is employed to ensure a non-overlapping and statistically uniform aggregate distribution within the computational domain.

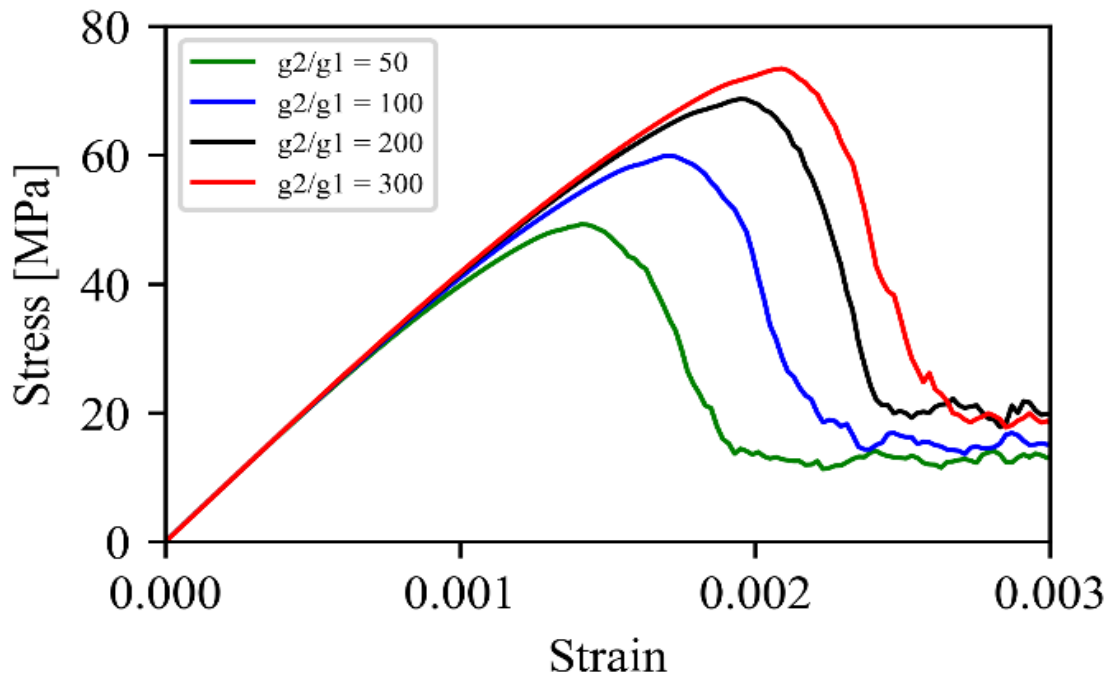


Fig. 5. Compares the simulated stress–strain responses for various values of g_2 / g_1

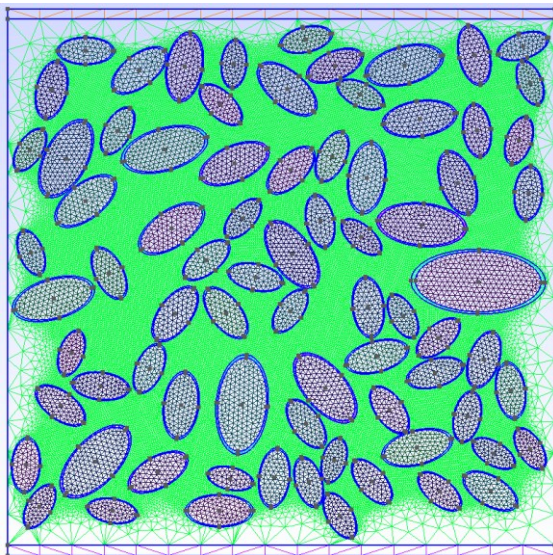


Fig. 7. Triangular finite element mesh incorporating elliptical aggregate particles

Similarly, for the elliptical-aggregate configuration, a triangular finite element mesh is employed with a total number of elements comparable to that of the circular-aggregate model (Fig. 7). The mesh is locally refined along aggregate boundaries and within the ITZ regions to adequately capture stress concentration and strain localization induced by aggregate shape anisotropy. The same mesh density criteria relative to the phase-field length scale are maintained to ensure consistent resolution of the diffusive crack

zone and numerical accuracy across both configurations.

