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Sujet de la thèse

**Effet de la forme et des caractéristiques de surface des
inclusions sur la fissuration du béton : étude expérimentale
et modélisation numérique**

**(Effect of shape and surface characteristics of inclusion on
concrete fracture: experimental investigation and numerical
simulation)**

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Titre alternatif

Étude expérimentale et modélisation numérique de la
fissuration du béton due au retrait de séchage : influence de
la forme des inclusions et de la zone de transition
interfaciale

(Experimental and numerical investigation of drying
shrinkage cracking in concrete: effect of inclusion shape and
interfacial transition zone)

Abstract

This thesis investigates the influence of inclusion shape and interfacial characteristics on drying shrinkage-induced cracking in cementitious composites, combining mesoscale experiments with advanced peridynamic modeling. A fully coupled three-dimensional hydro-mechanical peridynamic model, based on bond-based theory, was first developed to simulate cracking induced by drying shrinkage. After validation, the model was systematically applied to analyze the effects of aggregate geometry (spherical, flat, and elongated) on crack initiation and evolution. Results indicate that higher sphericity tends to reduce cracking, whereas elongated or flattened shapes promote the formation of anisotropic crack networks.

To capture interfacial debonding, a new peridynamic formulation for imperfect interfaces, based on the ordinary state approach, was introduced. This model incorporates independent parameters for normal and tangential stiffness as well as fracture energy, enabling the representation of displacement discontinuities and mixed-mode fracture. It successfully reproduces crack deviation, penetration, and arrest in weak interfacial transition zones (ITZ). Complementary X-ray microtomography experiments on samples containing smooth and rough glass inclusions highlight the critical role of interfacial properties. Parametric numerical analyses further reveal that fracture energy exhibits threshold effects, while interfacial stiffness governs crack propagation when toughness is sufficiently high. Numerical simulations accurately reproduce experimental observations, confirming the robustness of the proposed peridynamic framework for describing ITZ-governed fracture.

Overall, the results demonstrate that inclusion geometry and interfacial characteristics are key mesoscale factors controlling drying shrinkage-induced cracking. By linking experimental insights with innovative peridynamic formulations, this thesis advances the mechanistic understanding of ITZ-induced fracture processes and provides predictive modeling strategies to guide the design of more durable and resilient concrete.

Keywords: concrete cracking; inclusion geometry; interfacial characteristics; drying shrinkage; peridynamic modeling

Résumé

Cette thèse étudie l'influence de la forme des inclusions et des caractéristiques interfaciales sur la fissuration induite par le retrait au séchage dans les composites cimentaires, en combinant des expérimentations à l'échelle mésoscopique et une modélisation périodynamique avancée. Un modèle périodynamique tridimensionnel hydromécanique entièrement couplé, fondé sur la théorie des liaisons (Bond-based), a d'abord été développé pour simuler la fissuration liée au retrait au séchage. Après validation, ce modèle a été appliqué pour analyser systématiquement les effets de la géométrie des granulats (sphériques, plats et allongés) sur l'initiation et l'évolution des fissures. Les résultats montrent qu'une sphéricité accrue tend à réduire la fissuration, tandis que les formes allongées ou aplaties favorisent la formation de réseaux de fissures anisotropes.

Pour mieux représenter le décollement interfacial, une nouvelle formulation périodynamique à interface imparfaite, basée sur l'état ordinaire, a été introduite. Cette approche intègre des paramètres indépendants de rigidité normale et tangentielle ainsi que d'énergie de rupture, permettant de modéliser les discontinuités de déplacement et la rupture en mode mixte. Elle reproduit avec succès la déviation, la pénétration et l'arrêt des fissures dans les zones de transition interfaciales (ITZ) à faible cohésion. Des expériences complémentaires de microtomographie à rayons X sur des échantillons comportant des inclusions de verre lisses et rugueuses mettent en évidence le rôle déterminant des propriétés interfaciales. Les analyses numériques paramétriques révèlent par ailleurs que l'énergie de rupture présente des effets de seuil, tandis que la rigidité interfaciale contrôle la propagation des fissures lorsque la ténacité est suffisante. Les simulations numériques reproduisent fidèlement les observations expérimentales, confirmant la robustesse du cadre périodynamique proposé pour décrire la fracture gouvernée par les ITZ.

Dans l'ensemble, les résultats démontrent que la géométrie des inclusions et leurs caractéristiques interfaciales constituent des facteurs mésoscopiques clés régissant la fissuration due au retrait au séchage. En reliant des observations expérimentales à des formulations périodynamiques innovantes, cette thèse approfondit la compréhension mécanistique des processus de fracture induits par les ITZ et propose des outils prédictifs de modélisation pour la conception de bétons plus durables et résistants.

Mots-clés: fissuration du béton ; géométrie des inclusions ; caractéristiques interfaciales ; retrait au séchage ; modélisation périodynamique

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General Introduction

Concrete is one of the most widely used construction materials, serving as a cornerstone of modern infrastructure, from buildings and bridges to dams and nuclear facilities. Despite its ubiquity, concrete remains highly susceptible to cracking, which compromises structural integrity and durability. Cracking in concrete arises from multiple factors, including drying shrinkage, thermal fluctuations, external loading, chemical reactions, and corrosion. Among these, drying shrinkage has been identified as one of the critical drivers of crack formation, as it originates from pore water loss and induces internal stresses that exceed the tensile capacity of the material ([Mao et al., 2021](#); [Mukhtar and El-Tohfa, 2023](#)). Understanding the mechanisms underlying crack initiation and propagation is therefore essential for designing durable concrete structures.

Concrete is inherently a multi-scale heterogeneous composite, composed of cement paste, aggregates, and the interfacial transition zone (ITZ). Its macroscopic fracture behavior is governed by complex interactions across multiple length scales: from the pore- and hydrate-dominated microscale, through the mesoscale defined by aggregates, mortar, and ITZs, up to the structural macroscale ([Unger and Eckardt, 2011](#)). At the mesoscale, aggregates not only provide stiffness and strength but also influence shrinkage, fracture energy dissipation, and long-term durability ([Sáez-Pérez et al., 2020](#); [Talaat et al., 2021](#)). Experimental studies have revealed that aggregate-related properties—including size ([Akcaoglu et al., 2004](#); [Szczesniak et al., 2013](#); [Yu et al., 2019](#)), stiffness ([Li et al., 2020b](#); [Vyhřídál et al., 2021](#); [Zhang et al., 2014](#)), volume fraction ([Bischoff and Van Mier, 2002](#)), shape ([Jiang and Shen, 2022](#); [Jiang et al., 2021](#); [Rocco and Elices, 2009](#)), and surface characteristics ([Jia and Gu, 2021](#); [Königsberger et al., 2014](#))—play important roles in determining crack initiation, propagation paths, and connectivity. Complementary experimental techniques, such as X-ray computed tomography (XCT), scanning electron microscopy (SEM), digital image correlation (DIC), and acoustic emission monitoring, provide valuable insights into crack morphology and damage evolution at this scale ([Gao et al., 2020](#); [Skarżyński and Tejchman, 2016](#); [Van Steen et al., 2024](#); [Zheng et al., 2022](#)).

These mesoscale observations highlight critical mechanisms of damage localization and interfacial debonding that cannot be captured solely through macroscale testing.

Numerical modeling offers a powerful complement to experimental studies, enabling systematic exploration of fracture mechanisms under controlled parametric variations. At the mesoscale, several approaches have been developed. Continuum-based methods, such as FEM and XFEM, represent material heterogeneity within the continuum mechanics framework and can reproduce nonlinear stress redistribution and fracture processes (Ozbolt et al., 2014; Xue et al., 2019). Discrete methods, such as DEM, explicitly model aggregates and ITZs as separate entities, naturally describing crack initiation and coalescence through particle interactions (Lisjak and Grasselli, 2014; Wang et al., 2020b). More recently, nonlocal approaches such as the Phase-Field Method (PFM) (Chen, 2002) and Peridynamics (PD) (Silling, 2000; Silling et al., 2007) have emerged as promising alternatives. PD, in particular, employs an integral formulation that inherently accommodates displacement discontinuities and evolving crack networks without requiring remeshing. Applications to cementitious composites have demonstrated its ability to capture complex fracture phenomena such as crack branching, aggregate–mortar debonding, and shrinkage-induced cracking (Gerstle et al., 2007; Huang et al., 2011; Jin et al., 2021, 2023). These developments establish PD as a framework for bridging mesoscale heterogeneity with macroscale fracture performance.

The objective of this study is to analyze the influence of aggregate properties on the cracking behavior of cementitious materials during drying through a series of numerical simulations. Accordingly, this thesis is organized into five chapters:

Chapter I reviews mesoscale experiments and numerical simulation methods, with a focus on strategies for mesoscale model construction and constitutive modeling. Different approaches for ITZ representation are discussed. The advantages and limitations of FEM/XFEM and DEM are compared, followed by an introduction to peridynamic theory, including Bond-Based PD (BB-PD), Ordinary State-Based PD (OSB-PD), and Non-Ordinary State-Based PD (NOSB-PD). Recent advances in multiscale modeling and hybrid coupling strategies are also outlined.

Chapter II summarizes the experimental results on the effects of aggregate stiffness and size on shrinkage cracking in cementitious materials. The influence of aggregate surface roughness is then examined, with crack morphology analyzed using XCMT. In addition, experimental attempts were presented to investigate the role of aggregate shape.

Chapter III develops and implements a fully coupled three-dimensional hydro–mechanical BB-PD model to simulate drying-induced cracking. The model is first verified against

experimental observations of shrinkage crack morphologies. A three-phase mesoscale concrete model incorporating aggregates of varying shapes (spherical, flat, elongated) is then established, and systematic analyses quantify the role of aggregate geometry in crack initiation, width, length, and volume.

Chapter IV introduces a novel OSB-PD-based imperfect-interface formulation that permits displacement discontinuities and prescribes independent normal and tangential stiffnesses, together with a mixed-mode energy-based failure criterion. The method accounts for evolving interface normals during deformation. Validation examples demonstrate its capability to reproduce crack deflection, penetration, and arrest at weak interfaces.

Chapter V conducts parametric studies to evaluate the effects of interfacial stiffness and fracture energy on shrinkage-induced cracking. Experimental findings are then compared with numerical results to assess the model's ability to capture the role of surface roughness in crack evolution.

Chapter VI presents the conclusions and perspectives.

Chapter I

State of Art

1 Introduction

Concrete, a vital material in contemporary society extensively employed in diverse engineering applications from construction to nuclear plants, is prone to cracking due to various factors such as drying, loading, temperature changes, chemical reactions, and corrosion. The emergence of cracks threatens its structural integrity and severely compromises its durability, potentially resulting in catastrophic consequences. Thus, comprehending the causes and mechanisms of concrete cracking is imperative for the effective design and maintenance of concrete structures. The causes of concrete cracking vary, primarily influenced by shrinkage, thermal stresses, and loading ([Mehndi et al., 2014](#)). Notably, the shrinkage performance of concrete is critical as it represents the stress-inducing element leading to cracking, caused by changes in pore water content during drying or wetting processes ([Mao et al., 2021](#); [Mastali et al., 2018b](#); [Mukhtar and El-Tohfa, 2023](#)). Thermal stresses arise from temperature fluctuations, causing uncoordinated thermal strain due to different coefficients of thermal expansion in the concrete composition. Loading induces stress and strain in concrete, potentially leading to cracks if the stress surpasses its strength.

Drying shrinkage is a critical time-dependent deformation in cement-based materials that profoundly influences the long-term performance, serviceability, and durability of concrete structures ([Tran et al., 2021](#)). The phenomenon originates from moisture loss within the porous cement matrix, leading to volumetric contraction and, consequently, internal tensile stress development. Such stresses, when exceeding the tensile strength of the concrete, manifest as micro- or macro-cracks that serve as ingress pathways for aggressive agents, including chlorides and sulphates, accelerating reinforcement corrosion and structural deterioration ([Bazant et al., 1988](#); [Mehta and Monteiro, 2014](#)). Statisti-

cal analyses of construction performance underscore the economic significance of drying shrinkage-induced cracking. In the French construction industry, repair and maintenance costs associated with cracking-related defects constitute a significant budgetary burden, highlighting the economic scale of this issue (Tran et al., 2021). Beyond financial impact, shrinkage-induced cracking compromises durability and sustainability by necessitating premature repair and replacement, thereby increasing embodied carbon emissions from cement production (Neville, 2011; Thomas, 2013). Consequently, understanding the mechanisms and mitigation of drying shrinkage is imperative for designing durable and sustainable concrete.

The heterogeneous nature of concrete, composed of cement paste, aggregates, and the interfacial transition zone (ITZ), plays a critical role in determining its mechanical behavior and fracture resistance. Aggregates not only influence the strength and stiffness of concrete, but also affect its shrinkage, cracking potential, and long-term durability (Sáez-Pérez et al., 2020; Talaat et al., 2021). This state of art first introduces the mesoscopic mechanisms underlying crack initiation and propagation in cementitious materials, emphasizing the role of aggregate geometry and ITZ properties. It then presents an overview of various numerical modelling strategies—namely continuum-based, discrete element, and peridynamic methods—used to simulate the fracture behavior of concrete at the mesoscale. Finally, the recent progress and applications of the nonlocal peridynamic method are discussed, with a focus on its potential for capturing discontinuities and complex fracture phenomena in heterogeneous cement-based materials.

2 Drying shrinkage in cementitious materials

Shrinkage in cementitious materials is a complex volumetric instability that develops from early hydration to the long-term service life of concrete. It arises from a combination of physical and chemical processes that cause a reduction in internal moisture or microstructural rearrangement of the hydrated matrix. The overall shrinkage can be classified into four primary categories: plastic shrinkage, autogenous shrinkage, drying shrinkage, and carbonation shrinkage (Mastali et al., 2018a).

Plastic shrinkage occurs in the early hours after casting, when rapid evaporation from the surface outpaces bleeding, generating capillary stresses in the fresh matrix that often lead to surface cracking (Qu et al., 2024). Autogenous shrinkage develops during hydration as self-desiccation within low water-to-cement ratio systems induces internal stresses, which is particularly pronounced in high-performance concretes (HPC) with $w/c < 0.35$.

(Jensen, 2000; Tazawa, 1999). Carbonation shrinkage, a slower and secondary process, is driven by the reaction between calcium hydroxide and atmospheric carbon dioxide, leading to the formation of calcium carbonate and an associated decrease in solid volume (Ye et al., 2017).

Among these categories, **drying shrinkage** predominates in conventional concrete, particularly for mixtures with $w/c > 0.40$ (Tran et al., 2021). When the w/c ratio exceeds approximately 0.42–0.45, excess pore water remains after hydration, which subsequently evaporates under ambient drying conditions, resulting in capillary tension within the pore network and consequent macroscopic contraction (Mehta and Monteiro, 2014; Neville, 2011). The process is primarily governed by the movement of moisture within the porous cementitious matrix towards equilibrium with external relative humidity (RH). The magnitude of drying shrinkage depends on several factors, including pore size distribution, internal RH, curing conditions, and the morphology of the hydration products (Ayano and Wittmann, 2002; Bazant and Baweja, 2000; Powers, 1958).

2.1 Core Theoretical Mechanisms of Drying Shrinkage

Drying shrinkage in cementitious materials results from complex physicochemical interactions between pore water, solid hydrates, and the external environment. The phenomenon is fundamentally driven by the loss of moisture from the capillary and gel pore network as the system strives to reach hygral equilibrium with the ambient relative humidity (RH). The associated decrease in internal RH induces differential stresses in the hydrated matrix, giving rise to macroscopic volume contraction. Several fundamental theories have been developed to explain this behaviour, including (1) the surface free energy or Gibbs–Bangham effect, (2) capillary tension theory, (3) disjoining pressure, and (4) interlayer water movement within the calcium–silicate–hydrate (C–S–H) gel (Ayano and Wittmann, 2002; Bazant and Baweja, 2000; Powers, 1958; Soroka, 1993; Tran et al., 2021). Each mechanism predominates under a specific range of RH and contributes to the overall deformation in different degrees.

2.1.1 Surface Free Energy (Gibbs–Bangham Effect)

At low relative humidity (typically $RH < 40\%$), the shrinkage and swelling of the C–S–H gel are primarily controlled by changes in the surface free energy of the solid–liquid interface. The removal of physically adsorbed water layers from the surfaces of C–S–H particles increases the surface energy of the solid phase. This rise in surface free energy induces attractive forces among adjacent gel particles, resulting in contraction of the

solid skeleton and irreversible microstructural densification (Feldman and Sereda, 1968; Jennings, 2000; Muller et al., 2013).

This mechanism is thermodynamically explained by the Gibbs–Batham relationship, which correlates the change in surface free energy ($\Delta\gamma$) to the change in adsorption (ΔA) as:

$$\Delta\gamma = - \int p dV \quad (\text{I. 1})$$

where p is the vapor pressure corresponding to the desorption isotherm and V is the adsorbed volume of water. The progressive desorption of adsorbed water films in mesopores (2–50 nm) increases the tensile stress on the pore walls, producing measurable shrinkage even with minimal moisture loss (Mindess et al., 2003; Tran et al., 2021). As RH falls below 20%, the C–S–H layers approach direct contact, leading to van der Waals bonding and a permanent reduction in interparticle distance (Jennings, 2000).

2.1.2 Capillary Tension Mechanism

The capillary tension theory provides the most widely accepted explanation for drying shrinkage in the practical range of RH between 40–95%, which encompasses most field exposure conditions (Bazant and Baweja, 2000; Neville, 2011; Tran et al., 2021). As water evaporates from partially filled pores, menisci with a certain curvature radius r form at the liquid–vapor interfaces. The pressure difference (p_c) is given by the Laplace equation:

$$p_c = \frac{2\gamma\cos\theta}{r} \quad (\text{I. 2})$$

where γ is specific surface energy of water, and θ is the contact angle at the water–vapour interface within the capillary. If $\cos\theta$ is positive then the liquid wets the capillary surface and penetrates the capillary under tension created by the curvature of the air–liquid interface. If $\cos\theta$ is zero or negative then the liquid does not wet the capillary surface and has to be pressed into the capillary. In the water–concrete system θ is zero so p_c is equal to $2\gamma/r$. This pressure induces tensile stress on the pore walls and compressive stress within the solid skeleton, resulting in bulk contraction (Fig. I. 1).

As pore sizes decrease to the nanoscale, capillary stresses can reach magnitudes of 10–100 MPa, depending on pore geometry and RH (Ayano and Wittmann, 2002; Powers, 1958). The overall volumetric strain (ε_{sh}) due to capillary tension can be approximated as:

$$\varepsilon_{sh} = \frac{p_c}{E_c} \phi \quad (\text{I. 3})$$

where E_c is the composite elastic modulus and ϕ the porosity fraction. Experimental results show that shrinkage is largely irreversible once menisci collapse in finer pores (<

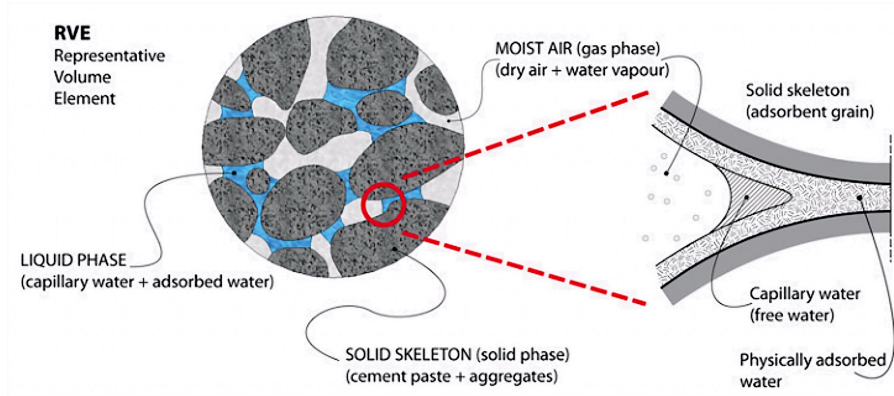


Figure I. 1: A schematic representation of the moist concrete as a multiphase porous material (Gawin and Pesavento, 2012)

50 nm), leading to partial pore closure (Feldman and Sereda, 1968; Jennings, 2000). The predominance of this mechanism in most structural concretes explains why surface tension-reducing admixtures or internal curing are effective in mitigating drying shrinkage.

2.1.3 Disjoining Pressure

Disjoining pressure (Π) arises from molecular interactions acting between two solid surfaces separated by a thin liquid film and is described by a combination of van der Waals, electrostatic, and structural forces (Churaev et al., 2013). Within the C-S-H interlayer, when the adsorbed water film thins as RH decreases, the reduction in repulsive forces allows adjacent layers to draw closer, producing a net attractive stress that contributes to shrinkage (Jennings, 2008; Muller et al., 2013). The disjoining pressure can be represented as:

$$\Pi(h) = \Pi_{vdW}(h) + \Pi_{el}(h) + \Pi_{str}(h) \quad (\text{I. 4})$$

where h is the separation distance between solid layers, and the three terms denote the van der Waals, electrostatic, and structural contributions, respectively.

At high RH ($> 50\%$), electrostatic repulsion dominates, maintaining the separation of C-S-H sheets; as RH declines, the reduced ion concentration in the pore solution weakens the electrostatic double layer, and van der Waals attraction prevails. This induces compressive stress on the solid skeleton and long-term shrinkage even after the cessation of drying (Feldman and Sereda, 1968; Tran et al., 2021). Disjoining pressure thus bridges the micro- and nano-scale mechanisms governing drying shrinkage.

2.1.4 Interlayer Water Movement

At very low humidity ($RH \leq 25\%$), the removal of interlayer water between C–S–H lamellae becomes significant. The polarized water molecules adsorbed within the C–S–H interlayers are strongly bound through hydrogen bonding and electrostatic attraction, forming a quasi-solid film. When external drying progresses, the partial migration or loss of this interlayer water narrows the interlaminar spacing and induces pronounced contraction (Feldman and Sereda, 1968; Jennings, 2000; Muller et al., 2013).

Experimental data from small-angle X-ray scattering (SAXS) and nuclear magnetic resonance (NMR) confirm that the reduction of interlayer spacing from approximately 1.1 nm to 0.9 nm correlates with macroscopic shrinkage strains on the order of 10^{-4} to 10^{-3} (Thomas et al., 1999). Because this mechanism requires significant desorption energy, it is only activated under severe drying ($RH < 15\%$), and is partially irreversible upon rewetting. The phenomenon explains the persistent residual strains observed in long-term shrinkage experiments even after saturation cycles (Bazant and Baweja, 2000; Tran et al., 2021).

2.1.5 Combined Mechanistic Behaviour

The four mechanisms described above act concurrently across the humidity spectrum. In practical exposure conditions, capillary tension predominates in the RH range of 40–95%, while surface free energy and disjoining pressure dominate at lower humidity levels ($< 40\%$) (Ayano and Wittmann, 2002; Tran et al., 2021). The transition region between 40–50% RH marks the point where capillary stresses reach a maximum, and the influence of surface energy mechanisms begins to emerge. A schematic summary of these mechanisms as a function of RH is provided in Fig. I. 2.

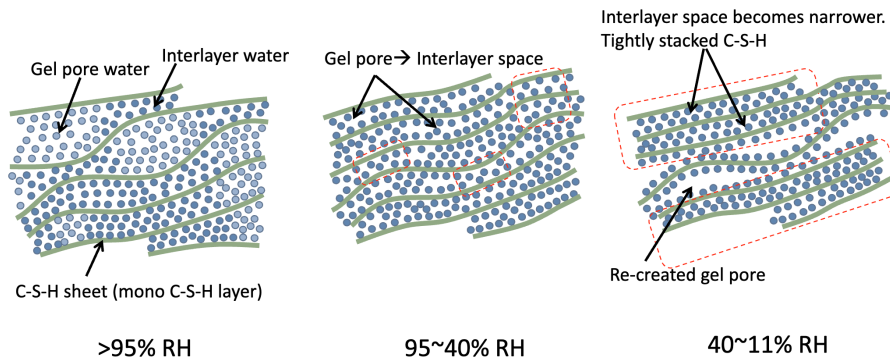


Figure I. 2: A schematic diagram depicting the re-arrangement of C–S–H laminar sheet and interlayer water during drying progress (Maruyama et al., 2019)

The integrated understanding of these mechanisms underpins the design of modern mitigation strategies. By manipulating capillary tension through shrinkage-reducing admixtures, refining pore structure using supplementary cementitious materials, or providing internal restraints via aggregates and fibres, it becomes possible to control or delay the onset of critical stresses associated with drying shrinkage. Such mechanistic insight forms the foundation for developing high-durability, shrinkage-resistant concretes essential for sustainable infrastructure systems.