All material parameters, including elastic properties, fracture energies, and phase-field length scale, are retained unchanged from the circular-aggregate model. In particular, aggregates are assumed to remain undamaged, with tensile fracture energy set to 10 times that of the cement paste, while the ITZ stiffness is taken as 50% of the corresponding matrix modulus. The same calibration strategy for tensile and compressive fracture energies (g_1, g_2) is applied.

Fig. 8 depicts the evolution of damage patterns for the elliptical-aggregate model at successive displacement levels of $u = -(0.105-0.140)$ mm. Compared to the circular-aggregate case, the presence of geometrically anisotropic aggregates leads to a more directionally biased crack evolution, with damage preferentially initiating along ITZ regions aligned with the major axes of the ellipses. As loading progresses, localized microcracks progressively interact and merge, resulting in the formation of an inclined and more concentrated shear-dominated failure zone. This behavior highlights the role of aggregate morphology in influencing stress

redistribution and crack path tortuosity at the mesoscale.

The corresponding stress–strain responses for the elliptical-aggregate models are presented in Fig. 9. While the overall compressive response remains consistent with experimental trends, noticeable differences in post-peak behavior are observed when compared to the circular-aggregate configuration. In particular, the elliptical aggregates promote enhanced strain localization and a slightly more pronounced post-peak softening response, attributable to increased stress concentrations induced by aggregate shape anisotropy. These results further confirm the ability of the proposed mesoscale phase-field framework to capture the combined effects of tensile-induced microcracking and compressive crushing, while also revealing the sensitivity of concrete failure mechanisms to aggregate geometry. Compared with the model using circular aggregates, the peak stress values of the elliptical-aggregate cases are slightly lower, with corresponding values of 61.65 MPa, 68.54 MPa, and 76.90 MPa.

The slight reduction in peak stress observed in the models with elliptical aggregates can be attributed to the increased stress concentration induced by the geometric anisotropy of the aggregates. Compared with circular aggregates, elliptical particles promote non-uniform load transfer and amplify local tensile stresses at the aggregate–matrix interfaces, which accelerates microcrack initiation and coalescence. As a result, macroscopic failure occurs at a lower peak stress, despite the overall compressive response remaining comparable to that of the circular-aggregate models.

Overall, the extended mesoscale–phase-field model provides a robust computational framework for evaluating the compressive behavior of concrete. The combination of heterogeneous material representation, dual damage mechanisms, and cohesive-enhanced phase-field formulation results in a realistic simulation of failure processes, offering valuable insights for material design optimization and structural analysis.