2.2 Influence of Inclusions on Drying Shrinkage

In cementitious composites, the dimensional stability of the material is also affected by the type and characteristics of its inclusions. These inclusions, aggregates, fibres, fillers, and supplementary cementitious materials (SCMs), govern the mechanical, hygral, and microstructural response of the composite during drying. Each inclusion type contributes to shrinkage control through specific restraint mechanisms, including geometric confinement, load transfer, crack bridging, and microstructural densification (Mehta and Monteiro, 2014; Neville, 2011; Tran et al., 2021). The efficiency of these mechanisms depends on the inclusion's size, stiffness, volume fraction, and interfacial bond with the surrounding cement paste.

In this section, different inclusion types are discussed in detail. In cementitious materials, the principal categories of inclusions are: (i) aggregates, (ii) fibres, (iii) fine fillers and powders, and (iv) supplementary cementitious materials (SCMs). The restraining mechanisms associated with these inclusions are analyzed below.

2.2.1 Restraint Mechanisms of Inclusions

The restraining action of inclusions can be broadly categorized into three coupled mechanisms: (i) *mechanical restraint*, arising from elastic incompatibility between inclusions and cement paste (Hobbs, 1974; Zhang et al., 2013); (ii) *hygral restraint*, related to water absorption, desorption, and internal curing effects (Bentz and Snyder, 1999); and (iii) *interfacial restraint*, resulting from stress transfer and confinement at the inclusion–matrix boundary (Ollivier et al., 1995). These mechanisms act concurrently and are strongly coupled—moisture gradients generate local stress incompatibilities, while interfacial stiffness and permeability influence both mechanical and hygral responses across multiple scales.

Mechanical restraint develops when aggregates or fibres with a higher modulus of elasticity than the cement matrix resist the tensile stresses induced by drying. Rigid inclusions constrain the surrounding paste, inducing internal compressive stresses that

counteract shrinkage deformation (Ayano and Wittmann, 2002; Bazant and Baweja, 2000). The degree of mechanical restraint (R_m) can be expressed as:

$$R_m = \frac{E_i V_i}{E_m(1 - V_i) + E_i V_i} \quad (\text{I. 5})$$

where E_i and E_m are the elastic moduli of the inclusion and the matrix, respectively, and V_i is the inclusion volume fraction. A higher R_m corresponds to stronger shrinkage suppression.

Hygral restraint is governed by the inclusion's ability to regulate internal moisture gradients. Dense aggregates with low water absorption limit evaporation and capillary tension, whereas pre-saturated porous inclusions (e.g., lightweight aggregates or hydrophilic fibres) provide internal curing by releasing stored water, maintaining internal relative humidity (RH), and reducing desiccation stresses (Jensen, 2000; Liu et al., 2017).

Interfacial restraint arises from the bond characteristics between inclusions and paste. Fibres and angular aggregates generate interfacial shear stresses that redistribute localized shrinkage strains and delay crack formation (Banthia and Gupta, 2006; Wu et al., 2019a). The effectiveness of this mechanism depends on the surface morphology, roughness, and chemical compatibility at the interface.

Overall, these mechanisms act synergistically and depend on inclusion geometry and microstructural integration. Rigid, non-absorptive inclusions primarily provide mechanical restraint, while porous or hydrophilic inclusions offer combined mechanical and hygral restraint.

2.2.2 Types of Inclusions in Cementitious Composites

Aggregates constitute 60–80% of concrete volume and are typically categorized as coarse or fine. Coarse aggregates (e.g., crushed granite, basalt, gravel) provide structural rigidity and reduce paste content, while fine aggregates (sand) improve packing density and workability (Mehta and Monteiro, 2014; Neville, 2011). Aggregates primarily contribute mechanical restraint due to their stiffness relative to the paste (Bazant and Baweja, 2000).

Fibres are discontinuous reinforcements used to enhance tensile strength, crack resistance, and post-cracking ductility. Common types include steel fibres (high modulus and ductility), polymeric fibres such as polypropylene (PP) and polyethylene (PE) for crack control, alkali-resistant (AR) glass fibres for strength enhancement, and natural fibres (e.g., cellulose, hemp, jute) for sustainable solutions (Banthia and Gupta, 2006; Li, 2019; Wu et al., 2019a).

Fine mineral fillers (e.g., limestone powder, fly ash fines) occupy voids between cement grains, improving particle packing and reducing permeability. They indirectly reduce shrinkage by lowering capillary porosity rather than through mechanical confinement (Bentz and Weiss, 2011; Mehta and Monteiro, 2014).

SCMs such as fly ash, ground granulated blast furnace slag (GGBFS), and silica fume react with calcium hydroxide to form additional calcium silicate hydrate (C-S-H), refining pore structure and strengthening the ITZ (Neville, 2011; Thomas, 2013). These reactions improve both moisture stability and mechanical restraint. The effects of aggregates and fibres will be analysed in detail in the following.

2.2.3 Effect of Aggregates

Aggregates provide the dominant internal restraint against drying shrinkage. Their effectiveness depends on the mismatch in stiffness and shrinkage coefficient between aggregate and matrix phases (Mehta and Monteiro, 2014; Neville, 2011; Tran et al., 2021).

Increasing aggregate size and volume fraction enhances mechanical restraint, as the total interfacial area per unit paste volume decreases, limiting the extent of shrinkage deformation (Chen et al., 2018; Rao, 2001). Using 3D digital image correlation, Chen et al. (2018) demonstrated that aggregates larger than 10 mm suppressed shrinkage by up to 60% through localized compressive zones. Similarly, Rao (2001) reported a 69.8% shrinkage reduction when increasing fine aggregate size from 1.18 to 2.36 mm under 65% RH. These findings align with the “aggregate skeleton dispersion” model, where stiff aggregates form a network that transfers and counterbalances shrinkage stresses (Zhu et al., 2016).

Aggregate mineralogy and porosity influence hygral restraint. Dense aggregates such as granite, basalt, or quartz limit water loss and capillary tension, whereas porous or recycled aggregates (RCA) tend to amplify shrinkage due to uneven moisture exchange (Ismail and Ramli, 2014; Kou et al., 2011). Surface treatments of RCA (e.g., silicate or polymer coatings) can restore surface density and reduce shrinkage deformation to levels comparable to natural aggregates (Ismail and Ramli, 2014).

Pre-saturated lightweight aggregates provide internal curing by releasing stored water during drying, maintaining internal RH and reducing desiccation stress (Fig. I. 3) (Jensen, 2000). Liu et al. (2019) observed a 20% shrinkage reduction at 91 days with 10% sand replaced by pre-wetted fine lightweight aggregates. Ling et al. (2011) found a 17% reduction using recycled glass aggregates (<10 mm), attributing this to low permeability and surface rigidity. Conversely, finer glass particles (<2 mm) increased shrinkage due to poor bonding and stress concentration (Penacho et al., 2014).

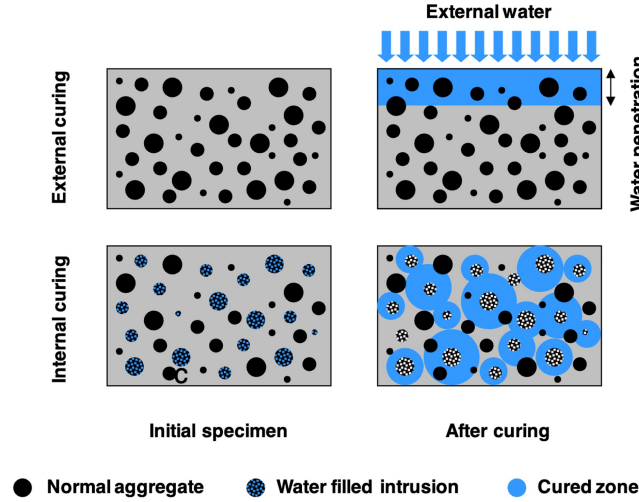


Figure I. 3: Illustration of external versus internal curing, showing uniformly distributed water-filled inclusions ensuring moisture coverage throughout the cement paste (Castro et al., 2010)

2.2.4 Effect of Fibres

Fibres provide restraint primarily through stress transfer across the matrix–fibre interface, delaying crack initiation and limiting shrinkage-induced deformation. The restraining mechanisms of fibres are governed by three interrelated parameters: fibre modulus, bond strength, and distribution uniformity (Banthia and Gupta, 2006; Tran et al., 2021). Polymeric fibres such as polypropylene (PP), polyvinyl alcohol (PVA), and polyacrylonitrile (PAN) introduce micro-level restraint by bridging microcracks and reducing strain localization. PP fibres, despite being hydrophobic, have demonstrated 10–25% shrinkage reductions through internal reinforcement and improved microstructural integrity (Mohammadhosseini et al., 2018; Zhang and fu Li, 2013). PAN fibres, with high surface area and hydrophilicity, further reduce shrinkage (up to 60–70%) by providing nucleation sites for C–S–H growth and promoting water retention at early ages (Fig. I. 4) (Chinchillas-Chinchillas et al., 2019) .

Inorganic fibres, such as steel, carbon, and glass, act predominantly through mechanical restraint. Their high modulus of elasticity enhances stiffness and counters the tensile stresses induced by capillary tension. Wu et al. (2019b) observed that increasing steel fibre volume from 1% to 3% reduced drying shrinkage by 29% after 91 days. Hooked or corrugated shapes further improved interfacial anchorage, providing an additional 10–15% reduction.

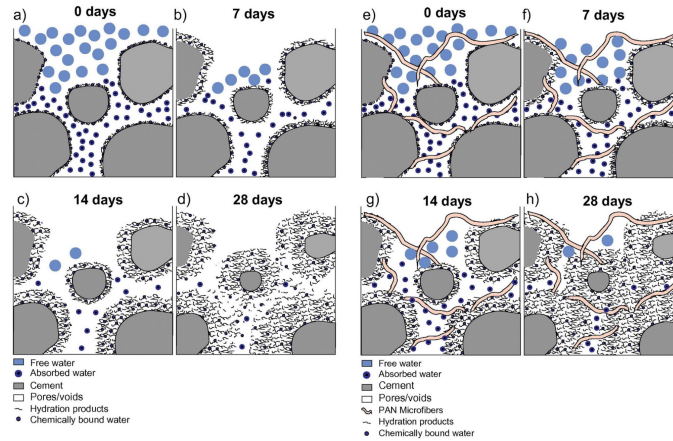


Figure I. 4: Schematic representation of the effect of fibres on water retention during drying: (a–d) without fibres and (e–h) with fibres ([Chinchillas-Chinchillas et al., 2019](#))

Natural fibres (e.g., sisal, coconut, and luffa) exhibit a dual effect due to their porous microstructure. Although untreated fibres can increase shrinkage by forming moisture pathways, alkaline or peroxide surface treatment enhances interfacial bonding and allows pre-wetted fibres to act as internal water reservoirs, supplying hygral restraint during early drying. [Tong et al. \(2014\)](#) reported a 30% reduction in shrinkage after 90 days using treated luffa fibres, relative to untreated counterparts.

2.2.5 Combined Restraint and Design Implications

Aggregates and fibres act complementarily to provide multiscale shrinkage resistance. Aggregates contribute macro-level restraint by constraining paste deformation and stabilizing internal RH, while fibres operate at micro- and meso-scales to bridge cracks and delay coalescence. This synergy can be expressed as:

$$\varepsilon_{ds} = \varepsilon_0(1 - R_{m,a})(1 - R_{m,f})(1 - R_h) \quad (\text{I. 6})$$

where ε_{ds} is the effective drying shrinkage strain, ε_0 is the free shrinkage strain, and $R_{m,a}$, $R_{m,f}$, and R_h represent mechanical restraint of aggregates, fibres, and hygral restraint, respectively.

Optimizing these parameters through mixture design, balancing aggregate stiffness, volume fraction, and fibre type, provides a practical pathway to develop shrinkage-resistant, durable, and sustainable concrete systems. Drying shrinkage represents a fundamental limitation to the dimensional stability and durability of cementitious materials. It originates from complex moisture–solid interactions driven by surface free energy changes,

capillary tension, disjoining pressure, and interlayer water migration. The mitigation of drying shrinkage requires understanding these mechanisms and controlling microstructural evolution through material design. In this context, a mesoscopic investigation of drying shrinkage-induced cracking is essential to investigate the relationships between inclusion characteristics, moisture transport, and stress development within the composite system.

3 Meso-Scale Analysis of drying shrinkage-induced cracking of cementitious materials

Concrete is a typical multi-scale heterogeneous material, whose macroscopic mechanical behavior is governed by complex interactions across multiple length scales, including the macro-scale (e.g., structural components), meso-scale (e.g., aggregates, mortar, and ITZs), and micro-scale (e.g., pores and hydrates). As illustrated in Fig. I. 5, this hierarchical structure provides the physical basis for understanding damage evolution, transport phenomena, and fracture processes in cementitious composites.

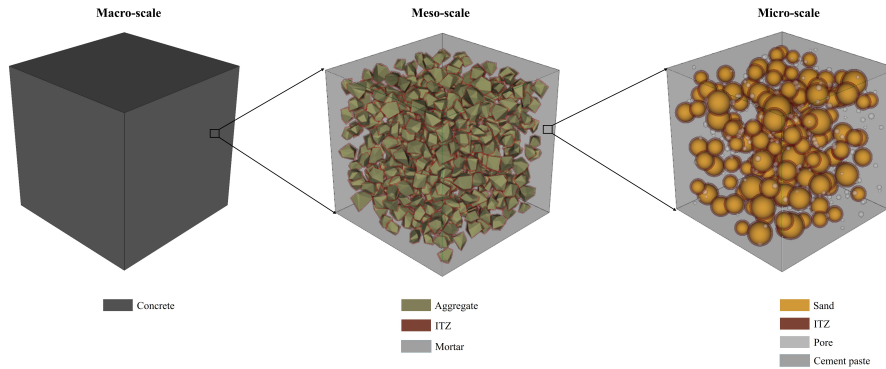


Figure I. 5: Multiscale representation of concrete: from macroscale to meso- and microscale heterogeneity

Among the different length scales, meso-scale research has attracted growing attention for its ability to explicitly capture the geometric and mechanical heterogeneities introduced by aggregates and the surrounding ITZs (Unger and Eckardt, 2011; Zhang et al., 2017a). In particular, meso-scale experimental studies have provided valuable insights into the role of aggregates in fracture behavior. Early work by Creath et al. (1969) showed that aggregate particles significantly alter local strain distributions within mortar under multi-axial loading. Since then, a variety of experimental approaches—including uniaxial tension/compression (Naderi and Kaboudan, 2021), bending (Peng et al., 2019), shear (Sherwood et al., 2007), and dynamic loading (Jiang et al., 2021)—have been em-

ployed to examine how aggregate properties influence fracture.

Advanced imaging techniques, such as X-ray computed tomography (XCT) and X-ray Microtomography (XMT), are also widely used to investigate meso-scale cracking in concrete. These methods consistently reveal that aggregates, which form the structural skeleton of concrete, exert a dominant influence on its mechanical properties, including strength, elasticity, thermal behavior, dimensional stability, and durability (Sáez-Pérez et al., 2020; Talaat et al., 2021). Consequently, aggregate characteristics—such as size (Yu et al., 2019), stiffness (Li et al., 2020b), and shape (Jin et al., 2018)—are critical for understanding their impact on crack initiation and propagation. These studies are frequently complemented by advanced diagnostic techniques, including acoustic emission (AE) monitoring (Van Steen et al., 2024), scanning electron microscopy (SEM) (Zheng et al., 2022), digital image correlation (DIC) (Gao et al., 2020), and X-ray micro-computed tomography (XMCT) (Chen et al., 2022a; Guo et al., 2023; Skarżyński and Tejchman, 2016; Zhang et al., 2022), which enable in-situ characterization of damage evolution and crack morphology.

In summary, a wide range of aggregate-related properties—including size, volume fraction, stiffness, shape, and surface characteristics—have been identified as key factors governing fracture performance. The following subsections examine in detail how each of these factors influences the mechanical response and crack behavior of concrete.

3.1 Effect of aggregate size

In the previous research, several researchers have shown that the diameter of aggregates had a significant impact on the strength of concrete. For example, Akcaoglu et al. (2004) studied the influence of the coarse aggregate size on the formation of ITZ and subsequently on the failure process of concrete under uniaxial compression by using single spherical steel aggregates of different sizes. In Fig. 1. 6, we can observe that the larger aggregate size decrease the tensile strength of the concrete, and it will strengthen the compressive strength of concrete to a certain extent, but this strengthening effect will be limited as the size increases.

The study conducted by Sim et al. (2013) demonstrated that an excessive increase in aggregate size leads to elevated stresses at the interface between aggregate particles and cement paste. Based on the XMCT analysis, Szczesniak et al. (2013) observed that the cracking pattern in cementitious composites with glass rigid aggregates was strongly dependent on the diameter of the aggregates, with smaller aggregates leading to a different cracking network and potentially influencing the global mechanical behavior of the

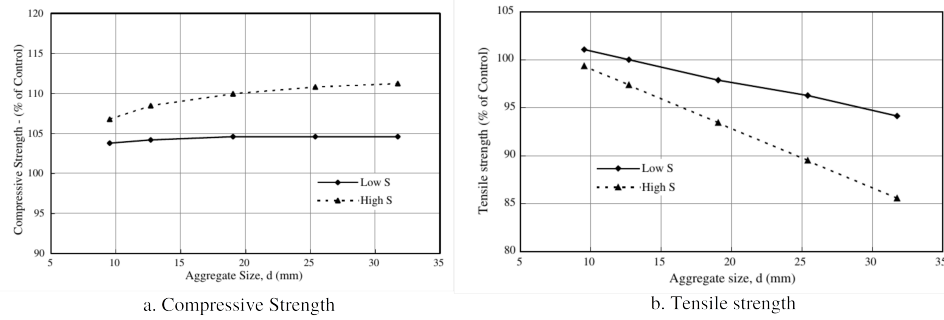


Figure I. 6: Effect of aggregate size on strength of low and high strength concrete (Akcaoglu et al., 2004)

composite under compressive loadings (Fig. I. 7).

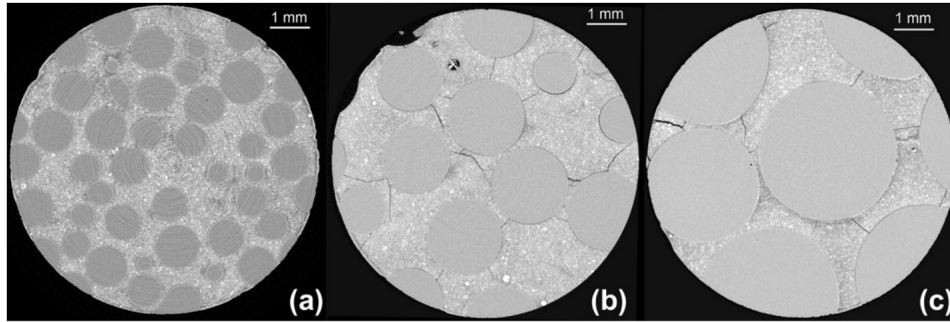


Figure I. 7: Microphotograph of composites after drying: (a) 1mm; (b) 2mm; (c) 4mm (Szczesniak et al., 2013)

3.2 Effect of aggregate rigidity

Aggregates limit the shrinkage of concrete due to temperature changes and moisture variations. The shrinkage of concrete generally decreases as the rigidity of aggregates increase (Zhang et al., 2014). However, this restriction may cause cracks to form during concrete shrinkage. By using the XCMT technique, the effects of aggregate rigidity on drying cracks were studied Li et al. (2020b). The study found that samples with more rigid aggregates showed a greater increase in crack surface compared to samples with less rigid aggregates (Fig. I. 8). This indicates that the rigidity of aggregates affects the formation and propagation of cracks during drying. Vyhlídal et al. (2021) analyses how the rock aggregates affects the mechanical fracture parameters of cement-based composites, such as fracture energy and critical stress intensity factor. They used different types of rocks (limestone, granite, basalt) as aggregates and performs 3-point bending tests on notched

specimens concluding that rock aggregates with higher rigidity and lower porosity lead to higher fracture energy and critical stress intensity factor.

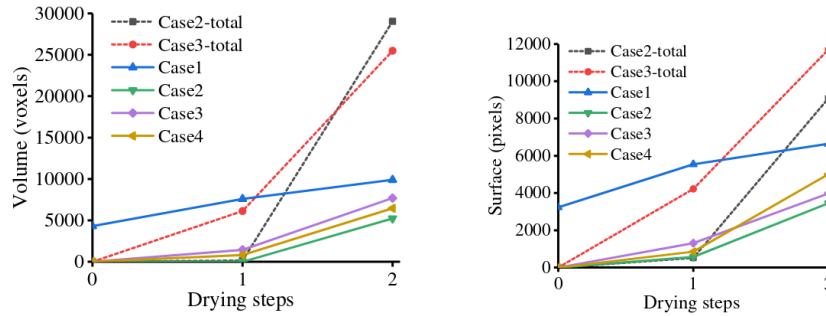


Figure I. 8: Evolution of the volume and area of crack space with drying steps with different rigid aggregate (Li et al., 2020b)

3.3 Effect of aggregate volume fraction

Bisschop and Van Mier (2002) investigated the effect of aggregate volume fraction on drying shrinkage micro-cracking in cement-based composites. They conducted experiments using cement-based composites containing spherical glass particles as aggregates. The micro-cracks were made visible using an impregnation technique and optical microscopy, and crack patterns were quantified using image analysis software. The results show that the quantity of glass spheres (aggregate volume fraction) affects drying shrinkage micro-cracking, with more spheres leading to smaller total crack length for the composites. As the aggregate volume fraction increases, the direction of the cracks becomes more isotropic (Fig. I. 9). Lager aggregate volume fraction resulted in lower maximum micro-cracking depth for the composites with 0.5 mm, 1 mm and 2 mm particles, but larger maximum micro-cracking depth for the composites with 4 mm and 6 mm particles.(Fig. I. 10).

3.4 Effect of aggregate shape

Regarding the influence of aggregate shape on concrete properties, researchers first conducted a qualitative study by comparing aggregates with regular and irregular shape. According to a study by Rocco and Elices (2009), the aggregate shape influences concrete fracture energy, tensile strength and elasticity modulus (Fig. I. 11). Stempkowska et al. (2020) demonstrated that the geometrical parameters of dolomite coarse aggregate have a significant impact on the thermal and mechanic properties of preplaced aggregate concrete. Jiang and Shen (2022); Jiang et al. (2021) investigated the effect of aggregate shape on

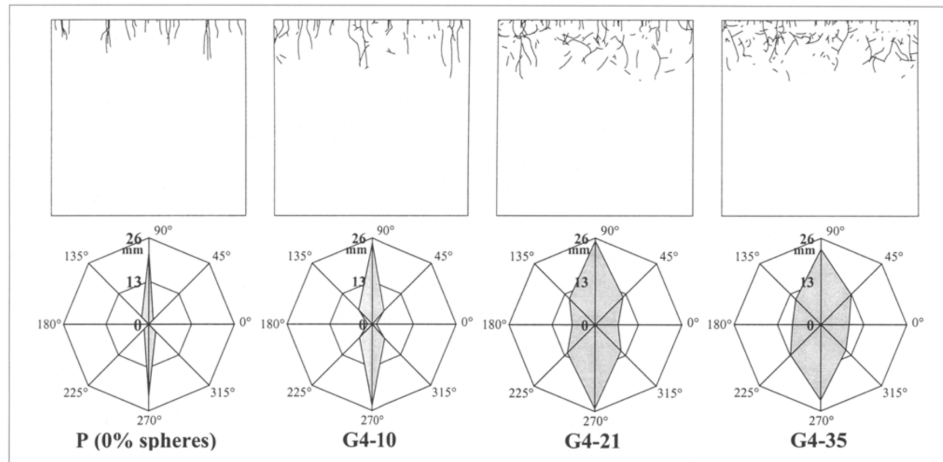


Figure I. 9: Effect of aggregate volume fraction on drying shrinkage micro-cracking for composites and cement paste (Bisschop and Van Mier, 2002)

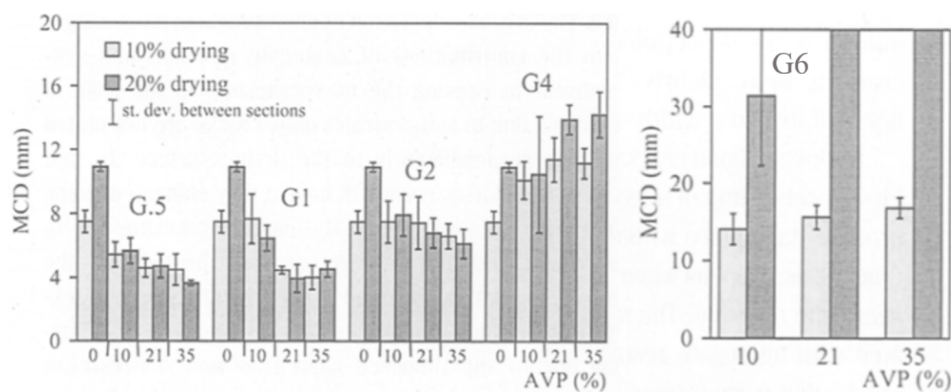


Figure I. 10: Maximum depth of drying shrinkage micro-cracking in cementitious composites and cement paste (Bisschop and Van Mier, 2002)

the cracking characteristics and compressive strength of cementitious mortar under high strain rates. The results show that the shape of the aggregates influences the failure patterns and particle size distribution, with irregular-shaped aggregates leading to more severe failure and smaller particle sizes. The compressive strength of the mortar is lower for irregular-shaped aggregates due to the presence of more ITZs.

In order to obtain a more accurate description of the affect of aggregate shapes on concrete, researchers use some methods for aggregate's shape characterization typically involve the use of global shape parameters derived from projected images (Kwan et al., 1999). One common approach is to use global shape parameters derived from projected images (Fig. I. 12). These parameters include:

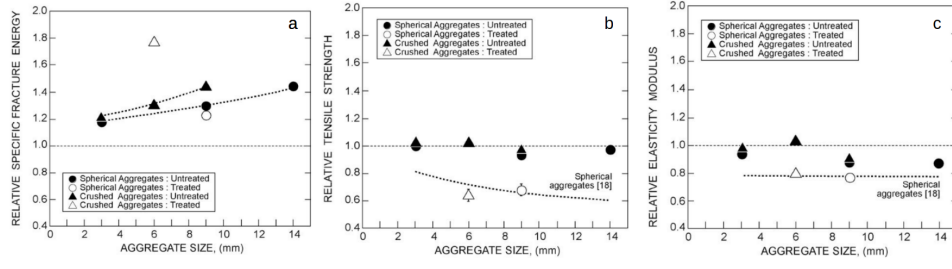


Figure I. 11: Different size spherical and crushed aggregates with different kinds of matrix-aggregate interfaces (a) Relative specific fracture energy; (b) Relative tensile strength; (c) Relative elasticity modulus (Rocco and Elices, 2009)

$$\text{Elongation ratio} = \text{Length} / \text{Width}$$

$$\text{Flakiness ratio } (\lambda) = \text{Thickness} / \text{Width}$$

$$\text{Circularity} = (\text{Perimeter})^2 / (4\pi * \text{Area})$$

$$\text{Rectangularity} = \text{Area} / (\text{Area of bounding rectangular})$$

$$\text{Aspect ratio} = F_{\max} / F_{\min},$$

where $F_{\max}$ and $F_{\min}$ are maximum and minimum Feret Diameter

$$\text{Fullness} = \text{Area} / (F_{\max} * F_{\min})$$

$$\text{Sphericity ratio} = \sqrt[3]{\lambda(\text{Width}/\text{length})}$$

$$\text{Shape factor} = \lambda * \sqrt{(\text{Width}/\text{length})}$$

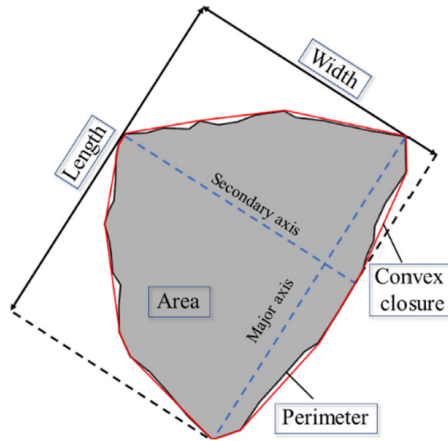


Figure I. 12: Calculated diagram of the aggregate shape properties (Zhou et al., 2019)

These parameters provide information about the approximation of the particle profile to certain geometric shapes, such as circles or rectangles, as well as the similarity of the particle to a sphere.

3.5 Effect of surface characteristics

The ITZ between matrix and aggregate seriously affects bond strength (Königsberger et al., 2014). The characteristics of ITZ depend on surface characteristics of aggregate. For aggregates with well-polished surfaces, the interaction between the two phases is weak. For porous aggregates or aggregates with rough surfaces, hydration products can penetrate into surface cavities, which strengthened the bond between them. Jia and Gu (2021) used a scanning microscope to scan the surface of aggregates in concrete to observe surface morphology. The results showed that the surface morphology components of coarse aggregates were varying at different scanning scales, which included waviness and roughness. The uniaxial compression and direct tension tests were conducted to examine the effects of coarse aggregate surface morphology (CASM) on the mechanical behaviors of concrete. It was found that different surface features affect interface mechanical performance differently. Roughness influences ITZ mechanical properties, while waviness not only expands the actual bonding area but also impacts the mechanical interlocking between the cement matrix and coarse aggregates (Fig. I. 13).

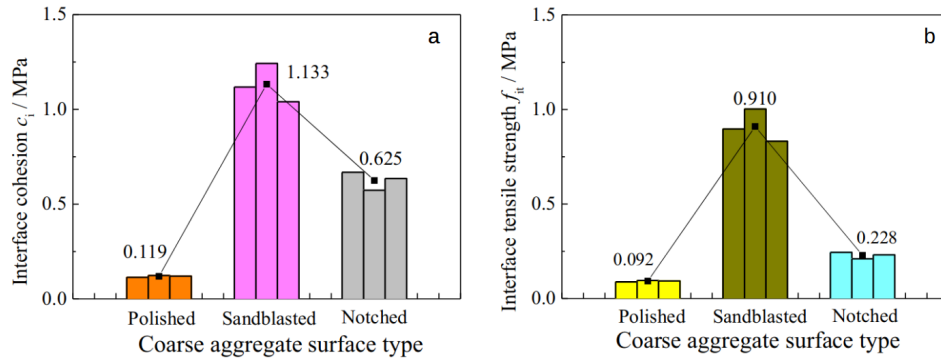


Figure I. 13: (a) The cohesion and (b) the tension strength of interface surface types with different CASMs (Jia and Gu, 2021)

In summary, meso-scale experimental studies have revealed that aggregate-related parameters—such as size, stiffness, volume fraction, shape, and surface characteristics—play critical roles in governing the initiation and evolution of cracks in concrete. These experiments have uncovered key mechanisms of damage localization, energy dissipation, and interface debonding that cannot be captured through purely macro-scale observations. The quantitative insights gained from meso-scale experiments not only deepen our understanding of concrete fracture behavior, but also serve as a valuable foundation for the development and validation of numerical models. These models, informed by experimentally observed mechanisms at the meso-scale, can more accurately simulate crack patterns

and mechanical degradation in concrete under various loading and environmental conditions, thus enabling predictive and mechanism-based design of cementitious materials.

4 Meso-scale modelling of Cementitious materials

Building on these findings, meso-scale modeling provides a complementary framework that extends experimental observations. While experiments reveal fundamental mechanisms, numerical approaches enable systematic parameter variation and controlled exploration of fracture processes under conditions that are difficult to reproduce in the laboratory. Meso-scale modeling and numerical simulation of concrete fracture can be broadly divided into three categories. Continuum-based methods (e.g., FEM, XFEM) describe heterogeneous media within the framework of continuum mechanics (Duarte et al., 2017; Xue et al., 2019). Discontinuum-based methods (e.g., LEM, DEM) explicitly represent aggregates and interfaces as discrete entities, offering a natural description of crack initiation and coalescence (Irazábal et al., 2023; Qu et al., 2020; Wang et al., 2020b). Emerging methods, such as Peridynamics (PD) and the Phase-Field Method (PFM), provide powerful alternatives: PD employs a nonlocal formulation that naturally represents crack initiation and propagation (Silling et al., 2007), while PFM introduces a variational framework to model complex crack patterns within a continuum description (Chen, 2002). These novel approaches provide more flexible and robust frameworks for investigating fracture mechanisms in heterogeneous cementitious composites at the meso-scale. This section presents a review of representative mesoscale modeling methods for concrete, including strategies for mesostructural representation and the selection of appropriate constitutive models.

4.1 Mesoscopic modeling and numerical simulation - Continuous numerical methods

Continuous numerical methods remain the most widely applied approaches for meso-scale simulation of concrete fracture. The FEM provides a flexible framework to capture stress redistribution and nonlinear material response, while the Extended Finite Element Method (XFEM) further enhances this capability by representing crack initiation and propagation independently of the mesh (Ozbolt et al., 2014; Xue et al., 2019; Yang et al., 2024). Within FEM- and XFEM-based frameworks, meso-scale modeling can be considered from two complementary aspects: (1) Representation of material heterogeneity, where aggregates, mortar matrix, and ITZs are explicitly modeled as distinct phases with their own geometric and mechanical properties; and (2) Constitutive description of each phase,

in which appropriate material models—such as linear elasticity for aggregates, damage or plasticity models for the mortar matrix, and cohesive or interface elements for ITZs—are assigned to capture their individual and collective contributions to fracture behavior.

4.1.1 Mesoscale model construction strategies for concrete

At the mesoscale, concrete is typically idealized as a three-phase composite consisting of the mortar matrix, coarse aggregates, and the ITZs. The construction of mesoscale models is a prerequisite for accurately simulating the fracture behavior of cementitious composites. Different strategies have been developed to represent aggregates, mortar matrix, and ITZs, each with its own advantages in terms of geometric realism, computational efficiency, and adaptability to experimental data. Depending on the available information and the targeted level of detail, mesoscale models are generally generated either from experimental imaging data or through parametric and algorithmic descriptions of aggregate geometry. The former emphasizes realism by directly reconstructing the internal structure of concrete, while the latter provides flexibility and computational efficiency for large-scale simulations.

1. Digital image processing based method: This approach reconstructs mesoscale models directly from experimental images, such as optical micrographs or XCT scans. Depending on the available imaging technique, different levels of model fidelity can be achieved. Two-dimensional models can be obtained from thin-section micrographs by image segmentation and thresholding, which allow aggregates and mortar phases to be distinguished in planar representations (Ren et al., 2015). Three-dimensional mesoscale models can be reconstructed from XCT scans, where serial slices are stacked to capture the spatial distribution and connectivity of aggregates. In addition, the external morphology of real aggregates can be scanned using optical or laser-based techniques and subsequently packed into a mortar matrix through placement algorithms to generate realistic concrete models. The main advantage of these image-based methods is their ability to realistically capture the size, shape, and orientation of aggregates as well as the heterogeneity of the surrounding mortar. However, they are computationally expensive and strongly dependent on imaging resolution and sample preparation quality (Jiang et al., 2023; Liu et al., 2018).

2. Parametric generation method: In parametric approaches, aggregates are represented using simplified but representative geometric shapes. Commonly adopted forms include ellipsoids, spheres, convex polyhedra, and other regular polygons. These idealized

geometries enable systematic control of particle size, volume fraction, and orientation. Representative examples of such 2D and 3D parametric aggregate models are shown in Fig. I. 14.

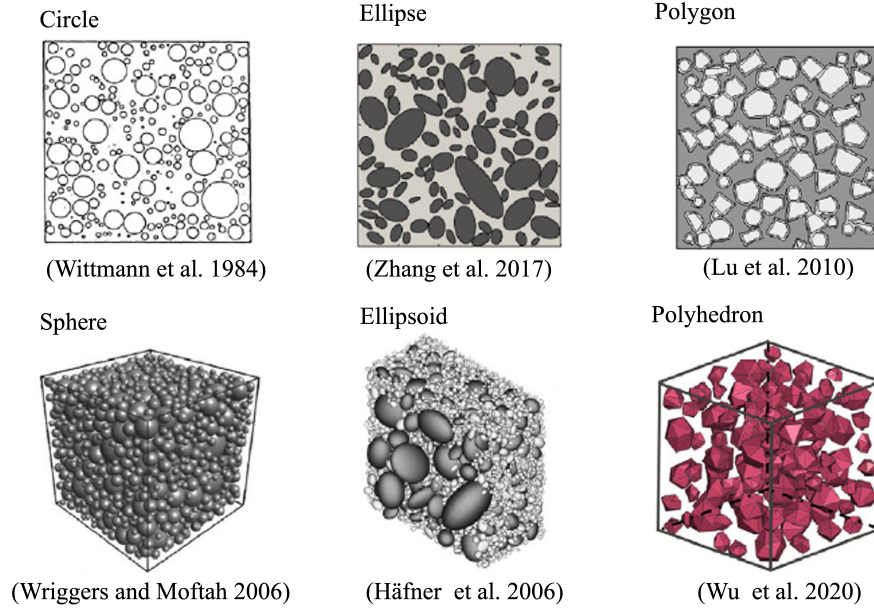


Figure I. 14: Typical 2D/3D parametric models representing coarse aggregates in concrete (Häfner et al., 2006; Lu et al., 2010; Wittmann et al., 1985; Wriggers and Moftah, 2006; Wu et al., 2020; Zhang et al., 2017b)

Beyond these idealized shapes, more advanced parametric strategies employ Voronoi (tessellated) polyhedra. In this approach, the modeling domain is partitioned into space-filling convex cells through Voronoi tessellation, where each cell corresponds to the region closest to a randomly distributed seed point. By selecting and scaling cells according to the target particle size distribution, aggregates with angular morphologies closer to real particles can be generated. The examples of Voronoi-based aggregate generation is shown in Fig. I. 15. Compared with regular ellipsoids or polyhedra, the Voronoi-based method more effectively reproduces the angularity and randomness of natural aggregates, thereby improving the fidelity of mesoscale representations. Owing to these advantages, Voronoi tessellations have been widely applied in mesoscale modeling to reproduce aggregate interlocking and realistic crack paths (Bayar and Bilir, 2023; Li et al., 2020a). Compared with image-based reconstruction, parametric methods—particularly those enhanced by Voronoi tessellations or irregular polyhedra—provide a balance between computational efficiency and geometric realism, making them suitable for large-scale simulations and systematic

parametric studies.

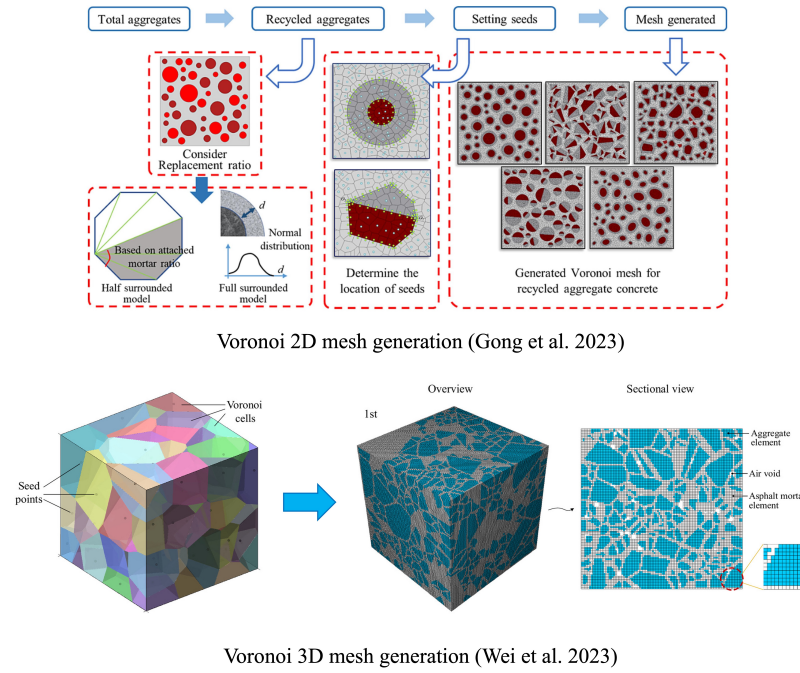


Figure I. 15: Voronoi tessellation-based mesh generation for concrete aggregates (Gong et al., 2023; Wei et al., 2023)

4.1.2 ITZ geometry generation

In mesoscale numerical models, the ITZ is usually treated as a distinct phase due to its weaker mechanical properties compared to the bulk mortar. The ITZ is a thin region surrounding aggregates. This region is characterized by higher porosity, lower hydration degree, and increased microcrack density, which together make it mechanically weaker and more brittle than either the aggregates or the bulk mortar. Experimental observations have consistently shown that cracks often initiate or propagate preferentially along ITZs, highlighting their decisive role in determining the fracture behavior of concrete. Consequently, an accurate representation of ITZ geometry and constitutive response is essential in mesoscale modeling, as it directly governs damage localization, aggregate–mortar debonding, and the overall macroscopic strength and toughness of concrete (Xu et al., 2022). A number of strategies have been developed to represent ITZ geometry and its mechanical behavior, which can be broadly summarized as follows:

- **Explicit thin-layer modeling:** The ITZ is modeled as a separate concentric layer surrounding each aggregate, typically with a thickness of 20–100 μm (Gu et al.,

2015). This approach provides a direct representation of ITZ geometry and allows the use of specific constitutive laws for the interfacial zone. However, because the real ITZ thickness is much smaller than typical finite element sizes, directly resolving such thin layers would lead to prohibitively fine meshes and high computational cost. For this reason, most mesoscale studies adopt an enlarged ITZ thickness, often several times greater than the physical value, to maintain computational efficiency while still reflecting the mechanical weakening effect of the ITZ (Du et al., 2014; Feng et al., 2022; Wu et al., 2021).

- **Interface or joint elements:** Instead of meshing a thin ITZ layer, cohesive zone models (CZMs) or zero-thickness interface elements can be inserted between aggregates and mortar. These elements follow traction–separation laws and are particularly effective for simulating crack initiation, debonding, and progressive failure along interfaces. Cohesive formulations are more computationally efficient than explicit thin layers, as they avoid excessive mesh refinement, but they require careful calibration of fracture energy and stiffness parameters (Chen et al., 2022b; Wu and Wriggers, 2015; Zhang et al., 2021).
- **Enrichment scheme in XFEM:** The ITZ can be treated through enrichment functions that allow displacement discontinuities to occur independently of the mesh. The aggregate–mortar boundary is represented as an internal interface where special enrichment functions account for debonding. This enables crack initiation and propagation along ITZs without remeshing and provides higher efficiency for large-scale simulations, though it requires more complex numerical implementation (Deng et al., 2022; Sukumar et al., 2004; Yu et al., 2010).

Overall, the choice of ITZ modeling strategy in FEM/XFEM depends on the desired trade-off between geometric fidelity and computational efficiency. Explicit ITZ layers are more realistic, while interface/joint element approaches are more practical for large-scale simulations.

4.1.3 Constitutive model for different phases

Each phase of concrete exhibits distinct mechanical properties and failure mechanisms, which need to be properly characterized in numerical models in order to reproduce its heterogeneous fracture behavior. The mortar phase controls the overall stiffness of the composite and serves as the primary medium for microcrack initiation and growth. Aggregates contribute strength and rigidity, governing crack deflection and load transfer across the

material. The ITZs, in contrast, act as preferential weak regions where cracks frequently nucleate and propagate. To capture these diverse roles, different constitutive formulations are typically assigned to each phase, ranging from simple linear elasticity to more advanced damage–plasticity or cohesive models, depending on the required balance between fidelity and computational efficiency. The following subsections summarize representative constitutive models for the mortar, aggregate, and ITZ phases in mesoscale simulations.

1. Mortar phase: At the mesoscale, the mortar matrix represents the continuous phase that binds aggregates together and plays a dominant role in overall stress transfer and crack development. Its constitutive behavior is typically modeled using linear elasticity in the pre-cracking regime, followed by nonlinear softening to capture tensile cracking and compressive crushing. Various constitutive models have been employed, including continuum damage mechanics models (Mazars and Pijaudier-Cabot, 1989; Sun and Xu, 2022) and plastic–damage formulations (Chen et al., 2010; Wang et al., 2020a). Among these, the Concrete Damage Plasticity (CDP) model, originally proposed by Lubliner et al. (1989) and later extended by Lee and Fenves (1998), has been widely applied in mesoscale FEM simulations. The CDP model combines isotropic damage with non-associated plasticity, enabling the description of both tensile cracking and compressive crushing, and remains one of the most popular constitutive laws for mortar due to its balance between accuracy and computational efficiency. Many researchers have employed the CDP model to simulate mesoscale fracture processes of concrete under different loading conditions (Naderi et al., 2021; Thirumalaiselvi et al., 2019; Zheng et al., 2023; Zhou et al., 2019), as shown in Fig. I. 16. However, a notable limitation of the CDP model is that damage is represented only through the degradation of stiffness, without explicitly resolving discrete cracks. As a result, it cannot accurately capture crack paths, branching, or the localized geometry of fracture surfaces, which restricts its ability to provide detailed information on mesoscale crack morphology.

2. Aggregate phase: Coarse aggregates are typically considered the stiffest and strongest phase in concrete. At the mesoscale, they are most often represented as linear elastic and isotropic materials, given their significantly higher stiffness compared to mortar and ITZ (Liu et al., 2018; Mazzucco et al., 2018). This assumption simplifies numerical modeling while still reproducing the stress-bridging and crack-deflection effects induced by aggregates. In some studies, aggregates are further assumed to be brittle, with damage or fracture criteria applied to capture aggregate cracking under extreme loading conditions (Wu et al., 2020).