3.2. Compression test

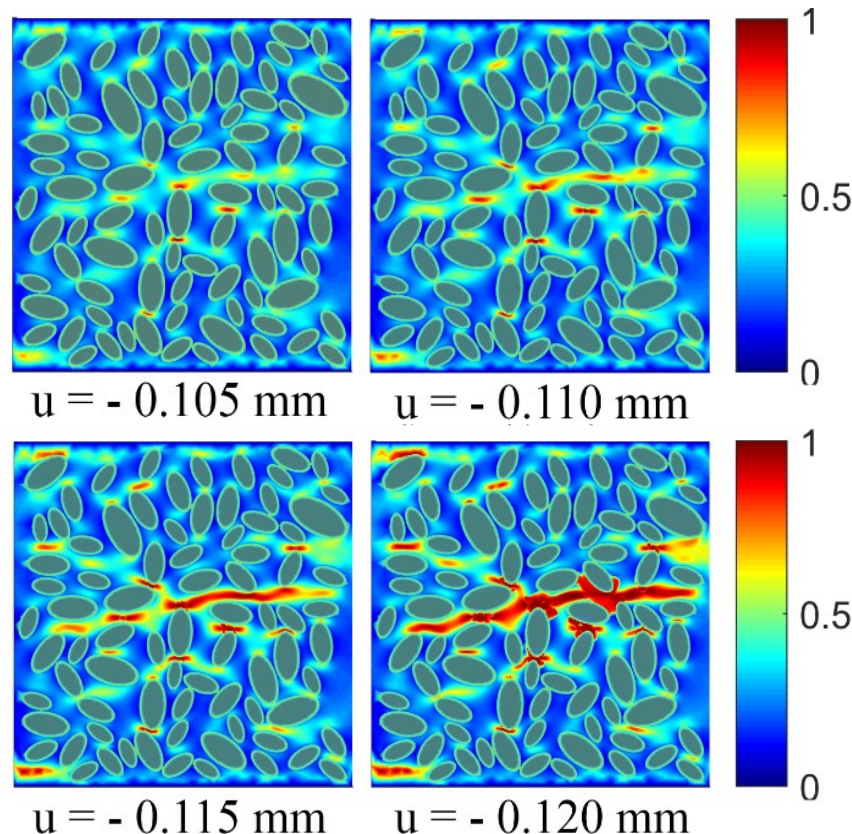


Fig. 8. Crack pattern with elliptical aggregate

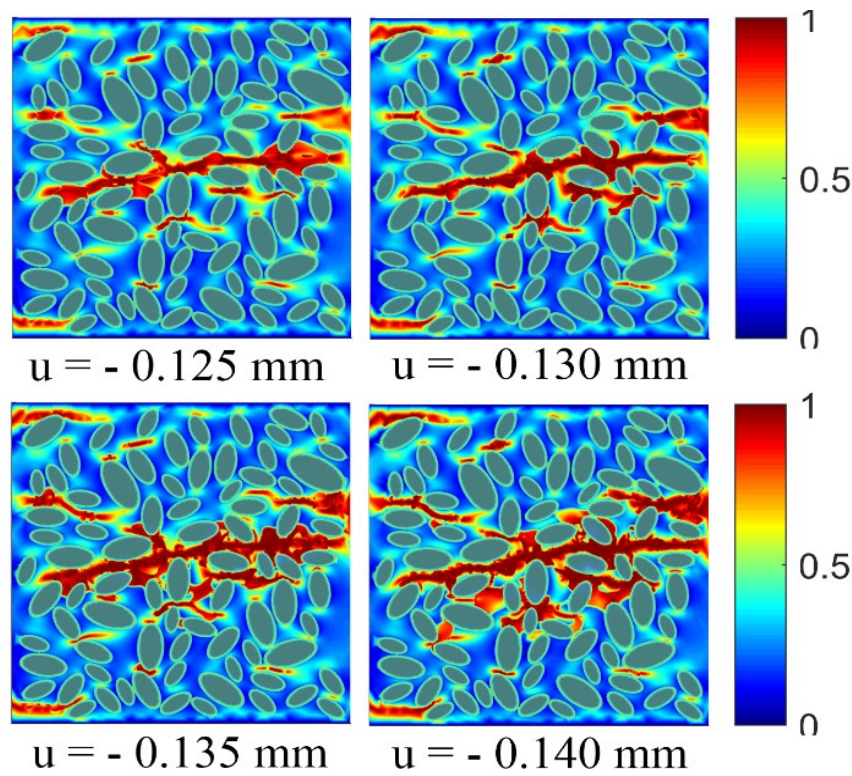


Fig. 8. (continued)