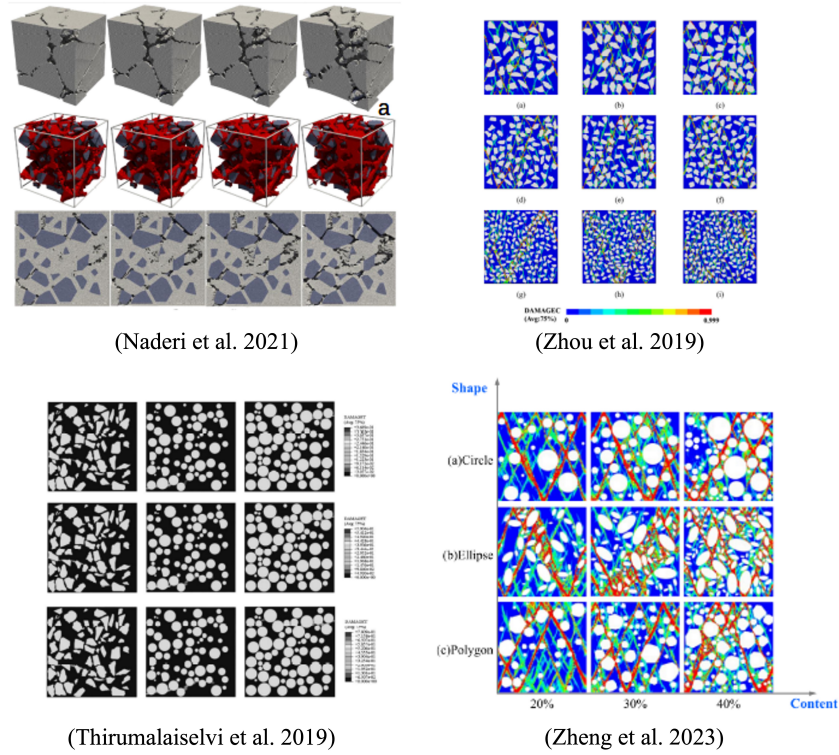


Figure I. 16: Simulation results about the effect of aggregate properties on concrete fracture by using CDP model under FEM method (Naderi et al., 2021; Thirumalaiselvi et al., 2019; Zheng et al., 2023; Zhou et al., 2019)

3. ITZ phase: Three main categories of constitutive descriptions are commonly used. First, elastic-damage models assign reduced elastic modulus and tensile strength to ITZ elements to account for their weakness, often combined with strain-softening laws calibrated against micromechanical tests (Häfner et al., 2006; Yan et al., 2016). Second, CZM represent ITZ by traction–separation relations that capture progressive debonding and crack opening (Caballero et al., 2006; Wu and Wriggers, 2015). More advanced formulations have introduced nonlinear fracture energy dependence or rate effects to capture ITZ performance under dynamic or environmental loading (Lu et al., 2010).

4.2 Mesoscale modeling and numerical simulation - Discrete element method

The Discrete Element Method (DEM) is a powerful numerical approach used to simulate the behavior of materials and systems where discontinuities, such as cracks and fractures, play a crucial role (Lisjak and Grasselli, 2014). DEM is particularly well-suited

for modeling brittle materials like concrete, where traditional continuum-based methods may struggle to capture complex failure mechanisms. Within this method, equilibrium forces and displacements of a group of particles are determined through a calculation that traces the movements of these particles or elements. In concrete modeling, these elements often correspond to aggregates, cement matrix, and ITZ. Each element follows Newton's laws of motion, where the interactions between elements are governed by contact models that can account for normal, tangential, and rotational forces, as well as bonding between particles (Beckmann et al., 2012).

4.2.1 Generation of mesoscale models

In the DEM, aggregates can be represented at different levels of geometric fidelity. The simplest approach uses a single particle to depict one aggregate (Nitka and Teichman, 2015), while more advanced strategies adopt a clump of bonded rigid particles or a cluster of smaller particles to mimic irregular aggregate shapes (Wang et al., 2020b).

1. Single particle representation of aggregates: In this approach, each aggregate is modeled as a single spherical or circular particle. This method provides a simple and computationally efficient way to generate concrete mesoscale models, as illustrated in Fig. I. 17(a). Although it cannot capture the angularity or irregular geometry of real aggregates, it is suitable for large-scale simulations where computational cost is a concern, or for parametric studies where only the statistical effect of aggregate size and volume fraction is of interest (Nitka and Teichman, 2015).

2. Cluster of particles representation of aggregates: To reproduce the irregularity and angularity of real aggregates, aggregates can be modeled as a clump or cluster of bonded particles. In this scheme, each aggregate is constructed by grouping multiple spherical particles that are rigidly or elastically bonded together, thus approximating polyhedral or irregular shapes, as shown in Fig. I. 17(b). This approach significantly improves the fidelity of DEM models in terms of stress transfer, crack deflection, and interlocking effects, albeit at a higher computational cost (Wang et al., 2020b).

4.2.2 Constitutive model in discrete element method

In DEM, the constitutive behavior of concrete is described at the particle–particle contact level rather than through continuum constitutive equations as in FEM. The macroscopic response of the material emerges from the interaction of large numbers of particles,

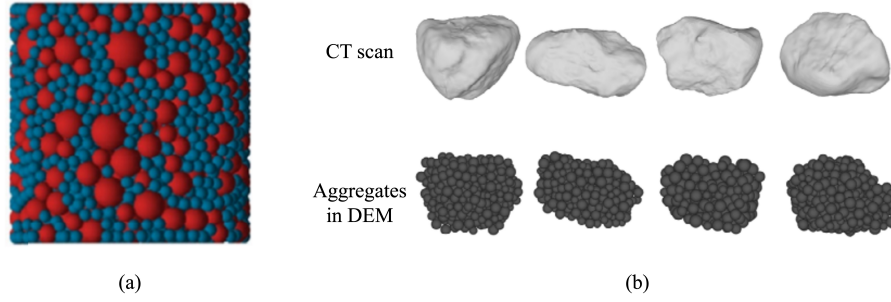


Figure I. 17: Generation of mesoscale DEM models: (a) single-particle representation of aggregates (Nitka and Tejchman, 2015), and (b) cluster-of-particles representation (Wang et al., 2020b).

making the choice of contact law critical. Several representative contact models have been widely applied in mesoscale DEM simulations of concrete.

Bonded-particle model (BPM): The BPM represents rock-like materials as a dense assembly of non-uniform circular or spherical particles bonded at their contact points. These bonds are capable of transmitting normal, shear, bending, and torsional forces, thereby capturing the microstructural interactions between grains (Potyondy and Cundall, 2004). A key advantage of BPM is its ability to replicate both the granular microstructure and the emergent macroscopic behavior of rock-like materials, including plasticity and viscoelastic responses under various loading conditions. However, this realism comes at the expense of high computational cost and the need for extensive parameter calibration (Ren et al., 2018; Song et al., 2019).

Parallel bond model (PBM): The PBM is a specific implementation of the BPM and has been extensively employed in mesoscale simulations of concrete (Potyondy and Cundall, 2004). In this formulation, each particle contact is represented by an elastic spring operating in parallel with a bonding element. The parallel bond is capable of transmitting normal and shear forces as well as bending and torsional moments, thereby reproducing the mechanical effects of mortar bridges or interfacial bonding between aggregate particles. When the bond strength is exceeded, failure occurs and the interaction reduces to a simple linear elastic frictional contact. This transition enables DEM to naturally reproduce the processes of crack initiation, growth, and coalescence within cementitious composites (Huang et al., 2022; Shen et al., 2022; Zhou et al., 2023).

Building on the classical BPM and its parallel-bond implementation, numerous exten-

sions of DEM have been developed through improvements in contact algorithms and the incorporation of different failure criteria. These advancements include models that allow for more realistic representation of inter-particle bonding (e.g., flat-joint models), cohesive contact formulations that embed traction–separation laws, and hybrid approaches that introduce rate-dependence or damage–plasticity at contacts (Li et al., 2022b). Such modifications enhance the capability of DEM to reproduce complex fracture processes in concrete, including crack initiation, propagation, and coalescence across mortar, aggregates, and ITZs, thereby bridging the gap between idealized particle bonding and experimentally observed meso-scale behavior (Mazzucco et al., 2021). Calibration of DEM parameters (stiffnesses, bond strengths, friction coefficients) is essential since they cannot be directly measured from experiments. Typically, mesoscale DEM models are calibrated against macroscopic test results such as uniaxial compression, Brazilian splitting, or three-point bending tests. Despite simplifications, DEM constitutive laws are powerful in capturing fracture processes governed by aggregate–mortar interactions.

In summary, while FEM and XFEM provide accuracy in stress analysis, their difficulty in capturing displacement discontinuities limits their efficiency in fracture simulations. DEM naturally describe discrete cracking but depend heavily on parameter calibration. These limitations have spurred the development of emerging approaches, like Peridynamics, which offer nonlocal and variational frameworks capable of simulating complex crack initiation, branching, and coalescence at the mesoscale. The following section reviews Peridynamics methods and their applications in concrete fracture analysis.

4.3 Mesoscopic modeling and numerical simulation – Peridynamic method

Peridynamics (PD) is a nonlocal solid mechanics theory originally proposed by Silling (2000) to overcome the limitations of classical continuum mechanics in dealing with singularities and displacement discontinuities. Unlike the partial differential form of classical theory, PD reformulates the governing equations as spatial integral expressions, which inherently allow for the natural initiation, propagation, branching, and coalescence of cracks. In PD, the computational domain is discretized into a set of material points that interact within a finite horizon through bonds, as illustrated in Fig. I. 18. These bonds transmit forces based on relative displacements, enabling the direct incorporation of nonlocal effects into the material response.

Applications of PD in concrete fracture have demonstrated its ability to capture complex failure processes across scales. For example, Gerstle et al. (2007) and Huang et al. (2011) incorporated strength-based failure criteria to simulate concrete fracture under

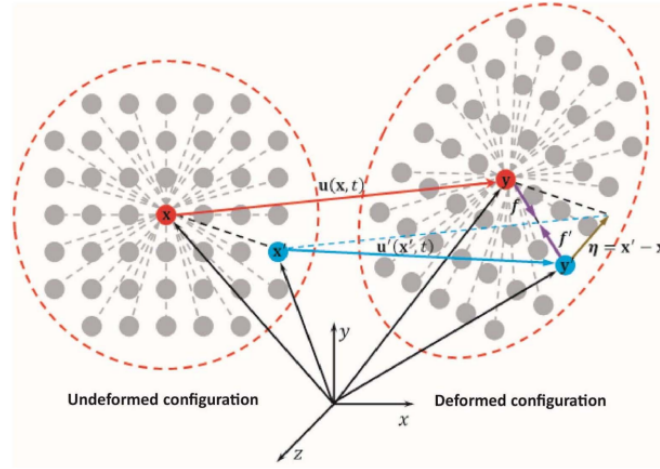


Figure I. 18: Principle of peridynamic theory in reference and deformed configurations.

various loading conditions. Wang et al. (2017) extended the framework by introducing conjugated bond interactions, accounting for both bond stretch and bond rotation, to model crack propagation and coalescence in pre-flawed concrete specimens under compression. Gu et al. (2016) further developed a peridynamic approach to simulate the dynamic fracture behavior of concrete disks in SHPB tests, achieving good agreement with experimental observations (Fig. I. 19).

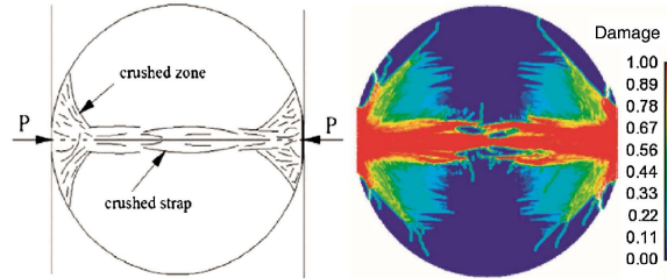


Figure I. 19: Peridynamic simulation of dynamic fracture in concrete Brazilian disk tests (Gu et al., 2016).

At the mesoscale, PD has been increasingly applied to explicitly account for heterogeneities in cementitious composites. For instance, (Jin et al., 2021, 2023) investigated the influence of aggregate stiffness and size on drying-shrinkage-induced cracking, demonstrating the ability of PD to reproduce realistic crack initiation and propagation patterns in heterogeneous microstructures (Fig. I. 20). Such studies highlight the potential of PD as a multiscale modeling tool for cementitious materials, bridging microscopic damage

mechanisms with macroscopic fracture behavior.

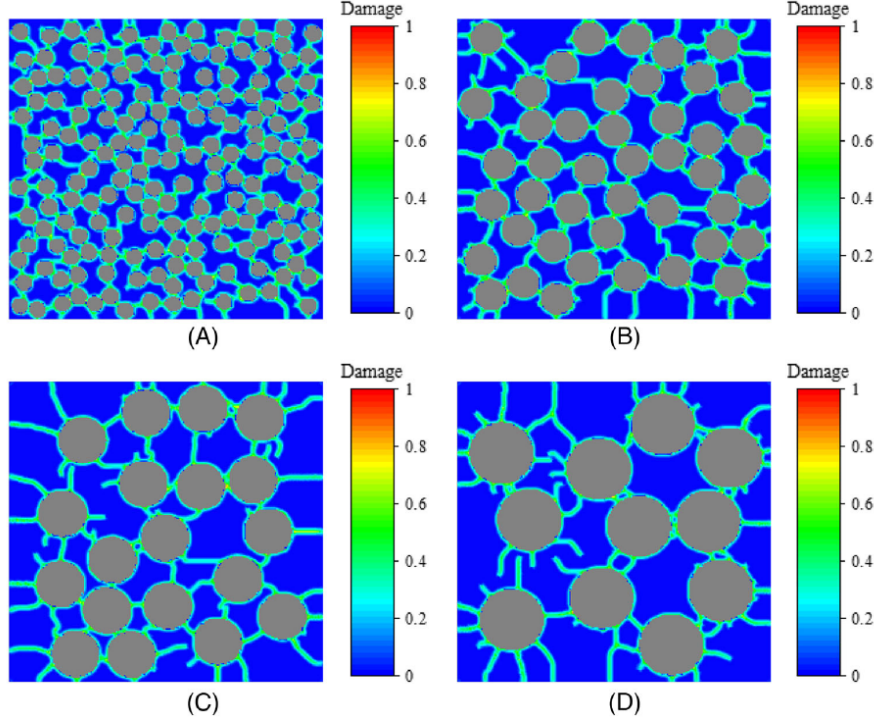


Figure I. 20: Mesoscale peridynamic simulation of drying-shrinkage cracking in concrete (Jin et al., 2023).

4.3.1 Generation of mesoscale models

The generation of mesoscale models is a prerequisite for applying peridynamics to concrete fracture analysis, as it determines how heterogeneity is represented in the numerical domain. Similar to FEM- or DEM-based approaches, mesoscale peridynamic models of concrete are typically constructed using either image-based or parametric methods. In image-based approaches, high-resolution experimental data, such as XCT or optical microscopy, are employed to directly reconstruct aggregate shapes, orientations, and spatial distributions. This provides a high degree of realism in terms of aggregate–mortar–ITZ morphology, enabling direct validation against experimental observations. However, image-based PD models are computationally demanding due to the large number of material points required to discretize complex geometries. In contrast, parametric approaches approximate aggregates using idealized geometries such as spheres, ellipsoids, convex polyhedra, or Voronoi-based tessellations. These methods enable efficient generation of statistically representative aggregate distributions that satisfy prescribed

particle size distributions and volume fractions. Compared to image-based reconstructions, parametric models are computationally more efficient and well-suited for large-scale simulations, though they inevitably sacrifice some geometric realism. Moreover, because the discretization size in peridynamics must be chosen in relation to the nonlocal interaction horizon, most mesoscale PD studies adopt uniform grids for model construction, which ensures consistency between horizon definition and particle spacing while simplifying numerical implementation (Madenci and Oterkus, 2016; Peng et al., 2025).

For ITZ modeling in mesoscale PD, two strategies are commonly adopted: (1) explicit discretization of the ITZ as a thin layer of peridynamic material points surrounding each aggregate, often with artificially enlarged thickness to avoid excessive discretization cost (Dong et al., 2021); and (2) modification of bond parameters between aggregate and matrix to implicitly represent weaker ITZ behavior (Geng et al., 2025; Jin et al., 2021). The choice between explicit and implicit approaches depends on the desired balance between accuracy and efficiency.

4.3.2 Different types of peridynamic methods for concrete

Over the past two decades, several peridynamic (PD) formulations have been developed and applied to model the complex fracture behavior of concrete, including bond-based peridynamics (BB-PD), ordinary state-based peridynamics (OSB-PD), and non-ordinary state-based peridynamics (NOSB-PD). Each formulation offers specific advantages and limitations in terms of computational efficiency, constitutive flexibility, and ability to capture heterogeneous fracture processes.

1. Bond-based peridynamics (BB-PD): The bond-based PD (BB-PD), originally introduced by Silling (2000), is the simplest formulation, in which material points interact through pairwise bonds that act as independent springs. As shown in Fig. I. 21(a), the bond force is always collinear with the relative position vector of the interacting particles, meaning that only axial deformation (stretch) is transmitted through the bond. Bond breakage is used to represent crack initiation and growth. Owing to its simplicity and ease of implementation, BB-PD has been widely used for simulating fracture in brittle cementitious materials (Gerstle et al., 2007; Huang et al., 2011). However, BB-PD suffers from a fundamental limitation: the Poisson's ratio is restricted to fixed values ($1/4$ in 3D and $1/3$ in 2D), making it unsuitable for modeling general elastic responses of concrete. To overcome this limitation, extensions such as conjugate BB-PD models (Zhang et al., 2023b) and improved formulations (Li et al., 2025) have been proposed to account for

more realistic concrete fracture processes.

2. Ordinary state-based peridynamics (OSB-PD): The ordinary state-based PD (OSB-PD) was developed to overcome the fixed Poisson's ratio limitation of BB-PD. In OSB-PD, the force density vector depends not only on the relative position vector but also on the collective deformation of all bonds within the horizon, as shown in Fig. I. 21(b). Although the force remains parallel to the relative position vector, its magnitude is influenced by the overall deformation state, which allows OSB-PD to reproduce classical linear elasticity with arbitrary Poisson's ratios. This formulation also supports more flexible constitutive laws (Silling et al., 2007). For concrete, OSB-PD has been applied to simulate crack branching, aggregate–mortar debonding, and multiaxial fracture responses (Wu et al., 2020; Zhang et al., 2017b). Compared with BB-PD, OSB-PD provides more accurate mechanical responses, though at a higher computational cost due to the need for more complex constitutive evaluations.

3. Non-ordinary state-based peridynamics (NOSB-PD): The non-ordinary state-based PD (NOSB-PD) further generalizes the theory by removing the constraint that the force vector must be parallel to the bond direction, as shown in Fig. I. 21(c). In this framework, the force vector can take arbitrary directions depending on the constitutive state, enabling a direct correspondence with classical continuum mechanics, including full tensorial stress and strain measures. This flexibility allows NOSB-PD to incorporate complex constitutive models such as plasticity, viscoelasticity, or coupled thermo-hydro-mechanical effects (Amani et al., 2016; Madenci et al., 2022). For concrete, NOSB-PD has been used to investigate crack coalescence, mixed-mode fracture, and the influence of loading rate on dynamic fracture properties (Lu et al., 2019; Yang et al., 2023, 2021). Its versatility makes it particularly suited for modeling concrete subjected to complex multiscale and multiphysics loading condition, though at the expense of the highest computational cost among PD formulations.

4.3.3 Recent advances and hybrid approaches

Beyond the classical BB-PD, OSB-PD, and NOSB-PD formulations, recent studies have introduced hybrid or improved peridynamic models for concrete. Examples include coupled PD–FEM frameworks for computational efficiency (Sun et al., 2023), and multi-scale coupling approaches where PD is applied locally to regions of interest (e.g., crack zones) while FEM or DEM is used elsewhere (Liu et al., 2023). Such advances highlight

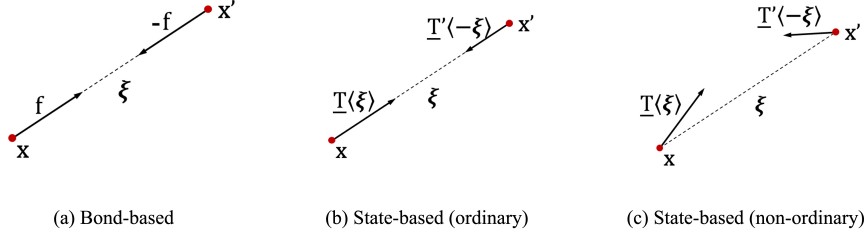


Figure I. 21: Different types of peridynamic methods and the characteristics of bond forces: (a) BB-PD; (b) OSB-PD; (c) NOSB-PD

the growing maturity of PD for concrete fracture modeling and its integration into broader multiscale and multiphysics simulation frameworks.

Overall, the choice of peridynamic formulation for concrete depends on the balance between computational efficiency and constitutive flexibility. BB-PD remains useful for brittle fracture in simple domains, OSB-PD offers improved elastic representation and meso-scale crack simulation, and NOSB-PD provides the most general framework for multiphysics and complex loading conditions.

5 Conclusions

Mesoscale studies have shown that aggregates and ITZs strongly govern crack initiation, propagation, and coalescence in concrete, with aggregates influencing stress redistribution and crack deflection, while ITZs act as preferential weak zones. These experimental insights provide critical benchmarks for validating numerical models.

Among numerical strategies, FEM and XFEM remain widely used for meso-scale simulations but face difficulties in explicitly describing displacement discontinuities. DEM naturally captures crack initiation and coalescence through particle interactions, though at the cost of extensive parameter calibration. Peridynamics offers a promising alternative: its nonlocal formulation inherently accommodates discontinuities and heterogeneous fracture without remeshing.

Overall, the state of art demonstrates progress in mesoscale fracture modeling but highlights persistent challenges in balancing geometric realism with computational tractability and bridging length scales. Peridynamics provides a powerful framework to address these challenges. Building on these insights, the present study employs an advanced peridynamic framework to investigate the influence of aggregate shape and surface characteristics on drying shrinkage-induced cracking in concrete.

Chapter II

Experiment Analysis of Inclusion Properties on Concrete Drying Fractures

1 Introduction

In this part, the focus is placed on the role of aggregate properties in controlling drying shrinkage-induced cracking in cementitious composites. As discussed in the state of the art, inclusions with different stiffness, size, shape and surface characteristics exhibit distinct effects on crack initiation and propagation. In concrete, due to the great variability of inclusion properties, and the complex interaction between inclusions and the cement matrix, it is challenging to isolate the mechanisms governing crack formation. To gain clearer insight, it is therefore useful to adopt simplified material systems in which selected aggregate parameters can be varied systematically. Based on this approach, the present study considers the influence of inclusion stiffness, size, and surface roughness on drying shrinkage cracking.

This chapter is organized as follows. First, a summary of previous experimental studies reported in [Li et al. \(2020b\)](#) and [Jin et al. \(2023\)](#) is provided, in which the influence of inclusion stiffness and size on drying shrinkage-induced cracking in cementitious composites was investigated. Building on the methodology and findings of these studies, and considering the additional effects of other aggregate properties on concrete behavior, the present work extends the analysis to examine the role of inclusion surface roughness on the morphology of shrinkage-induced cracks. The sample preparation procedure, experimental setup, and testing program are then described in detail, followed by quantitative

observations of the resulting crack patterns. The attempts to customize aggregate shape in order to investigate its role in crack evolution are presented.

2 Effect of inclusions rigidity

In this section, the experimental study and main findings of [Li et al. \(2020b\)](#) are presented. The primary objective of this work was to investigate the influence of inclusion rigidity on drying shrinkage-induced cracking in cementitious composites.

2.1 Sample preparation and experimental program

A typical CEM I 52.5 cement was used in accordance with European standards. The water-to-cement ratio (W/C) was fixed at 0.5, and the volume fraction of inclusions was set to 40%. Five types of artificial aggregates (inclusions) with different stiffness were employed: zirconium, titanium, glass, polyamide, and polyoxymethylene (see Fig. II. 1). Accordingly, five groups of composite samples were prepared. All inclusions were manufactured as smooth, spherical particles in order to minimize bonding at the interfaces between the cementitious matrix and the inclusions. The sphere diameter was chosen as 2 mm to ensure that crack openings would be sufficiently large to be detected with the available microtomography resolution of $7\ \mu\text{m}$. The inclusion volume fraction was fixed at 40% for all composites. To fit within the field of view of the camera used in the microtomographic analysis, cylindrical specimens with a diameter of 8 mm and a height of 15 mm were fabricated. The main properties of inclusions (density, Young's modulus, Poisson's ratio, Hardness, thermo-hydric properties) are given in the II. 1.

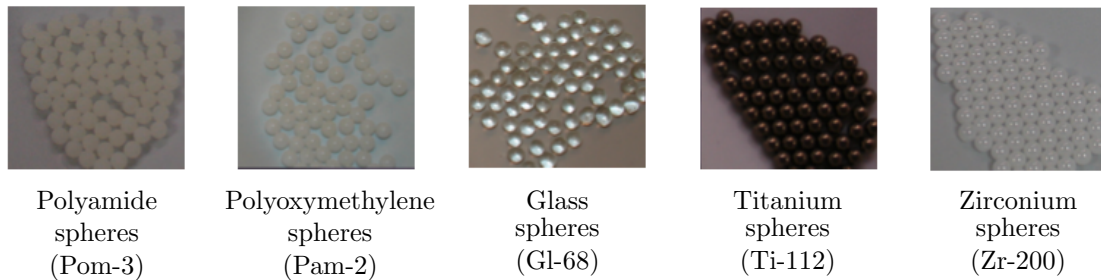


Figure II. 1: Inclusion with different rigidity used in this study

All samples were first cured in a lime-saturated solution at approximately $20\ ^\circ\text{C}$ to ensure proper hydration of the cement matrix and full water saturation. To accelerate the drying process and promote shrinkage-induced cracking, two successive accelerated drying steps under high moisture gradients were applied. In the first step, the fully saturated

specimens were placed in a climate chamber at a relative humidity (RH) of 12% and a temperature of 20 °C for 30 days, until mass stabilization was achieved. In the second step, the temperature was increased to 105 °C and maintained for about 20 days, after which the samples were cooled back to 20 °C.

2.2 Experimental results

The microstructural evolution and cracking patterns of dried samples were examined using X-ray microtomography (Limodin et al., 2013). Images were acquired at saturation, after the first drying step, and after the second step following cooling. Due to equipment limits, scans could not be performed at a constant 105,°C; thus, thermal expansion effects were not isolated, and no images were available at the start of the second stage. Quantitative crack analysis of stage2 was therefore not possible for Pam-2 and Pom-3. For Gl-68, Ti-112 and Zr-200, the low mismatch in thermal expansion with cement paste allows thermal effects to be considered negligible. Full 3D images were obtained, but only representative mid-height cross-sections are presented in Table II. 2. For samples with zirconium (Zr-200) inclusions, low matrix–aggregate contrast prevented clear crack reconstruction, and they are not presented in Table II. 2.

As drying progresses, an increasing number of cracks are observed in all specimens. The crack patterns of Pam-2 and Pom-3 differ from the others due to the water absorption and high thermal expansion of their inclusions. In the other cases, cracking develops in two dominant forms: (1) debonding at the matrix–inclusion interface and (2) radial cracks emanating from inclusions that link adjacent particles. Overall, the cracking behavior strongly depends on inclusion type. Moisture loss induces gradients in shrinkage, and rigid inclusions restrain the free deformation of the matrix. This restraint generates radial and tangential stresses around inclusions, producing both radial and interfacial microcracks. The intensity of these local effects increases with the Young’s modulus of the inclusions.

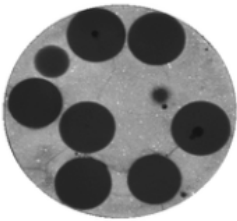
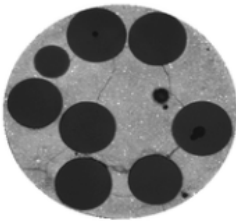
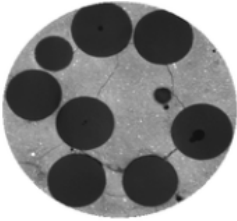
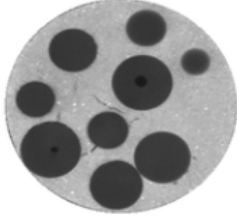
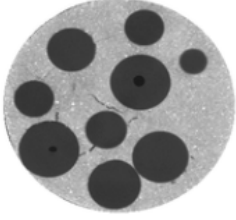
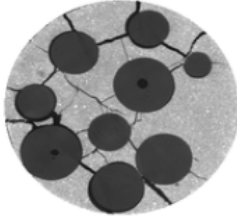
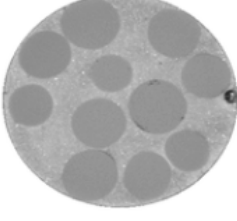
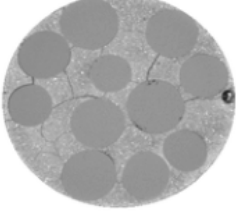
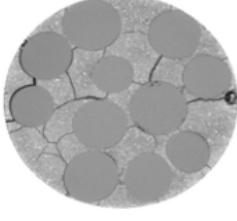
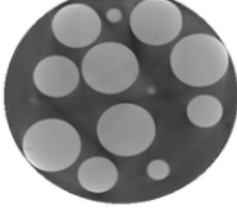
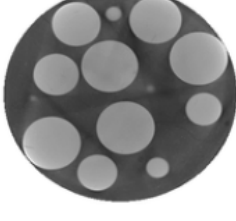
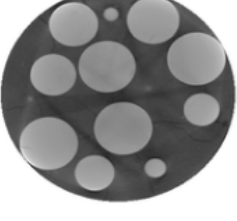
Table II. 1: Parameters for different materials of inclusions

Material	Polyamide	Polyoxymethylene	Glass	Titanium	Zirconium
Density (g/cm ³)	<u>1.14</u>	<u>1.40</u>	<u>2.50</u>	<u>4.45</u>	<u>6.05</u>
Young's modulus (GPa)	1.70–2.00	2.40–2.80	<u>68</u>	<u>112</u>	<u>200</u>
Hardness**	<u>100D</u> 78–121HRR 85–180 MPa BIH	<u>80D</u> 69–121HRR 30–179 MPa BIH	<u>465–585HK</u> 450–550HV	<u>28–42HRC</u> 290–420HV	<u>1100HV</u>
Coefficient of linear thermal expansion (10 ⁻⁶ /°C)	70–100	80–100	<u>9.6</u>	8.9	<u>10</u>
Thermal conductivity (W·m ⁻¹ ·K ⁻¹)	0.2–0.3	0.2–0.31	1	16	<u>2</u>
Water absorption	2–4%	0.25%	–	–	–
Poisson's ratio	0.38–0.45	0.35–0.43	0.17–0.25	0.26–0.34	0.23–0.32

* The underlined numbers are provided by the material production company; the others are compiled from literature/databooks for reference.

** HK: Knoop; D: Shore Durometer; HV: Vickers; HB: Brinell; HR: Rockwell; BIH: Ball Indentation Hardness. These methods measure different material responses; no unique exact conversion exists (only empirical relations).

Table II. 2: Reconstructed images of representative cross-sections in different samples at different steps of drying [Li et al. \(2020b\)](#)

	Saturated (T=20 °C)	Drying, end of step 1 (T=20 °C, RH=12%)	Drying, end of step 2 (T=105 °C)
Pam-2			
Pom-3			
Gl-68			
Ti-112			

In samples with higher Young’s modulus, crack surfaces increase markedly with inclusion stiffness, especially under severe drying at 105 °C. As shown in Fig. II. 2, this trend is evidenced by the titanium composite, which exhibits more numerous fine cracks and a greater cumulative crack length than the glass composite.

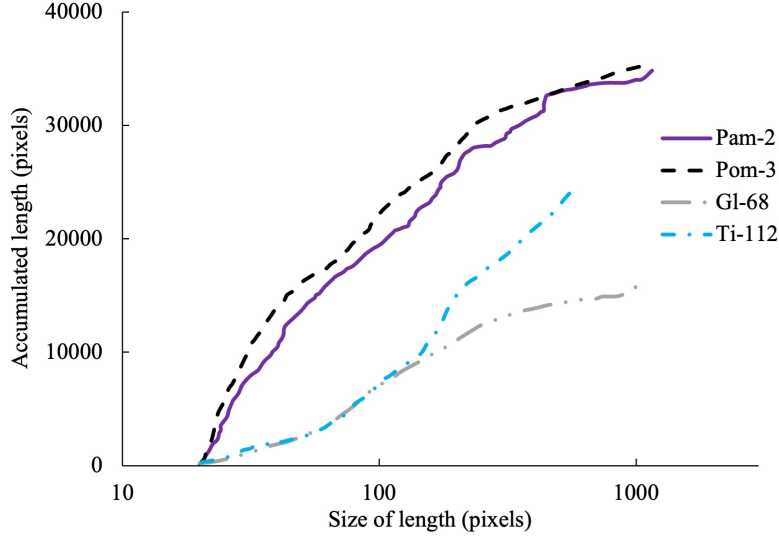


Figure II. 2: Accumulated length of cracks in different samples (step 2)

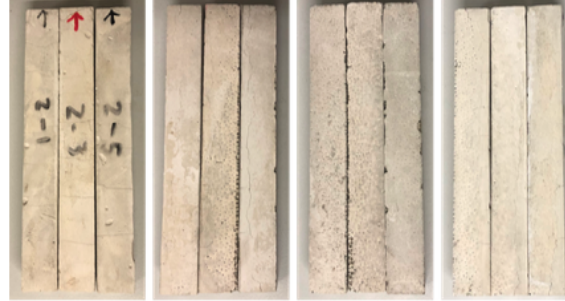
3 Effect of the inclusions size

In this section, the experimental study and main findings of [Jin et al. \(2023\)](#) are summarized. The work primarily investigated the effect of inclusion size on drying shrinkage-induced cracking in cementitious composites.

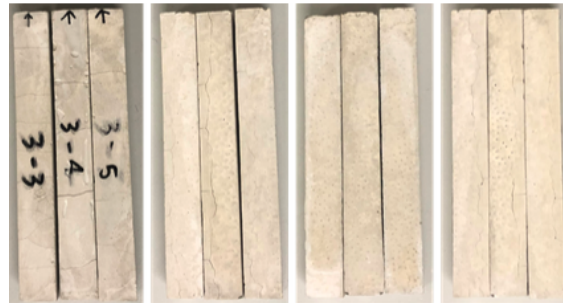
3.1 Sample preparation and experimental program

To investigate the effect of inclusion size on cracking, cementitious composites were prepared with 35% spherical inclusions and 65% cement paste. Glass beads of 2 mm and 3 mm diameter were selected, as their X-ray attenuation coefficient is sufficiently close to that of cement paste to minimize image artefacts at the matrix–inclusion interface while still enabling clear phase distinction, and their stiffness is comparable to that of common siliceous aggregates. The chosen diameters ensured that crack openings would be detectable at the available resolution ([Li et al., 2018](#)). Specimens were cast as prismatic bars ($20 \times 20 \times 160 \text{ mm}^3$). For each case, three replicate samples were prepared. CEM I 52.5 cement, compliant with European standards, was used with a water-to-cement ratio of 0.5 to allow proper casting without vibration. After casting, all specimens were cured in a lime-saturated solution at 20 °C for over one month to ensure advanced hydration and a stabilized microstructure. All samples were first cured in lime-saturated solution at 20 °C to ensure matrix maturation and full saturation, then dried at 25 °C and 50% RH in a controlled climatic chamber until mass stabilization (weight change $< 0.1\%$ over 7 days).

Fig. II. 3 presents the surfaces cracking of two specimens with different diameter inclusions after the drying process.



(a) Sample with inclusion of 2 mm



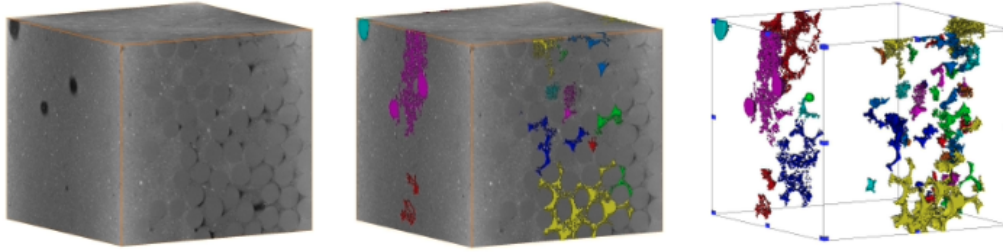
(b) Sample with inclusion of 3 mm

Figure II. 3: Images of different samples at the end of the drying procedure

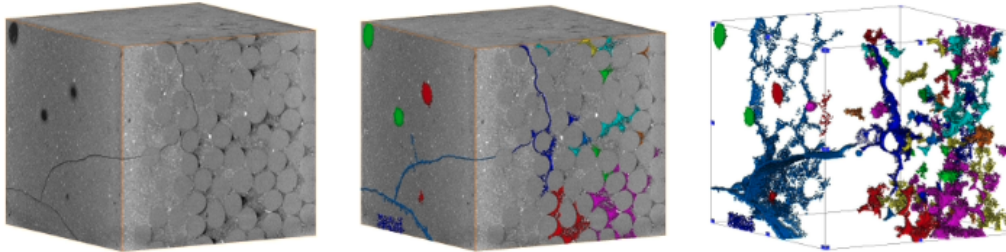
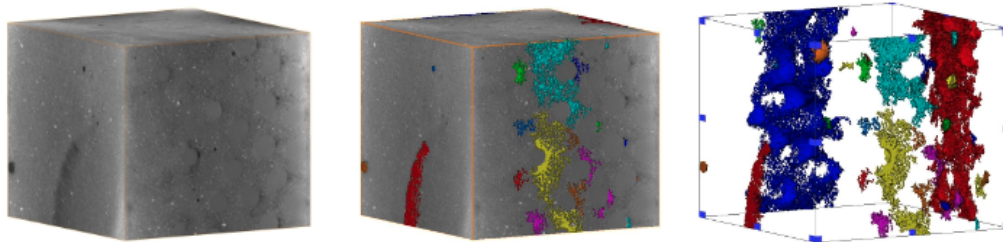
3.2 Experimental results

The crack networks of two types of cementitious composites are compared and analyzed. Image analysis was performed using segmentation based on voxel gray values, a semi-automated procedure that removes irrelevant structures and enables quantification of microstructural evolution, particularly cracking during drying. With this method, cracks can be clearly visualized in 3D reconstructed volumes (Fig. II. 4), where different colors denote distinct unconnected cracks, assigned randomly by the software. Surface voxels are often prone to bias, which explains the dense crack-like features visible at specimen surfaces in both saturated and dried states.

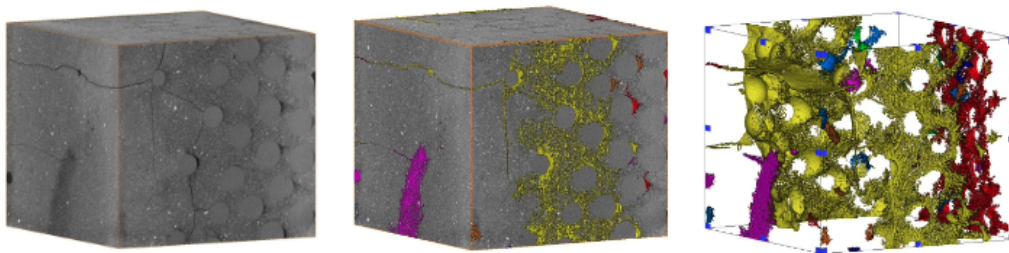
The analysis focuses on the evolution of crack networks with drying. Compared with the initial state, clear crack initiation and growth can be observed in the dried condition. Larger cracks appear in regions with a lower inclusion fraction, and the change in crack and pore volume reached 47% for the 3 mm sample, compared with 42% for the other sample type.



(a) Sample with inclusion of 2 mm (Saturated)

(b) Sample with inclusion of 2 mm ($T = 25\text{ }^{\circ}\text{C}$, HR=50%)

(c) Sample with inclusion of 3 mm (Saturated)

(d) Sample with inclusion of 3 mm ($T = 25\text{ }^{\circ}\text{C}$, HR=50%)**Figure II. 4:** Evolution of the 3D crack network in different samples

4 Effect of the inclusions surface roughness

As previously mentioned, the cracking behavior of concrete is significantly influenced by aggregate properties, with surface roughness playing a crucial role. This section investigates the effect of aggregate surface roughness as a key parameter governing crack initiation and propagation. Like previous experiments, this study follows the approach of [Shiotani et al. \(2003\)](#), employing simplified and representative conditions to isolate this factor, since the geometric complexity of real aggregates poses challenges for controlled analysis. Spherical aggregates were selected to further simplify the geometry and allow better control of boundary conditions during crack initiation and propagation.

4.1 Sample preparation

Spherical glass beads are adopted as inclusions to ensure geometric consistency, with two surface conditions considered: smooth and rough. The rough surface is prepared by mechanically abrading the originally smooth glass beads with sandpaper. By controlling other variables, the effect of surface roughness on crack initiation and development can be isolated and assessed.

As noted earlier, the sample size is determined by balancing representativeness and compatibility with X-ray microtomographic imaging. Inclusions with a diameter of 2 mm are sufficient to induce shrinkage cracks and are suitable for crack detection. In the experiment, a cone-beam X-ray setup is used, where image magnification depends on the relative positions of the X-ray source, specimen, and detector. To match the field of view and achieve a spatial resolution better than 10 μm , cylindrical specimens with a diameter of 8 mm and height of 15 mm are selected. The inclusion diameter is 2 mm, making the sample diameter four times larger than the inclusion. This configuration ensures adequate resolution and structural representativeness.

CEM I 52.5 cement, in accordance with European standard EN 197-1, is used in this study. A water-to-cement ratio (W/C) of 0.5 is adopted to ensure complete hydration and facilitate casting without the need for intensive vibration. One specimen is prepared for each type of cementitious composite, with a fixed inclusion volume fraction of 40%. All samples are cured in saturated limewater at 20°C for over one month to guarantee sufficient hydration and material stability.

4.2 Drying procedure and X-ray imaging acquisition

As shown in Fig. II. 5, all samples underwent four stages from preparation to drying. Following preparation, the specimens were stored in saturated limewater at 20 °C to ensure full water saturation. Thereafter, two consecutive drying steps were applied to investigate the formation of drying-induced cracks in cement paste under varying conditions. A marked contrast in relative humidity (RH) and temperature (T) between the two steps was introduced to enhance crack visibility, which is critical for accurate microtomographic observation.

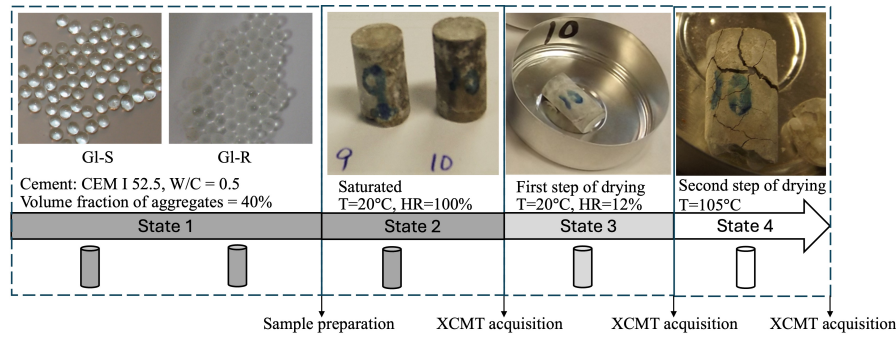


Figure II. 5: Drying steps of samples and corresponding micro-tomographic acquisition (GI-S=smooth-surfaced aggregates; GI-R=rough-surfaced aggregates.)

In the first stage, samples are placed in an environment at 20 °C with a low RH of 12%. Although this RH is considerably lower than typical environmental conditions, it is chosen deliberately to promote the formation and opening of cracks within the desired resolution. In the second stage, drying is conducted at 105 °C to achieve more complete desiccation of the matrix. Both drying steps are performed using a Vötsch[®] or Binder[®] climatic chamber, and each step continues until mass stabilization is reached. The weight of each sample is monitored using a balance with a precision of ± 0.01 g. Mass stabilization is defined as a weight change of less than 0.1% over seven consecutive days. A normalized weight loss of the cementitious matrix—assuming no mass loss from aggregates—is calculated instead of using the total specimen mass loss. The evolution of this normalized weight loss is presented in Fig. II. 6.

The evolution of microstructure during the drying process is monitored using X-ray micro-tomographic imaging. Initial scans of the fully saturated samples serve as a reference for comparison with those acquired after each of the two drying steps. The microtomographic acquisition is carried out on the ISIS4D platform (Limodin et al., 2013), as shown

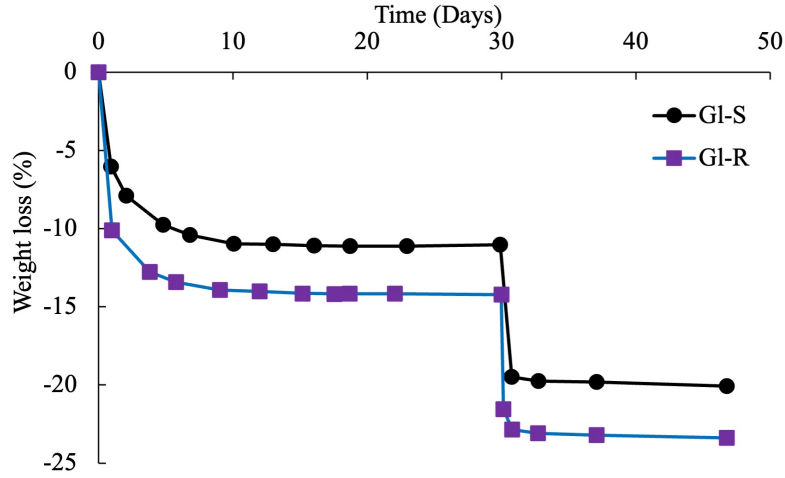


Figure II. 6: Evolution of normalized weight loss with drying time

in Fig. II. 7. This system uses a laboratory X-ray source equipped with a tungsten filament, and a 0.1 mm-thick aluminum filter is applied to minimize beam hardening effects. The reconstructed images have a spatial resolution of $7 \mu\text{m}$, meaning cracks narrower than $7 \mu\text{m}$ are not detected, and those between 7 and $14 \mu\text{m}$ are difficult to distinguish clearly (Lenoir et al., 2007).

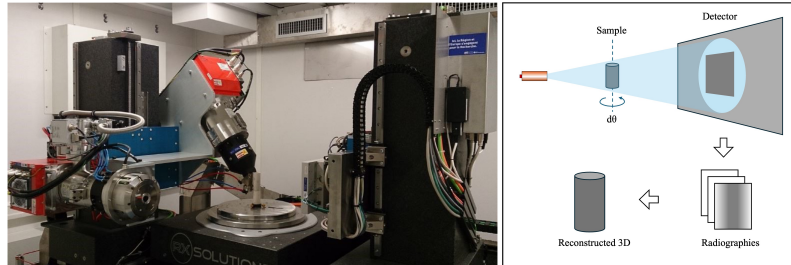


Figure II. 7: The micro-tomography equipment and the sketch of micro-tomographic acquisition and reconstruction

4.3 Image processing method

Drying-induced microcracks are visible in the X-ray microtomographic images, but the accuracy of quantitative analysis depends heavily on the quality of the reconstructed volumes. To mitigate inherent limitations of the imaging technique, several corrective measures are employed during image acquisition and reconstruction. For instance, appropriate choices of sampling frequency, detector sensitivity, and number of projections help prevent aliasing. The internal microstructure, particularly the distribution of cracks, is

visualized from reconstructed 3D greyscale volumes. The influence of surface roughness on crack patterns is assessed by examining crack width and propagation. Cracks are identified and quantified via image segmentation based on voxel greyscale intensity. Two main parameters are considered: the total volume and surface area of the crack space. The crack volume is computed from the number of crack voxels and the voxel volume (a^3), while surface area is estimated from the number of crack-surface facets multiplied by the facet area (a^2). For simplicity, voxel and pixel counts are used as proxies for volume and surface, respectively.

To improve segmentation reliability, several additional preprocessing steps are implemented. First, due to slight variations in sample positioning during each scan, reconstructed images are registered via rigid-body transformation using geometric references—namely, the positions of aggregates—to ensure spatial consistency across drying stages. Second, drying alters the moisture content of the cement paste, leading to changes in its X-ray attenuation coefficient. This manifests as a shift in the greyscale values in the reconstructed images, which is corrected by histogram calibration to allow consistent thresholding across all drying stages. Third, due to material heterogeneity and the partial volume effect, intermediate greyscale values may appear even in binary-phase materials. To enhance image quality, a median filter is applied to all data sets. These processing steps help reduce sensitivity to segmentation thresholds, thereby improving the reliability of the quantitative analysis, which is discussed further in the results section.