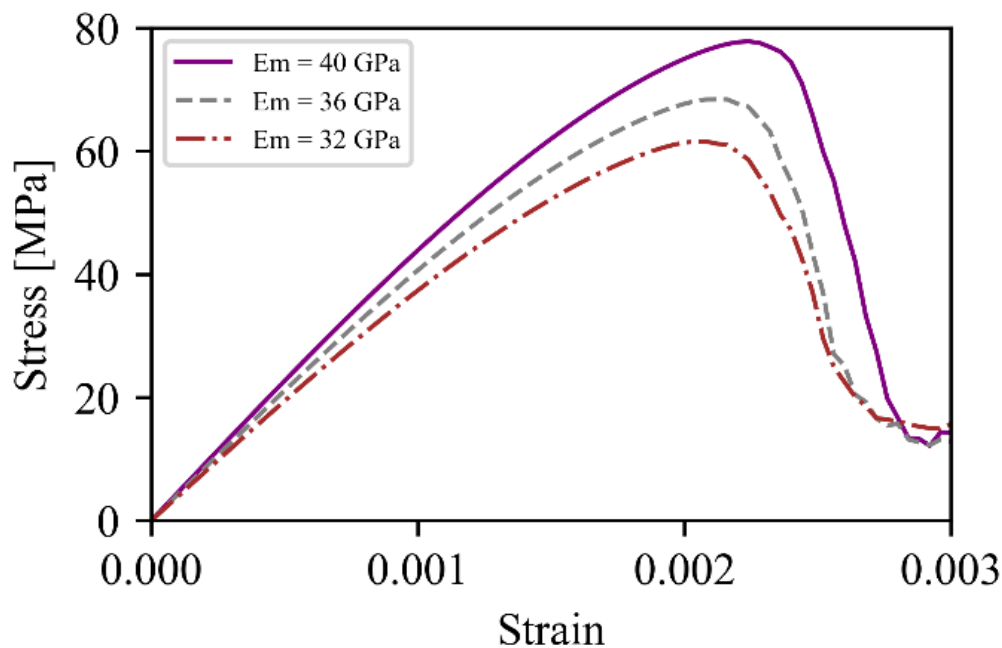


Fig. 9. Stress – strain curve with elliptical aggregate

The materials used in this study include Portland cement (PC) Fico PCB40 conforming to TCVN 6260:2020 [28]; natural yellow sand with a density of 2.63 g/cm^3 and particle sizes ranging from 0 to 4 mm; Class F fly ash with a density of 2.30 g/cm^3 ; and a polycarboxylate-based superplasticizer, ViscoCrete-8168 (Sika), with a solid content of 40%, light brown in color, and a

bulk density of 1.08 g/cm^3 at 25°C . The coarse aggregate consisted of crushed granite sourced from Tan Uyen quarry, Binh Duong province, which is commonly used in construction practice, with a density of 2.70 g/cm^3 . The granite aggregate with particle sizes of 4–12 mm satisfied the grading requirements specified in TCVN 7570:2006 [29] (Fig. 10). Prior to mixing, all materials were stored

under laboratory-controlled conditions to maintain stable moisture content and temperature, thereby minimizing variability in the properties of fresh concrete. The physical properties of the aggregates, including density and particle size distribution, were characterized in accordance with relevant Vietnamese standards to ensure consistency and reproducibility of the experimental program.

The workability of the concrete mixtures was

assessed using a slump test conducted with an Abrams cone. The measured slump values were 12 cm, 9 cm, and 5 cm for mixtures with water-to-cement (W/C) ratios of 0.50, 0.45, and 0.40, respectively (Fig. 11), indicating a systematic reduction in workability with decreasing water content. During casting, all mixtures were compacted using a needle vibrator in combination with a vibrating table to ensure uniform distribution of aggregates and adequate consolidation.



Fig. 10. Concrete constituent materials

For each concrete mix proportion, three standard cubic specimens with dimensions of 150 x 150 x 150 mm (Fig. 12) were cast in rigid steel molds in accordance with TCVN 3118:2022 [30]. Prior to casting, the inner surfaces of the molds were lightly oiled to facilitate demolding and prevent surface defects. Concrete was placed into the molds in three equal layers, each of which was compacted using a needle vibrator to minimize entrapped air and ensure homogeneous internal structure. The top surfaces of the specimens were carefully leveled to guarantee uniform load transfer during compression testing.

After casting, the specimens were covered with plastic sheets to prevent moisture loss and stored under laboratory ambient conditions for the first 24 hours. Subsequently, the specimens were demolded and transferred to a curing tank, where they were water-cured for 28 days under standard conditions, with a controlled temperature of $20 \pm 2^\circ\text{C}$ and relative humidity close to saturation, in accordance with TCVN 8828:2011 [31]. This curing regime was adopted to ensure sufficient hydration of cementitious materials and to provide a consistent basis for evaluating the mechanical properties of concrete at a mature age.

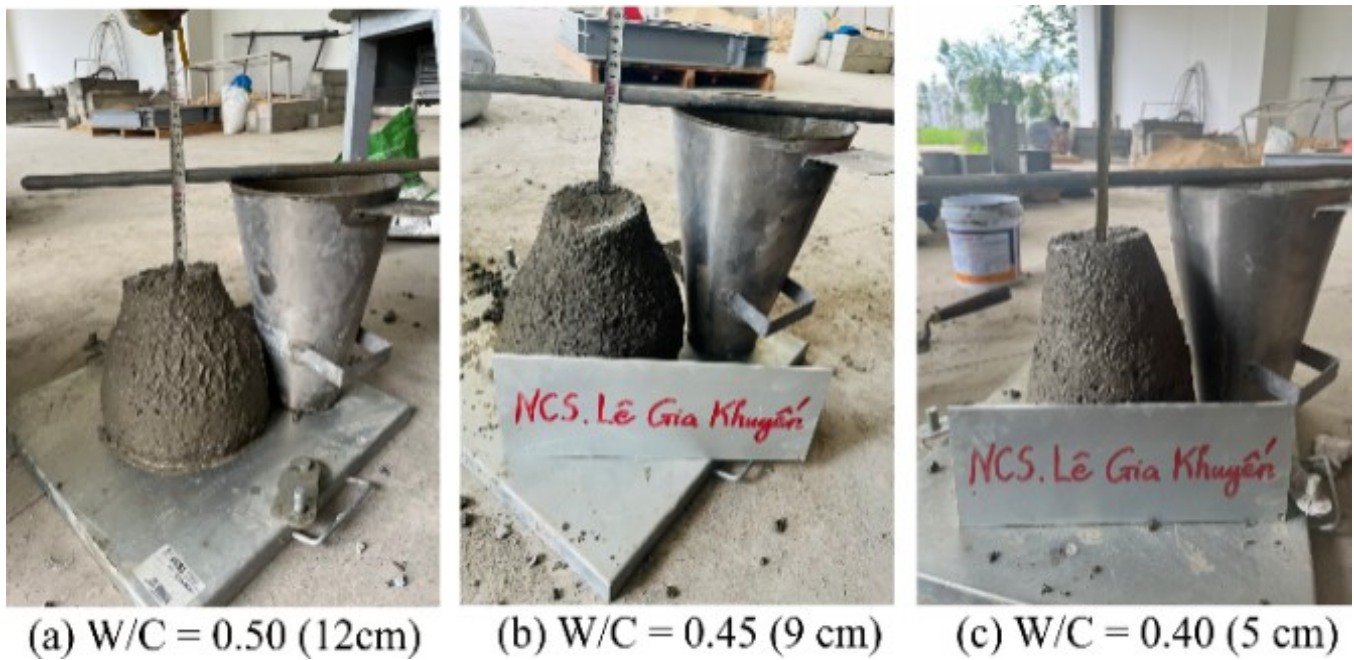


Fig. 11. Measurement of slump of concrete mixtures



Fig. 12. Cube mold for compressive strength testing

At the end of the curing period, the specimens were removed from the curing tank, surface-dried, and visually inspected for defects prior to testing. Compression tests were conducted using a servo-controlled hydraulic testing machine with a maximum load capacity of 2000 kN (Fig. 13). The compressive load was applied monotonically at a constant rate to promote stable crack development and enable reliable acquisition of

stress–strain responses. This standardized specimen preparation, curing, and testing protocol contributed to minimizing experimental variability and ensured the reproducibility and reliability of the measured compressive strength and failure characteristics.

Based on conventional concrete materials and practical considerations, this study designed high-workability concrete mixtures that exhibited

no segregation or bleeding while maintaining adequate viscosity for proper aggregate dispersion. This ensured mixture homogeneity and enhanced the mechanical contribution of

aggregates within the concrete matrix. The mix design results for the three concrete compositions corresponding to different W/C ratios are summarized in Table 2.