4.4 Experiment results

A 3D volume of each sample is reconstructed from denoised X-ray microtomographic images. Representative cross-sectional slices, primarily extracted from the mid-height of the specimens, are presented in Fig. II. 8. These images capture the evolution of the microstructure from the saturated state through the two successive drying stages. In particular, the effect of aggregate surface roughness on shrinkage-induced cracking in cementitious composites is revealed through detailed analysis of crack morphology and spatial distribution.

Different phases within the cementitious composites are distinguishable by their grey values, which correspond to varying X-ray attenuation coefficients. Cracks appear as dark regions, with lower grey value typically indicating wider openings due to the averaging effect of partial voxel occupancy. The cement paste generally exhibits a uniform grey tone, while denser anhydrous cement grains appear as bright spots. Occasionally, portlandite crystals are observed within air voids. Due to its heterogeneous nature—including pores

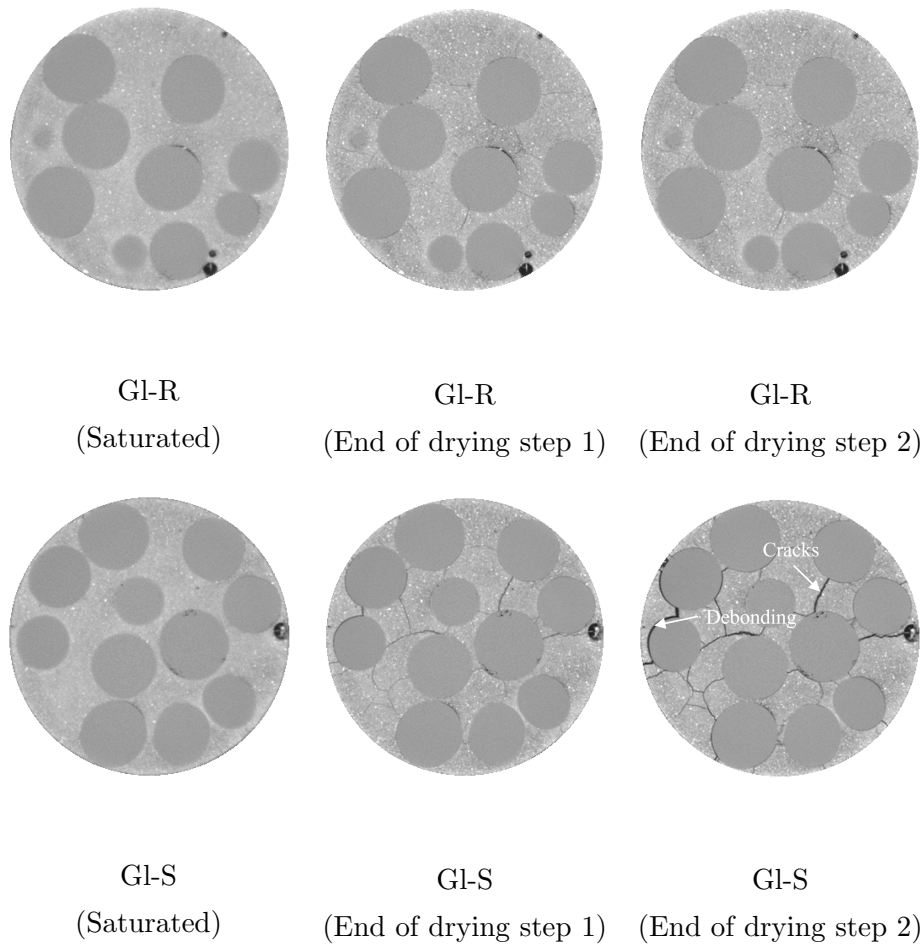


Figure II. 8: Representative cross-section images in different samples at different drying states

and hydration products—the greyscale of cement paste is more variable than that of the aggregates.

In the saturated state, only initial pores and entrapped air are detected, and no visible cracks are present. These images serve as the baseline for assessing crack development during drying. After the first drying step (20 °C, RH=12%), fine cracks begin to emerge. Notably, the extent and clarity of cracking vary with the surface condition of aggregates. Samples with smooth aggregates GI-S, display more frequent and distinct cracks compared to their rough-surfaced counterparts like GI-R.

Following the second drying step (105 °C), cracks become more pronounced, exhibiting increased width and length. The influence of surface roughness is more evident at this stage. Cracks are primarily observed in radial configurations and between aggregates. In

GI-S, the cracks are wider and more continuous, while in GI-R they tend to be finer and shorter. The presence of circumferential cracks around smooth aggregates indicates interfacial debonding, whereas rough aggregates appear to enhance matrix bonding, thereby limiting interface separation.

4.5 Identification and quantitative analysis of cracks

To enable a more comprehensive and quantitative analysis of the experimental results—beyond single cross-sectional observations—crack regions in all samples are extracted from the reconstructed 3D volumes using an image segmentation approach. This segmentation is performed based on a carefully selected threshold, determined from the grey value histogram of each sample. Accordingly, a brief overview of the histogram analysis and the rationale behind the threshold selection is first presented. This is followed by a detailed discussion of the quantitative results derived from the identified cracks.

It should be noted that the entire volume of each sample is not scanned or displayed in Fig. II. 9. Due to their fragility following the two drying stages, the samples could not remain intact. Additionally, image quality deteriorates near both ends of the specimens because of various interference factors. As a result, only selected sub-volumes are analyzed and presented. Within each of these subsets, the total volume of segmented cracks is calculated.

The radial cracks shown in Fig. II. 9 are visualized not merely in a single cross-section but within a more representative three-dimensional volume. A marked increase in radial crack development is observed in the GI-S samples after the first drying stage, as compared to GI-R. This observation aligns with prior cross-sectional analysis but provides a more robust and representative assessment. To substantiate these findings, quantitative data analysis is conducted to evaluate the influence of inclusion surface roughness on crack development.

The evolution of crack volume and area with respect to inclusion surface roughness is presented in Fig. II. 10. As the entire volume of each sample is not scanned and the analyzed sub-volumes vary among samples, the crack quantities are normalized and expressed per slice to allow meaningful comparison. The results indicate that, after the first drying stage, a greater number of cracks are observed in samples with smooth inclusion surfaces compared to those with rough surfaces. At this stage, many cracks are extremely fine and comprise only a few pixels, which can make radial cracks more difficult to detect, particularly in smoother samples. Additionally, circumferential cracks may form at the inclusion–cement interface, and any underrepresentation of these may lead to an

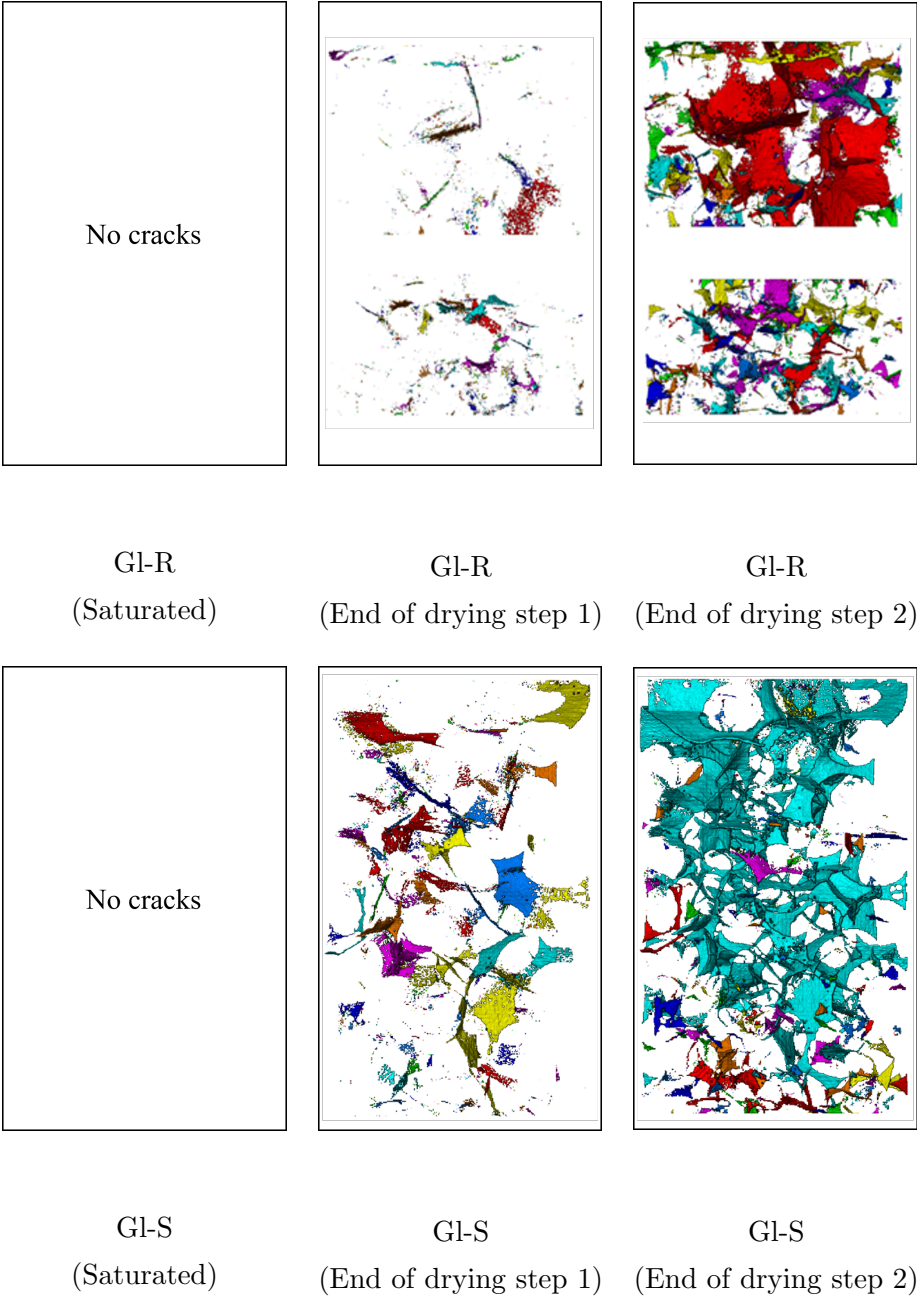


Figure II. 9: Evolution of crack in different samples

underestimation of the total crack quantity. Nevertheless, the quantitative results clearly demonstrate the significant influence of inclusion surface roughness on crack formation.

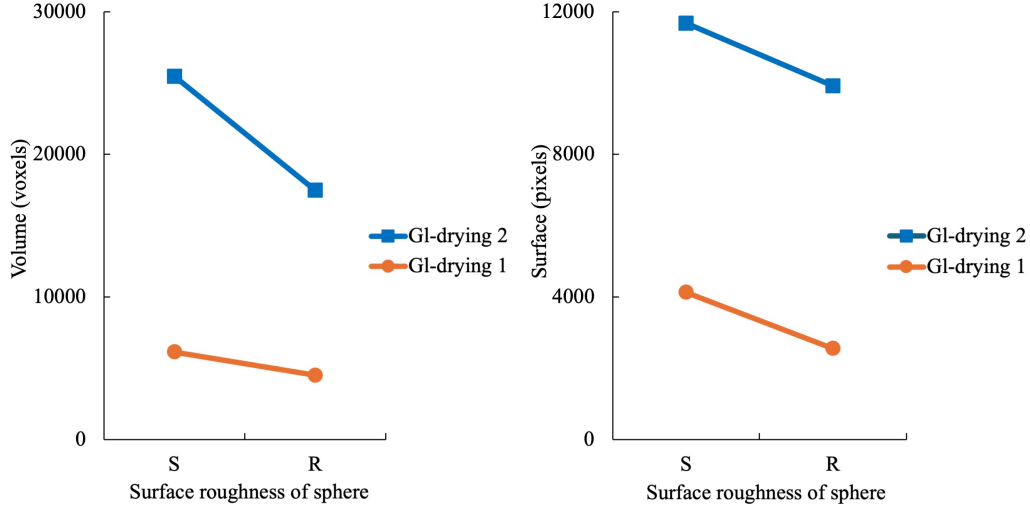


Figure II. 10: Evolution of the volume and area of crack space with surface roughness

In addition to crack quantity, other morphological characteristics are also influenced by the surface roughness of inclusions. Samples with smooth inclusion surfaces tend to exhibit wider, longer, and more interconnected cracks. To capture these differences in crack patterns, several quantitative measures are applied to the segmented cracks, including connected component analysis, as well as evaluations of crack width and length. Connected component analysis, in particular, is used to assess the connectivity of the crack network, with each connected region labeled in a distinct color in Fig. II. 9.

The accumulated crack volume as a function of connected component size for different samples, after the second drying stage, is shown in Fig. II. 11. The results indicate that larger connected crack structures are more prevalent in samples with smooth inclusion surfaces. This enhanced connectivity is likely facilitated by the presence of circumferential cracks at the interface, which further contribute to the integration of the crack network in these samples.

The measured crack widths in samples with different surface roughness are presented in Fig. II. 12 (a). Fewer cracks with widths less than 10 pixels are observed in samples containing smooth-surfaced spheres compared to those with rough-surfaced spheres. In contrast, a greater number of cracks with widths exceeding 10 pixels are found in the smooth-surface samples. This indicates that wider cracks tend to develop when inclusions have smoother surfaces. These findings are consistent with the previous observations regarding crack morphology and connectivity.

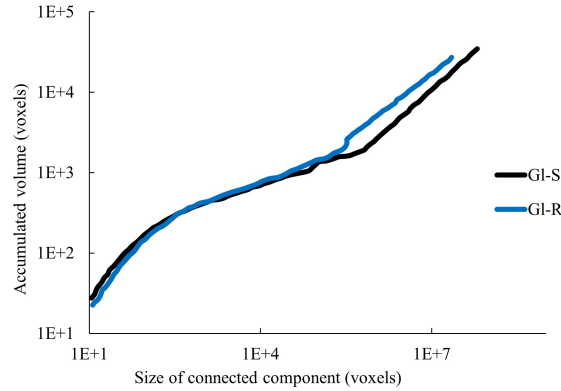


Figure II. 11: Accumulated volume of connected component in different samples (step 2)

Fig. II. 12 (b) shows the accumulated crack length in the different samples. For GI-S samples, a gradual increase in accumulated length is observed for small cracks, followed by a more rapid growth in the medium-length range. Notably, fewer short cracks (less than 100 pixels in length) are present in the GI-S samples. This further supports the conclusion that smoother inclusions tend to promote the formation of longer, more connected cracks rather than numerous small ones.

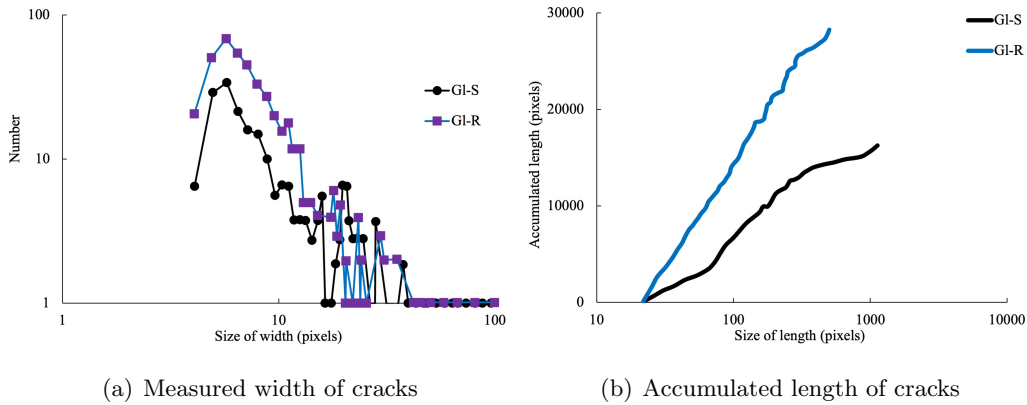


Figure II. 12: The information of cracks in different samples (step 2)

5 Effect of the inclusions shape

The shape of inclusions is a key factor influencing stress distribution and crack propagation in cementitious composites. To study this effect under controlled conditions, we attempted several methods to fabricate inclusions with tailored, regular geometries. The

motivation for using well-defined shapes is to reduce the uncertainty associated with the irregularity of natural aggregates and to enable a more systematic analysis of shape effects. By producing inclusions with controlled geometry, it becomes possible to characterize their morphology using quantitative shape parameters—such as aspect ratio, sphericity, or angularity—and to correlate these descriptors with the observed cracking behavior. The following section introduces the approaches explored for tailoring inclusion geometry and outlines the procedures adopted for preparing inclusions of different shapes.

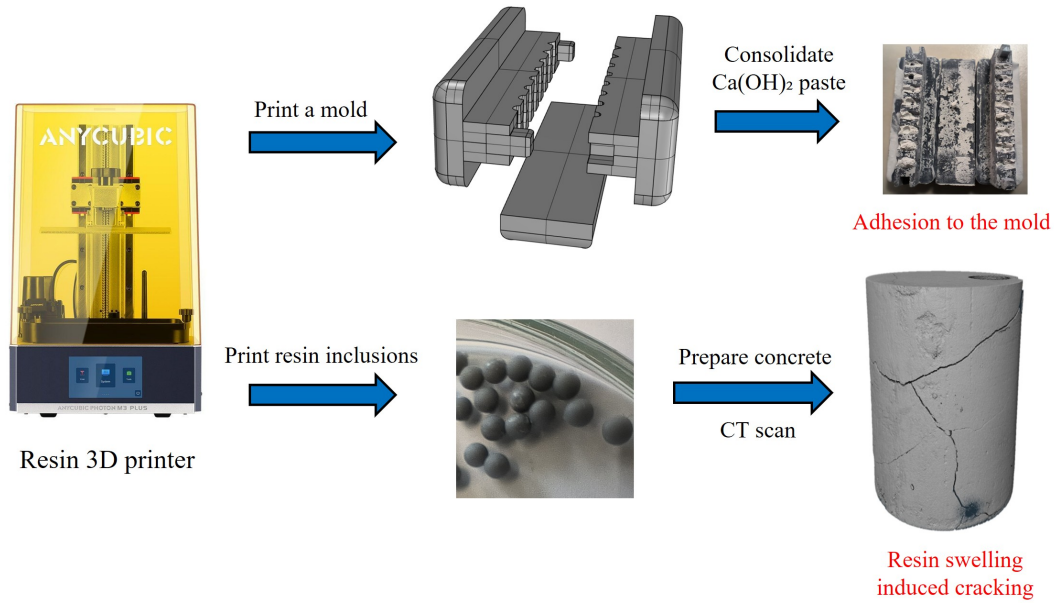
5.1 Experimental attempts

Based on the results of the previous experiments, an inclusion size of 2–3 mm was selected. This dimension was shown to be optimal for inducing shrinkage cracks while still allowing them to be clearly visualized in XMCT scans. With this target size in mind, several approaches were explored to fabricate inclusions of controlled geometry for use in cementitious composites.

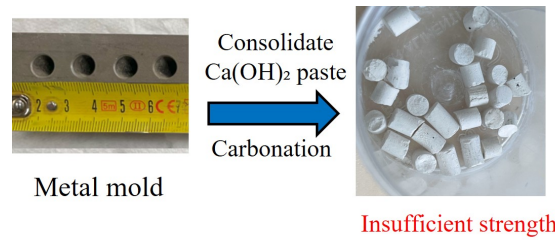
As shown in Fig. II. 13, several methods were explored for the preparation of inclusions. The first attempt involved 3D printing technology, in which two strategies were tested. In the first, a resin printer was used to fabricate molds of specific shapes, into which $\text{Ca}(\text{OH})_2$ paste was consolidated. However, during demolding, strong adhesion between the paste and the printed mold prevented the recovery of intact inclusions. In the second strategy, inclusions were directly printed from resin. Although this approach provided good dimensional accuracy, the resin material swelled during concrete curing, generating undesired internal stresses and causing premature cracking of the cement matrix. Consequently, this method proved unsuitable for reliable experimental use.

A second approach involved pressing $\text{Ca}(\text{OH})_2$ powder into metal molds, followed by carbonation to increase their strength. Although demolding was successful and inclusions with regular geometry were obtained, mechanical testing showed that their uniaxial compressive strength did not exceed 2 MPa. This value is far below the requirement for stable handling and mixing in cementitious composites. Consequently, many inclusions fractured prematurely, making this method unsuitable for producing reliable substitutes for natural aggregates.

These experimental attempts demonstrated the challenges of fabricating inclusions with tailored shapes while maintaining both the dimensional requirements and the mechanical compatibility with cement paste. Although promising in concept, further improvements are necessary to overcome the issues of adhesion, swelling, and inadequate strength encountered in the tested methods.



(a) Using 3D printing technology

(b) Inclusion prepared by pressing Ca(OH)_2 powder**Figure II. 13:** Two methods of inclusion preparation and the problems encountered

Following these attempts, we also explored the use of ceramic 3D printing resins to fabricate inclusions by printing and subsequently sintering the particles. Commercially available ceramic resins, typically composed of ceramic powders such as alumina or zirconia dispersed in a photocurable organic matrix, were employed for this purpose. After printing, the organic binder is removed by pyrolysis, and the remaining ceramic phase is densified through high-temperature sintering. Although this approach allowed us to obtain inclusions with controlled geometry, the material itself presented a major drawback: ceramic resins, particularly those containing high-density oxides like zirconia, exhibit a high X-ray absorption coefficient. This strong attenuation reduces image contrast and may hinder the accurate detection of fine cracks in microtomographic analyses, thereby limiting the usefulness of this method.

An additional attempt was made by sintering glass particles to shape glass inclusions with predefined geometries. In principle, this method could provide inclusions with X-ray attenuation closer to that of the cementitious matrix. However, because of the small target size (2–3 mm), the glass beads tended to coalesce during high-temperature sintering, leading to severe agglomeration and loss of the intended geometry. As a result, this method was also found unsuitable for producing well-defined inclusions.

In summary, multiple experimental routes were explored to fabricate inclusions with controlled shapes and sizes suitable for XMCT observations, including resin-based 3D printing, pressing and carbonating $\text{Ca}(\text{OH})_2$, ceramic resin printing with sintering, and glass sintering. Each method demonstrated certain advantages in terms of geometric control, but all exhibited critical limitations such as adhesion during demolding, swelling, insufficient mechanical strength, excessive X-ray absorption, or agglomeration at small scales. These outcomes highlight the significant practical challenges in producing artificial inclusions that simultaneously meet the requirements of geometry, mechanical compatibility, and imaging quality. Further refinement of processing techniques will be required before such inclusions can serve as reliable substitutes for natural aggregates in systematic studies of shape effects.

6 Conclusions

In the present work, experimental studies have been performed to investigate the influence of inclusion properties (rigidity, size, and surface roughness) on drying shrinkage-induced cracking in cementitious composites. Based on the obtained results and previous observations reported in [Li et al. \(2020b\)](#) and [Jin et al. \(2023\)](#), the following main remarks can be formulated:

- **Inclusion rigidity (Li et al., 2020):** X-ray microtomography enables detailed 3D observation of drying-induced crack evolution. Stiffer inclusions (e.g., Ti, Zr) intensify ITZ stress concentrations and promote radial and interfacial cracking. More compliant inclusions (e.g., Pam, Pom) reduce stress localization but show swelling or absorption effects, which alter the crack patterns.
- **Inclusion size (Jin et al., 2023):** Cracks are mainly generated at the inclusion–matrix interface and often propagate radially to connect neighboring inclusions. The overall quantity of cracks increases with inclusion size, with 3 mm beads producing a larger change in crack/pore volume than 2 mm beads. The crack distribution pattern, however, remains similar across sizes.