Fig. 13. Concrete compression testing machine

Table 2. Material composition for 1m³ of concrete

No.	Cement (kg)	Fly ash (kg)	Sand (kg)	Aggregate (kg)	Superplasticizer (kg)	Water (litre)	Ratio W/C
1	300	90	800	1012	1.8	150	0.50
2	300	90	817	1033	2.4	135	0.45
3	300	90	833	1053	3.6	120	0.40

Table 3. Comparison of the compressive strength (MPa) of concrete specimens between experimental results and numerical simulations

No.		Specimen 1	Specimen 2	Specimen 3	Average Exp.	Circular Model	Elliptical Model
1	W/C = 0.50	63.73	64.25	63.46	63.81	62.24	61.65
2	W/C = 0.45	69.87	68.56	70.29	69.57	68.61	68.54
3	W/C = 0.40	76.02	78.76	79.67	78.15	77.06	76.90

For each concrete mix proportion, three specimens were tested to obtain a representative average compressive strength. The experimental results were subsequently compared with

numerical simulations, with detailed quantitative comparisons presented in Table 3 and illustrated in Fig. 14 and Fig. 15.

Observation of the failure patterns of the

concrete specimens (Fig. 14), together with the comparison of stress–strain curves between experiments and numerical simulations (Fig. 15), reveals a clear agreement between the computational results and the experimental data. The findings indicate that a decrease in the W/C ratio, corresponding to an increase in the elastic

modulus of the cement paste phase, leads to an improvement in the compressive strength of the concrete mixture. Both visually and quantitatively, the three-phase model (aggregate, ITZ, and cement paste) demonstrates a strong capability to accurately capture the compressive damage behavior of concrete.



Fig. 14. Compression failure test specimen

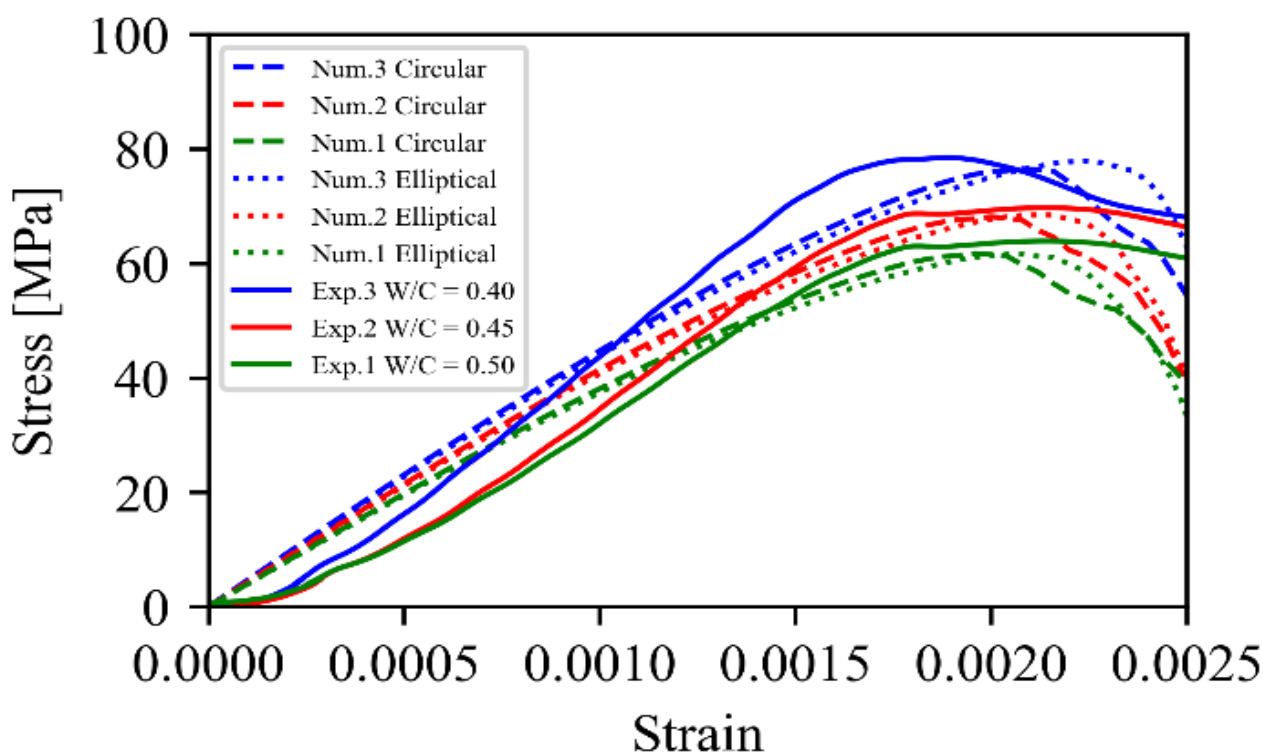


Fig. 15. Comparison of stress-strain curves between numerical model–experimental results

3.3. Limitations of the 2D assumption

It should be noted that the present simulations are performed within a two-dimensional framework under a plane stress assumption. While this idealization enables high-resolution mesoscale modeling of the aggregate–ITZ–matrix system with reasonable computational cost, it does not fully capture inherently three-dimensional effects observed in experimental concrete specimens.

In particular, the 2D model cannot represent out-of-plane crack tortuosity, spatial crack branching in the thickness direction, or possible confinement and triaxial stress effects that may arise in 3D cubic specimens. Moreover, absolute geometric size effects associated with specimen depth and volumetric crack interaction are not explicitly accounted for in the current formulation.

Nevertheless, the primary objective of this study is to investigate mesoscale damage initiation, crack interaction mechanisms, and the influence of aggregate morphology and W/C ratio on the nominal compressive response. These mechanisms are largely governed by in-plane stress redistribution and interfacial heterogeneity, which can be reasonably captured within a 2D representation. The comparison with experiments therefore focuses on global mechanical indicators—such as nominal stress–strain curves, peak compressive strength, and overall failure mode—rather than detailed three-dimensional crack topology.

Future work will extend the present framework to fully three-dimensional mesoscale models in order to further examine size effects and spatial crack evolution, and to provide a more comprehensive validation against experimental results.

4. Conclusions

In this paper, a new numerical model based on the phase-field method combined with cohesive zone theory was developed to describe the compressive behavior of concrete. The model represents concrete as a three-phase material

system, consisting of the aggregate phase, the cement mortar matrix phase, and the interfacial transition zone (ITZ) between the aggregate and the mortar, thereby enabling a clear investigation of the role of each phase as well as their mechanical interactions during loading. The model was applied to simulate concrete with two different aggregate shapes, namely circular and elliptical aggregates, allowing for an assessment of the influence of aggregate shape on the compressive strength of concrete. The simulation results obtained for both cases show good agreement with experimental data, particularly in reproducing the stress–strain curves and peak compressive strength. This close agreement demonstrates the high accuracy and reliability of the proposed model in predicting and reproducing the mechanical behavior of concrete under compressive loading. On this basis, the main conclusions of this study are drawn as follows:

The numerical model accurately reproduces the stress–strain relationship of concrete under compression, consistent with experimental observations.

The model can serve as an effective computational tool for reproducing the mechanical behavior of concrete under compressive loads, thereby reducing the need for extensive experimental testing.

With its ability to be calibrated and extended, the model has potential applications to various composite materials such as fiber-reinforced concrete or textile-reinforced concrete, thereby contributing to the development of sustainable and high-performance concretes.

Although the present study focuses on mesoscale modeling, several strategies can be considered to extend the framework toward structural-scale applications. One possible approach is RVE-based computational homogenization, in which effective elastic properties, fracture energies, and softening laws are extracted from mesoscale simulations and transferred to macroscopic constitutive models. Alternatively, a macroscopic phase-field

formulation with effective parameters calibrated from mesoscale results may be employed, avoiding explicit resolution of aggregates and ITZ at the structural level. A local multiscale (“zoom-in”) strategy, where mesoscale phase-field models are applied only in critical regions of large structures, also offers a balanced compromise between computational efficiency and mechanistic accuracy. These directions provide a clear pathway for future multiscale structural applications of the proposed framework.

Acknowledgments

This research is funded by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 107.02-2023.15

Declaration of Generative AI

During the preparation of this work, the authors did not use Generative AI and AI-assisted technology tools in order to generate the content of the manuscript.

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