- **Inclusion surface roughness:** Surface roughness strongly affects crack morphology and connectivity. Smooth inclusions tend to favor wider, longer, and more connected cracks, often accompanied by circumferential debonding. Rough inclusions, in contrast, enhance interfacial interlocking and lead to finer, shorter, and less connected crack networks.
- **On attempts to study inclusion shape:** Several methods were tested to fabricate inclusions with controlled geometries, including 3D-printed resin molds, direct resin printing, pressing and carbonating $\text{Ca}(\text{OH})_2$, ceramic resin printing with sintering, and glass sintering. All methods showed critical limitations such as adhesion, swelling, insufficient strength, excessive X-ray attenuation.

In summary, inclusion rigidity, size, and surface roughness were found to play decisive roles in drying shrinkage-induced cracking. However, due to the experimental challenges in preparing inclusions of different shapes, the influence of aggregate geometry will be further addressed through numerical simulations in the following chapter.

Chapter III

Numerical Analysis of Inclusion Shape on Concrete Drying Fractures

1 Introduction

In this chapter, a fully coupled three-dimensional hydro-mechanical bond-based peridynamic (BB-PD) model was developed to simulate crack evolution in cementitious materials under drying shrinkage conditions. The principles and implementation of the hydro-mechanical BB-PD model are first introduced, and its validity is rigorously verified through comparisons with experimental drying shrinkage crack patterns. Subsequently, a three-phase meso-scale concrete model is generated, and the effects of aggregate shape on drying shrinkage cracks are investigated. The obtained results provide new insights into the fracture behavior of cementitious materials under drying shrinkage, offering practical strategies to mitigate the detrimental effects of drying shrinkage cracks. This work not only advances the understanding of crack propagation in cementitious composites but also will guide engineers in optimizing material design and improving the durability of concrete under varying environmental conditions.

2 Hydro-mechanical bond-based peridynamic model for cementitious materials

This section presents the development of a fully coupled hydro-mechanical BB-PD model for cementitious materials in three dimensions. Following the theoretical formula-

tion, a BB-PD code will be developed to implement the proposed model.

The cementitious composites are assumed to be an isotropic porous medium saturated with liquid water (denoted by index f) and a gas mixture (denoted by index gz). The gas mixture is considered a perfect blend of dry air (denoted by index da) and vapor (denoted by index va). Since the variation in gas pressure is negligible compared to the liquid pressure during drying shrinkage processes, the gas pressure is neglected in this study, i.e., $p_{gz} = 0$. Only the liquid pressure p_f is considered in the present work.

2.1 Classic formulations

PD is a non-local continuum theory designed to address structural discontinuities, that traditional continuum mechanics cannot handle. In peridynamics, a material point within a body interacts with other points within a finite range, termed the "horizon δ ," as shown in Fig. III. 1. H is the neighborhood domain of the point $\mathbf{x}$, in three-dimensional (3D) problems, defined by:

$$H = H(\mathbf{x}, \delta) = \{\mathbf{x}' \in R : |\mathbf{x}' - \mathbf{x}| \leq \delta\} \quad (\text{III. 1})$$

The interaction between two material points $\mathbf{x}$ and $\mathbf{x}'$ is governed by a response function $\mathbf{f}$, which contains the constitutive properties of the material.

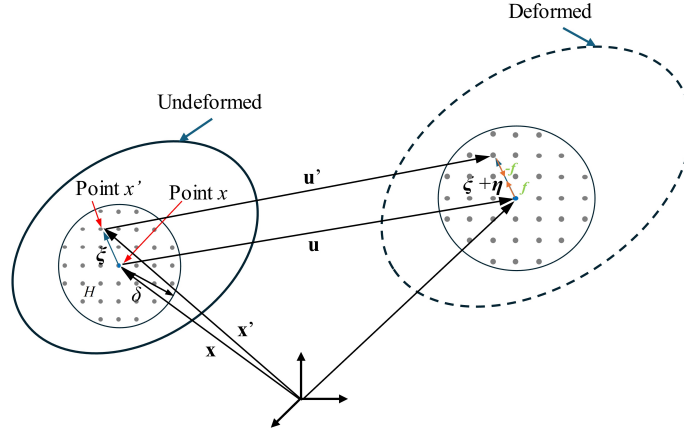


Figure III. 1: Principle of BB-PD theory in reference and deformed configuration

The peridynamic equation of motion at a reference position of $\mathbf{x}$ and time t , derived by Silling (2000), is given as:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_H \mathbf{f}(\mathbf{x}' - \mathbf{x}, \mathbf{u}' - \mathbf{u})dV + \mathbf{b}(\mathbf{x}, t) \quad (\text{III. 2})$$

where ρ is the mass density, $\ddot{\mathbf{u}}$ is the acceleration quantity vector, $\mathbf{b}$ is a prescribed body force density field; $\mathbf{u}'$ and $\mathbf{u}$ represent the displacements of points $\mathbf{x}'$ and $\mathbf{x}$, respectively. The response function $\mathbf{f}$, that defines the force between two material points, is written as

$$\mathbf{f} = cs \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|} \quad (\text{III. 3})$$

where $\mathbf{y}$ represents the position of the material point $\mathbf{x}$ in the deformed configuration : $\mathbf{y} = \mathbf{x} + \mathbf{u}$. The stretch s between the material points is defined as:

$$s = \frac{|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|}{|\mathbf{x}' - \mathbf{x}|} \quad (\text{III. 4})$$

The bond constant c is the micro modulus, in 3D, which is expressed as (Jin et al., 2023; Zhou et al., 2020):

$$c = \frac{12E}{\pi\delta^4} \quad (\text{III. 5})$$

where E is the material's elastic modulus.

2.2 Fluid flow field

Based on the research work of Biot (1941), fluid flow in the porous medium is described by Darcy's law. The governing equation for single-phase fluid flow in concrete is given as:

$$\frac{\partial(\rho_f \beta)}{\partial t} = -\nabla \cdot (\rho_f \mathbf{v}) + q_f \quad (\text{III. 6})$$

where ρ_f is the fluid density, q_f is the mass of fluid produced per unit volume per unit time, and β is the water content variation:

$$\beta = \alpha\theta + \frac{P}{Q_b} \quad (\text{III. 7})$$

where Q_b is the Biot modulus; α represent the Biot parameter; θ is the volumetric strain.

The fluid velocity $\mathbf{v}$ is expressed as

$$\mathbf{v} = -\frac{k_p}{\mu_v} \nabla P \quad (\text{III. 8})$$

where k_p is the permeability; μ_v is the fluid viscosity. Under three-dimensional conditions, PD permeability k_p is expressed as a function of intrinsic permeability k of porous medium:

$$k_p = \frac{6k}{\pi\mu_v\delta^4}, \text{ with } k = \begin{cases} k_{int} , \text{ intact domain} \\ \frac{\omega^3}{12} , \text{ fractured domain} \end{cases} \quad (\text{III. 9})$$

When the bond remains intact, permeability is equivalent to that of the intact material k_{int} . Otherwise, permeability matches that of the fractured domain. Based on previous work (Witherspoon et al., 1980), the cubic law is only valid under low Reynolds number conditions, where transmissivity becomes flow-rate-independent and scales with the cube of the mean hydraulic aperture (ω). To model the intrinsic permeability of fractured materials, this study adopts the cubic law for 3D cases (Eq. III. 9). Consequently, in fractured media, permeability is governed by ω , a parameter tied to the state of bond.

As the gas pressure is neglected in the present work, the fluid pressure P is given as (Callari and Abati, 2009):

$$P = p_f - \rho_f g z \quad (\text{III. 10})$$

where p_f is the fluid pressure; g is the gravitational acceleration; and z is depth. For constant material properties, as derived by Biot (1941), the governing equation (Eq. III. 6) for partially saturated porous medium can be rewritten as

$$\frac{1}{Q_b} \frac{\partial P}{\partial t} = \frac{k_r k_p}{\mu_v} \nabla^2 P - \alpha \frac{\partial \theta}{\partial t} + \frac{q_f}{\rho_f} \quad (\text{III. 11})$$

where k_r is the relative permeability. By adopting the analogy between poroelasticity and thermoelasticity (Oterkus et al., 2014), the peridynamic form of Eq. (III. 11) is derived as:

$$\frac{1}{Q_b} \dot{P}(\mathbf{x}, t) = \int_H \left(k_r k_p \frac{P(\mathbf{x}', t) - P(\mathbf{x}, t)}{|\mathbf{x}' - \mathbf{x}|} - \frac{c}{2} \alpha \gamma \dot{e} \right) dV + \frac{q_f}{\rho_f} \quad (\text{III. 12})$$

In PD (Silling, 2000), the extension between the material points is defined as:

$$e = |\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|, \quad (\text{III. 13})$$

As a result, the time rate of change of extension can be obtained:

$$\dot{e} = \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|} \cdot (\dot{\mathbf{u}}' - \dot{\mathbf{u}}) \quad (\text{III. 14})$$

The Biot modulus Q_b for partially saturated porous media is :

$$\frac{1}{Q_b} = \frac{S_l^2 (\alpha - \phi)}{K_s} + \frac{S_l \phi}{K_f} - \phi \frac{\partial S_l}{\partial p_c} \quad (\text{III. 15})$$

where K_s and K_f are the bulk modulus of solid and fluid, respectively; ϕ is porosity. S_l is the water saturation and is a function of the capillary pressure p_f , by using water retention curve. The van Genuchten function is employed to describe the water retention curve (van Genuchten, 1980) :

$$S_l = S_l^r + (1 - S_l^r) [1 + (\epsilon p_c)^n]^{-m}, \quad (\text{III. 16})$$

where S_l^r is the residual saturation degree; ϵ , m and n are empirical parameters and can be calibrated by experimental data.

2.3 Peridynamic equation of motion in cementitious material

To determine the bond state, the average pore water pressure between two material points is defined as

$$\bar{P}(\mathbf{x}, \mathbf{x}', t) = \frac{P(\mathbf{x}', t) + P(\mathbf{x}, t)}{2} \quad (\text{III. 17})$$

By exploiting the analogy between poroelasticity and thermoelasticity, the peridynamic equation of motion for a material point at x , incorporating fluid pressure, is expressed:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_H c\psi(\mathbf{x}, \mathbf{x}', t)(s - S_l\alpha\gamma\bar{P}(\mathbf{x}, \mathbf{x}', t)) \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|} dV + \mathbf{b}(\mathbf{x}, t) \quad (\text{III. 18})$$

where $\psi(\mathbf{x}, \mathbf{x}', t)$ is the bond state function, which will be introduced in section 2.4.; γ is the coefficient of fluid pore pressure:

$$\gamma = \frac{(1 - 2\nu)}{E} \quad (\text{III. 19})$$

with ν representing the Poisson's ratio.

2.4 Fracture criterion

In PD, crack initiation and propagation are represented by bond breaking. The state function of the interacting bond in a horizon can be defined as follows:

$$\psi(\mathbf{x}, \mathbf{x}', t) = \begin{cases} 0, & s \geq s_0 \\ 1, & s < s_0 \end{cases} \quad (\text{III. 20})$$

where $\psi(\mathbf{x}, \mathbf{x}', t)$ equaling 0 means that the bond is broken, while $\psi(\mathbf{x}, \mathbf{x}', t)$ equaling 1 means that the bond is intact; s_0 is the critical stretch of bonds, which can be obtained by the energy release rate G_0 of macroscopic material:

$$s_0 = \sqrt{\frac{5G_0}{6E\delta}} \quad (\text{III. 21})$$

The global damage at a material point is calculated based on the ratio of broken bonds to the total number of bonds within the horizon. Thus, the global damage function of material points is written as:

$$D(\mathbf{x}, t) = 1 - \frac{\int_H \psi(\mathbf{x}, \mathbf{x}', t) dV}{\int_H dV} \quad (\text{III. 22})$$

It's not possible to directly obtain geometric parameters of fractures, such as length and width. However, the damage value can serve as an indicator for tracking the initiation and propagation of cracks. Based on prior research (Qin et al., 2022), the $D(\mathbf{x}, t)$ value of 0.24 can be used to determine the presence of cracks. The crack width, ω_i , can be calculated by the following equation:

$$\omega_i = \mathbf{n} \cdot (\mathbf{u}' - \mathbf{u}) \quad (\text{III. 23})$$

where $\mathbf{n}$ is the unit normal vector of the fracture surface.

3 Numerical discretization and implementation

The development of the hydro-mechanical BB-PD model in Section 2 establishes the theoretical framework for simulating drying-induced crack evolution in cementitious composites. To operationalize this framework, this section details the numerical discretization and implementation strategies required to resolve the coupled hydro-mechanical equations. Key challenges include the non-local nature of peridynamic interactions, boundary effects in heterogeneous meso-scale models, and computational efficiency for quasi-static drying processes. The spatial discretization, surface/volume corrections, and adaptive time integration schemes presented here address these challenges, ensuring robust simulation of three-dimensional crack propagation under drying conditions.

3.1 Spatial discretization

The computational model, based on PD theory, discretizes the continuous medium into a series of regularly distributed particles with grid spacing Δx . Each material point $\mathbf{x}_i$ is assigned a volume ΔV_i , and the neighbourhood domain H_i of $\mathbf{x}_i$, defined by the horizon size δ , can be given as:

$$H_i := \mathbf{x}_j \mid \mathbf{x}_j \neq \mathbf{x}_i, \mathbf{x}_j - \mathbf{x}_i \leq \delta \quad (\text{III. 24})$$

As a result, the discretized form of the hydro-mechanical BB-PD equations for material point $\mathbf{x}_i$ is:

$$\rho(\mathbf{x}_i) \ddot{\mathbf{u}}(\mathbf{x}_i, t) = \sum_{\mathbf{x}_j \in H_i}^N c_{ij} \psi_{ij}(s_{ij} - S_l \alpha \gamma \bar{P}(\mathbf{x}, \mathbf{x}', t)) \frac{\mathbf{y}_j - \mathbf{y}_i}{|\mathbf{y}_j - \mathbf{y}_i|} \Delta V_i + \mathbf{b}(\mathbf{x}_i, t) \quad (\text{III. 25})$$

where c_{ij} is the bond constant, ψ_{ij} is the bond state function, and $\bar{P}(\mathbf{x}, \mathbf{x}', t)$ is the averaged pore pressure. Previous studies have validated the accuracy of this discretization for coupled hydro-mechanical applications through comparisons with finite element method (FEM) results (Jin et al., 2023).

3.2 Surface and volume correction

Surface and volume corrections are crucial in PD theory to mitigate boundary artifacts caused by incomplete neighbourhoods near material edges. These corrections ensure continuity of material properties and make more accurate the stress/strain prediction, which is the most important issue for modelling fracture propagation.

Firstly, to mitigate inaccuracies near the boundary of a neighborhood domain in PD theory, a volume correction factor will be introduced. The λ_{ij} adjusts the interaction weight between material points x_i and x_j based on the portion of their horizon intersecting the material domain, and is given by:

$$\lambda_{ij} = \begin{cases} 0 & \text{when } |\mathbf{y}_j - \mathbf{y}_i| \geq \delta \\ 1 & \text{when } |\mathbf{y}_j - \mathbf{y}_i| \leq \delta - r \\ \frac{\delta + r - \|\mathbf{y}_j - \mathbf{y}_i\|}{2r} & \text{when } \delta - r \leq |\mathbf{y}_j - \mathbf{y}_i| \leq \delta \end{cases} \quad (\text{III. 26})$$

with $r = \frac{\Delta x}{2}$.

Moreover, at the surface or boundary of the material, the horizon extends beyond the actual material geometry, causing some interactions to be "missing" compared to points deep within the material. This difference can result in inaccuracies in predicting stresses and strains at these boundary points, which are critical for assessing fracture propagation, material failure, and other stress-related phenomena. Therefore, a stiffening factor τ_{ij} , proposed by Le and Bobaru (2018) is employed to account for surface effects. Fig. III. 2 shows a bond connecting two material points $\mathbf{x}_i$ and $\mathbf{x}_j$. The point at $\mathbf{x}_i$ has a neighborhood volume $V(\mathbf{x}_i)$ and the point at $\mathbf{x}_j$ has neighborhood volume $V(\mathbf{x}_j)$. The stiffening factor τ is formulated as:

$$\tau_{ij} = \frac{2V_0}{V(\mathbf{x}_i) + V(\mathbf{x}_j)} \quad (\text{III. 27})$$

where $V_0 = \frac{4\pi\delta^3}{3}$ in three dimensions. Incorporating these corrections, the motion equation becomes:

$$\rho(\mathbf{x}_i)\ddot{\mathbf{u}}(\mathbf{x}_i, t) = \sum_{\mathbf{x}_j \in H_i}^N \tau_{ij} \mathbf{f}_{ij} \lambda_{ij} \Delta V_i + \mathbf{b}(\mathbf{x}_i, t) \quad (\text{III. 28})$$

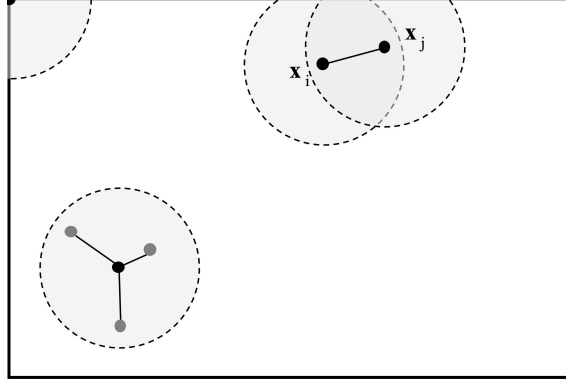


Figure III. 2: Neighborhood of PD points inside the body and near the surface

3.3 Time integration scheme

Concrete drying is a quasi-static process, but traditional explicit time integration in PD is computationally inefficient for such slow-evolving phenomena. To address this, an adaptive dynamic relaxation method, proposed by [Kilic and Madenci \(2010\)](#), is employed. This method adjusts damping parameter and time steps to stabilize convergence. Fig. [III. 3](#) illustrates the numerical workflow for the fully coupled hydro-mechanical BB-PD model, comprising the following stages: Firstly, the simulation begins with the generation and discretization of a meso-scale concrete model, incorporating aggregates of various shapes, and the initialization of calculation parameters such as bond networks, material parameters, surface correction parameters, and boundary conditions. Secondly, time integration starts at zero and progresses with the setting of fluid pressure boundary conditions and updating the fluid pressure at each material point. This step is followed by solving the fluid diffusion equation to calculate the rate of change of pressure. Thirdly, the bond status between material points is assessed and updated. Lastly, the simulation updates the damage values and nodal displacements, including the calculation of crack information. This iterative process continues until the simulation reaches the designated total time. The generation process for a cementitious composite at meso-scale, including cement matrix, aggregate and ITZs, will be detailed in next section.

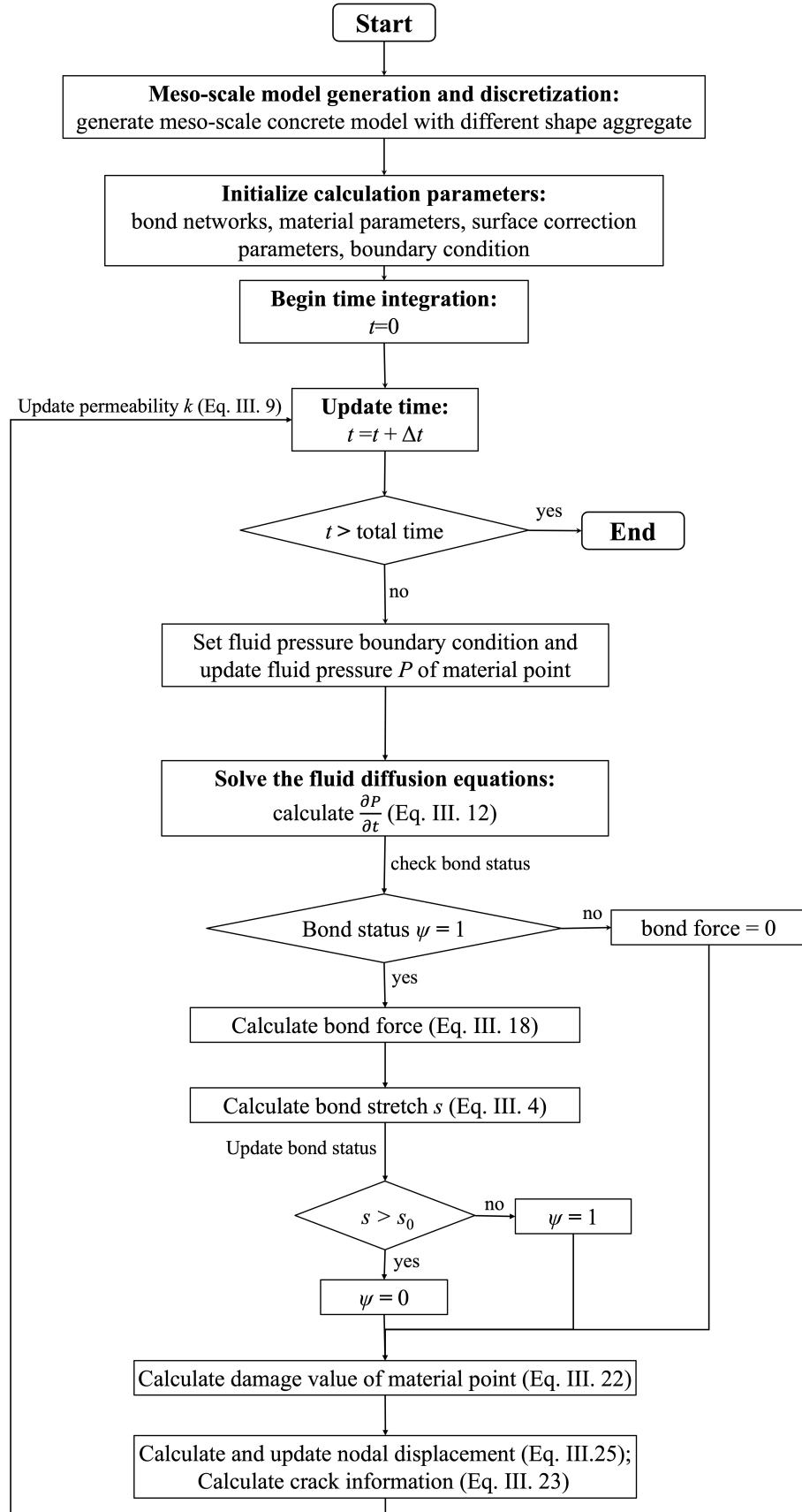


Figure III. 3: Flowchart for the coupled hydromechanical BB-PD model

4 Meso-scale modeling for concrete with aggregates

To investigate the fracture behavior of cementitious composites, a three-dimensional meso-scale model is first constructed, consisting of a cement matrix, coarse aggregates, and interfacial transition zones (ITZs) (Qin et al., 2020). The model generation process accounts for aggregate volume fraction, gradation, and distribution. In this study, a typical aggregate volume fraction of 40% is used (Naderi et al., 2021), and a uniform aggregate size is adopted to isolate the effects of other variables. Aggregates are randomly positioned within the cement matrix using a “Generate-and-Place” algorithm (Zhang et al., 2023a), which ensures non-overlapping placement. A flowchart of the meso-structure generation process is shown in Fig. III. 4.

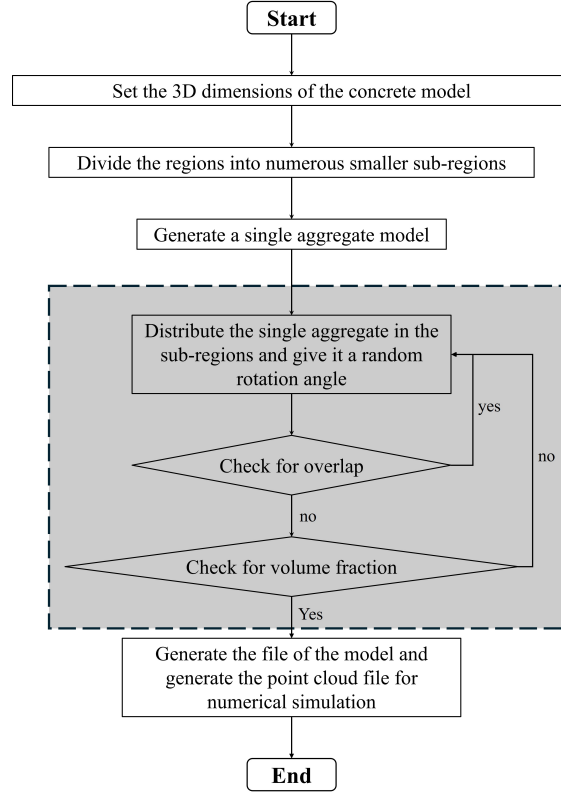


Figure III. 4: Flowchart of the meso-scale model generation process

Following model construction, the PD framework is calibrated using experimental data to ensure accurate representation of material behavior. The influence of aggregate surface roughness on drying shrinkage-induced cracking is first simulated using the calibrated parameters. The study is then extended to assess how aggregate shape affects crack initiation and propagation. Through quantitative comparisons between numerical results

and experimental observations, the meso-scale PD model systematically links ITZ strength and aggregate geometry to macroscopic cracking behavior, providing valuable insights for optimizing the durability of concrete materials.

4.1 Parameter calibration

Accurate parameter calibration is essential to ensure the fidelity of meso-scale simulations to real-world material behavior. The parameters are categorized into two groups: mechanical parameters and hydraulic parameters, as summarized in Table III. 1. Furthermore, the relationship between the water saturation (S_l) and the capillary pressure (p_c) is described by the water retention curve. Based on the experimental results of Li et al. (2018), the following parameters are used: $S_l^r = 0$, $\epsilon = 2.09\text{E-}8$, $n = 1.9$ and $m = 0.47$ are adopted and the water retention curve is then expressed as:

$$S_l = [1 + (2.09 \times 10^{-8} p_c)^{1.9}]^{-0.47} \quad (\text{III. 29})$$

The relative permeability of partially saturated porous medium is defined by the following function (Van Genuchten, 1980):

$$k_r = \sqrt{S_l} \left[1 - \left(1 - S_l^{1/1.9} \right)^{1.9} \right]^2 \quad (\text{III. 30})$$

The mechanical parameters were calibrated using the uniaxial stress-strain compression curves from pure cement mortar (Li et al., 2018). As shown in the Fig. III. 5, ten random damage points were selected from the simulation results. The obtained numerical results are compared with experimental results of Li and Li (2011). One observes that the simulation results align closely with the experimental data, validating the accuracy of the mechanical parameters.

To further validate the hydro-mechanical coupling framework, a concrete disk subjected to drying shrinkage is simulated. The experimental setup involved a concrete disk (100 mm diameter) with stainless steel aggregates (20 mm, 10 mm, and 6 mm diameters) at 41.2% volume fraction. The relationship between capillary pressure and relative humidity (RH) was described by Kelvin's law:

$$-p_c = \frac{RT \ln \text{RH}}{M} \quad (\text{III. 31})$$

where R is the universal gas constant; M is the molar volume of the liquid; T is temperature in Kelvin. The specimen was dried at 25°C and 45% RH for 30 days. In the numerical analysis, the permeability of the stainless steel aggregate is assumed to be zero.

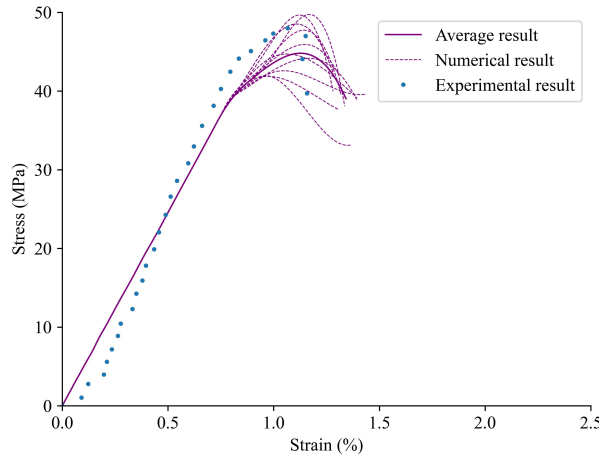


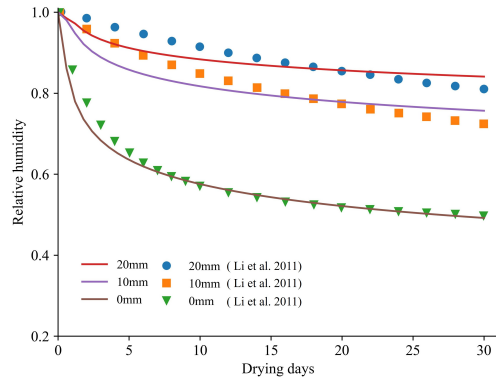
Figure III. 5: Comparison of the stress-strain curves from numerical simulations of uniaxial compression on cement mortar with calibrated parameters against experimental data

The numerical results are presented in Fig. III. 6. Cracks induced by drying shrinkage are predominantly concentrated within 10 to 20 mm from the sample edges (Fig. III. 6(a)). These cracks typically form along the outer sides of aggregates near the surface. The proximity of an aggregate's outer edge to the sample boundary, combined with its size, increases the susceptibility of the surrounding mortar to cracking during drying. Fig. III. 6(c) illustrates the simulated drying crack distribution, showing that shrinkage-induced cracks localize around aggregates. The simulated crack morphology closely matches the experimental observations reported by Li and Li (2011).

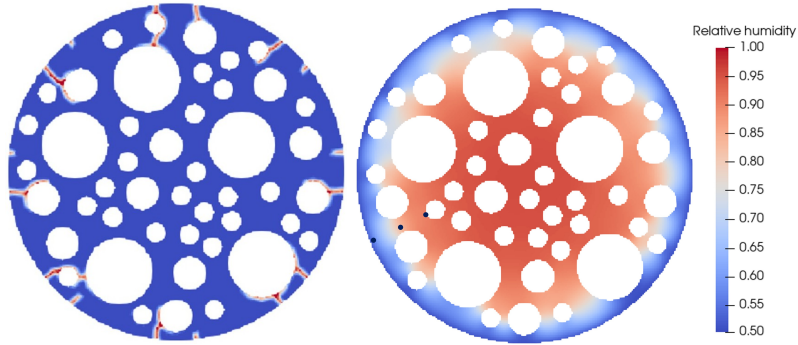
After 30 days of drying, the relative humidity (RH) distribution within the test disk is highly non-uniform (Fig. III. 6(d)). While the surface RH approaches the environmental RH, the interior RH remains above 80%. Significant RH variations are observed within 0–20 mm from the disk boundary. The RH variation at 0 mm, 10 mm, and 20 mm from the boundary is analyzed and presented in Fig. III. 6(b). The results indicate that the concrete disk desaturates progressively, with the desaturation rate decreasing as the distance from the sample boundary increases. These findings are compared with the experimental data from Li and Li (2011). The simulation results exhibit consistent trends and similar values, further validating the reliability of the numerical method.

Table III. 1: Mechanical and hydraulic parameters of cement paste and aggregate.

Parameters	cement paste	aggregate
Elastic modulus E (GPa)	15	68
Poisson's ratio ν	0.25	0.25
Energy release rate G_0 (N/mm)	0.03	0.5
Density ρ (kg/m ³)	1530	2500
Porosity ϕ	0.35	-
Biot coefficient α	0.63	-
Fluid viscosity (Pa·s)	1.00E-03	-
Permeability of intact porous medium k (mm ²)	1.00E-14	-



(a) The test sample and the crack distribution (white part) (b) Relative humidity curve with drying time at 0 mm, 10 mm and 20 mm away from the surface



(c) Drying crack distribution (red part) (d) Relative humidity distribution after 30 days

Figure III. 6: Comparison between experiment and numerical simulation

4.2 Numerical analysis of the influence of aggregate shape on the drying shrinkage cracks

In this section, the influence of aggregate shape on drying shrinkage-induced cracking is systematically analyzed. By employing meso-scale models with identical material properties and volume fractions, but varying aggregate geometries, the role of particle shape in governing crack patterns is isolated and examined. This analysis focuses on key shape descriptors—such as sphericity, flatness, and elongation—and their impact on stress distribution, ITZ development, and crack network connectivity. Through a comparative study of different aggregate shapes, the simulation results aim to reveal how geometric characteristics influence the fracture behavior of cementitious composites and contribute to the design of more crack-resistant concrete. In practice, coarse aggregates typically appear in two forms ([Erdogan et al., 2006](#)): (1) crushed stone, characterized by irregular, rough surfaces, and (2) gravel, which has smoother, rounded shapes. To investigate the effects of aggregate shape on drying shrinkage cracks, two aggregate types are considered: crushed stone, represented by four regular polyhedra (hexahedron, octahedron, dodecahedron, and icosahedron), and gravel, represented by ellipsoids with aspect ratios ranging from 1.25:1.25:1 to 2.0:1. In view of this, two groups of cementitious composites are developed to assess the influence of aggregate shape on drying shrinkage and cracking. The first employs regular polyhedra to represent crushed stone, while the second utilizes ellipsoids to approximate gravel geometry. These shapes are classified based on elongation (major/intermediate axis) and flatness (intermediate/minor axis), providing a quantitative framework for evaluating shape-induced effects on concrete performance.

As illustrated in Fig. III. 7, the concrete model is a cylinder with a diameter of 9 mm and a height of 18 mm. It incorporates spherical aggregates with a diameter of 3 mm, while the volumes of aggregates with other shapes are maintained consistent with the spherical aggregates.

As is well known, the main objective of the present work is to focus on the influence of aggregate shape on drying shrinkage cracks. In practice several characteristics are commonly used to describe aggregate shape, including angularity, sphericity, flatness, elongation, and surface texture. In the present work, sphericity, flatness, and elongation are taken as key aggregate characteristics to study drying shrinkage cracks. This choice is based on their ability to describe the geometric properties of aggregates that directly influence stress distribution and crack behavior in cementitious composites. Sphericity, which measures how closely an aggregate resembles a sphere, promotes uniform stress distribution and reduces cracking due to its smooth surfaces and lack of sharp edges. In

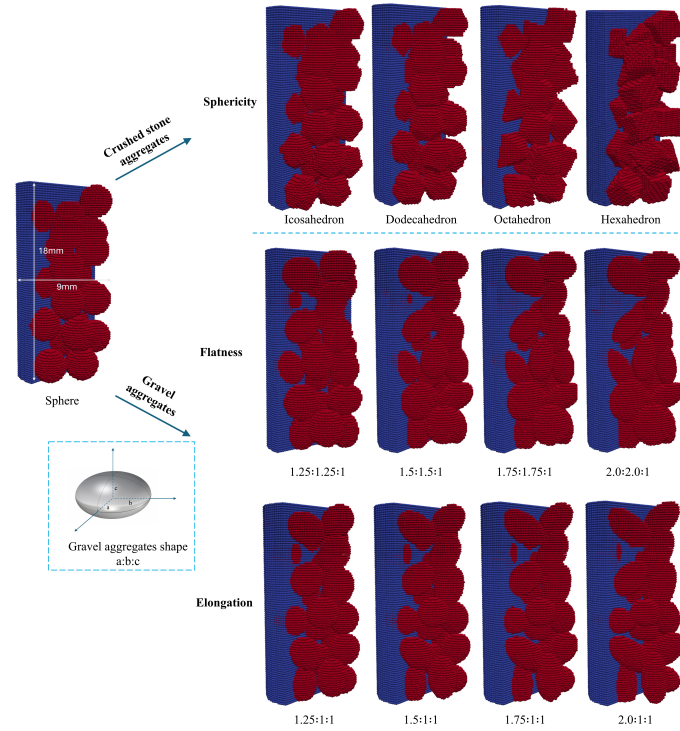


Figure III. 7: Meso-scale concrete model with aggregates of different shape

contrast, Flatness describes the ratio of the shortest dimension (thickness) to the intermediate dimension (width), while elongation refers to the ratio of the longest dimension (length) to the intermediate dimension (width). Therefore, flatness and elongation, which describe how "flat" or "elongated" an aggregate is, create stress concentrations at edges and corners, leading to anisotropic stress fields and directional crack propagation. Flat and elongated aggregates also increase the interfacial transition zone (ITZ) and restrict uniform shrinkage, exacerbating crack formation. Together, these characteristics provide a comprehensive understanding of how aggregate shape impacts drying shrinkage cracks, highlighting the importance of spherical aggregates in minimizing damage and the detrimental effects of flat and elongated aggregates.

4.2.1 Damage

The damage evolution and distribution in cementitious composites with different aggregate shapes are studied in this section. The results are divided into two subsections based on the type of aggregate: gravel aggregate and crushed stone aggregate. We begin with the results for cementitious materials containing gravel aggregate.

Gravel aggregate:

For gravel aggregates, the shape characteristics of elongation and flatness are relevant. Elongation is defined as the ratio of the longest dimension of a particle to its intermediate dimension, while flatness is the ratio of the intermediate dimension to the shortest dimension. These parameters describe the degree to which aggregates deviate from a spherical or equiaxial shape, with higher values indicating more elongated or flatter particles.

Damage distributions on the surface of samples containing aggregates with varying elongation and flatness are shown in Fig. III. 8. It is observed that as the elongation and flatness of the aggregates increase, surface cracks become more numerous and vertical cracks are more prevalent. This damage distribution illustrates the influence of aggregate shape on the mechanical behavior of cementitious composites. Elongated and flat aggregates tend to create anisotropic stress fields, leading to preferential crack propagation along certain directions.

It is important to note that the observed surface damage does not directly correspond to the actual crack distribution within the material. Based on Eq. (III. 23), crack widths in the samples are calculated. As the drying time increases, the crack distribution in samples with aggregates of varying elongation and flatness follows a similar pattern to that of crushed stone aggregates (Fig. III. 10). As shown in Fig. III. 9, by the end of the drying process, the increase in elongation and flatness of the aggregates causes the concrete to be filled with numerous small cracks, most of which are concentrated around the aggregates. Additionally, the crack width on the surface also increases. These results demonstrate that both flatness and elongation significantly influence the distribution of cracks within the concrete. Elongated and flat aggregates exacerbate cracking due to their tendency to create localized stress concentrations and anisotropic crack propagation paths.

Crushed stone aggregate:

Damage distributions on the surface of samples containing aggregates with varying sphericity are shown in Fig. III. 8. It is observed that as aggregate sphericity increases (i.e., aggregates become more spherical), the surface crack distribution becomes more uniform. Conversely, samples with lower sphericity (e.g., hexahedron-shaped aggregates) exhibit more localized and severe surface damage. This observation highlights the significant role of aggregate shape in determining the damage distribution within cementitious materials.

The crack distribution is analyzed at different drying times: $t = 1800$ s, $t = 3600$ s, and $t = 18000$ s. At the end of $t = 18000$ s, the samples are fully dry, marking the end of the drying process.

As shown in Fig. III. 10, significant differences in crack distribution are observed in samples with aggregates of different sphericity at each drying stage. During the early

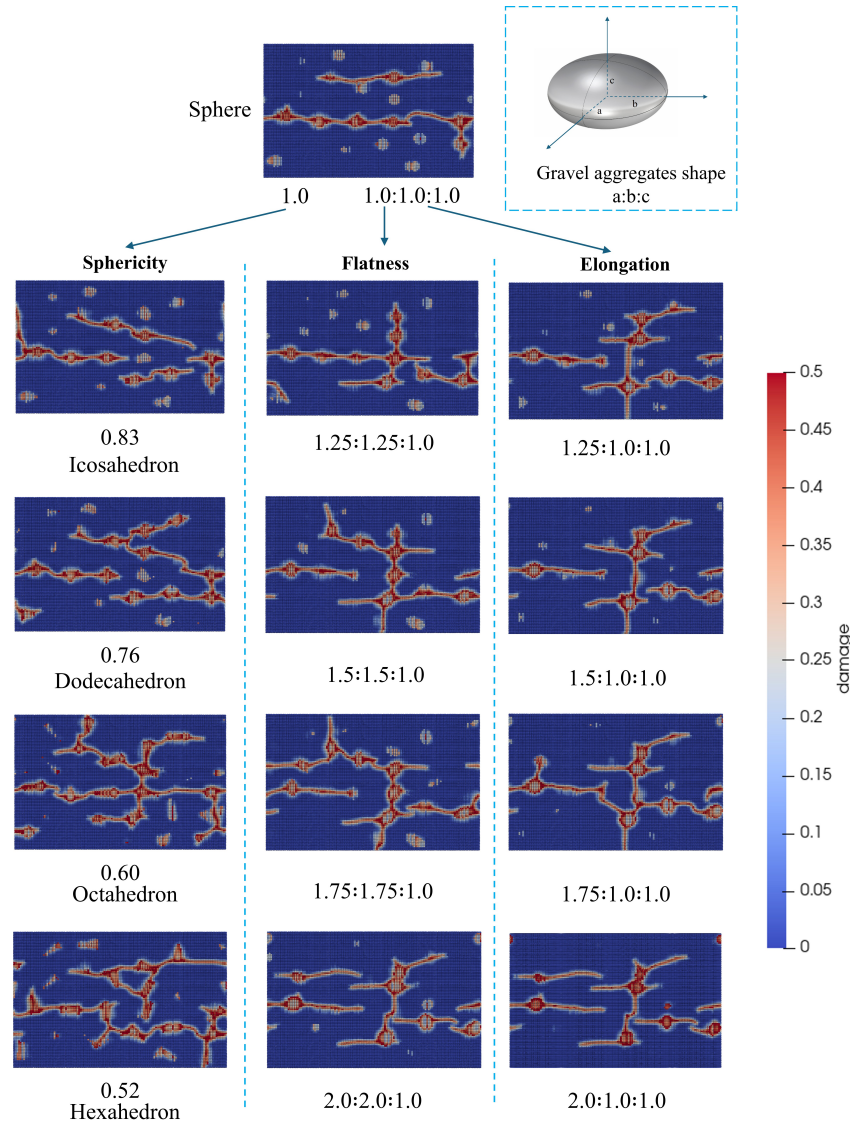


Figure III. 8: Damage distribution in surface of samples with aggregates of varying shape

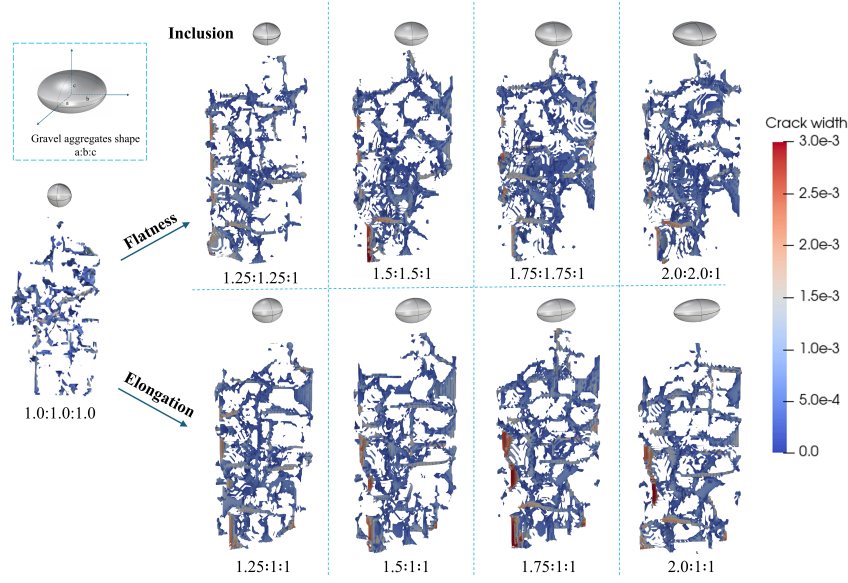


Figure III. 9: Distribution of cracks in samples with aggregates of varying flatness and elongation

drying stage (i.e. $t = 1800$ s), cracks primarily appear on the concrete surface and are relatively wide. As drying continues (i.e. $t = 3600$ s), these surface cracks expand, widening and extending partially into the sample interiors. At the end of the drying process (i.e. $t = 18000$ s), the interior of the concrete is filled with numerous small-width cracks, mostly concentrated around the aggregates. The spatial distribution of these internal cracks varies significantly with aggregate sphericity: as aggregate shapes become more spherical, the number of internal cracks in the samples decreases. This reduction in cracking is attributed to the more uniform stress distribution provided by spherical aggregates, which mitigates localized stress concentrations and crack initiation.

The comparison between crushed stone and gravel aggregates reveals distinct damage mechanisms influenced by aggregate shape. Spherical crushed stone aggregates promote more uniform stress distribution, reducing both surface and internal cracking. In contrast, gravel aggregates with high elongation and flatness create anisotropic stress fields, leading to increased cracking and more severe damage. These findings underscore the importance of aggregate shape in controlling the mechanical performance and durability of cementitious composites, particularly under drying conditions.

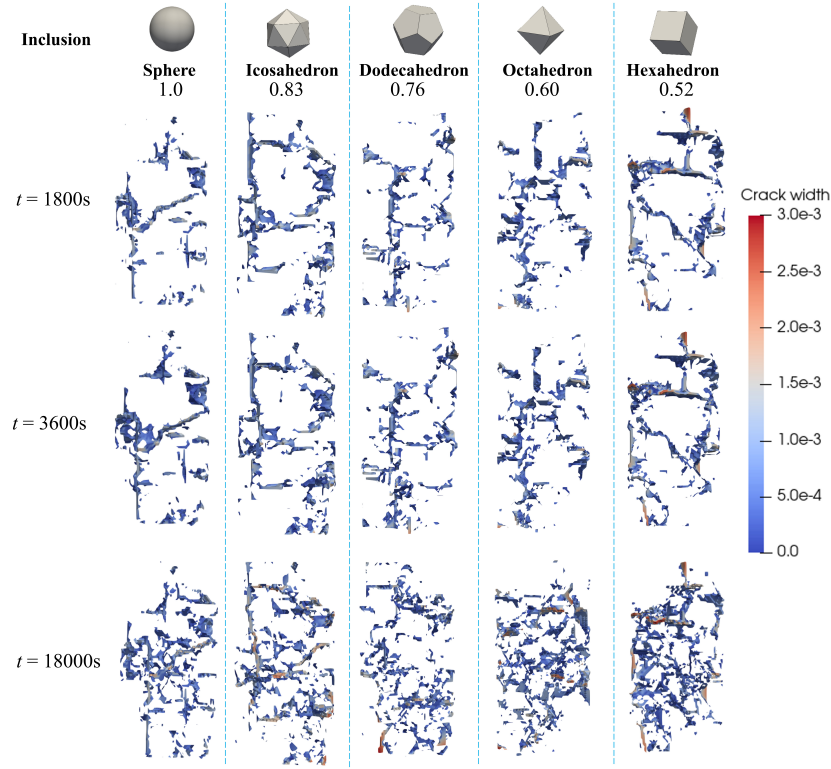


Figure III. 10: Distribution of cracks in samples with aggregates of varying sphericity at different drying times

4.2.2 Crack characteristics

To further examine the differences in cracking across samples, the crack characteristics in the samples are studied, including crack length, average crack width, and crack volume. To ensure representative results, five concrete models corresponding to each aggregate type are randomly generated and statistically analyzed.

The crack length l_c is calculated as the sum of the element sizes l_i divided by 2:

$$l_c = \sum_{i=1}^{n_c} l_i / 2 \quad (\text{III. 32})$$

where l_i denotes the element size Δx ; n_c is the number of cracked elements. The average crack width w_c is determined by averaging the width w_i of all cracks elements:

$$w_c = \frac{\sum_{i=1}^{n_c} w_i}{n_c} \quad (\text{III. 33})$$

where w_i is calculated by Eq. (III. 23). And the crack volume v_c is computed by

$$v_c = l_c w_c \Delta x \quad (\text{III. 34})$$

The influence of sphericity on the crack characteristics is firstly analysed. As shown in Fig. III. 11 (a), crack length decreases significantly as sphericity increases from 0.5 to 1.0, dropping from nearly 1600 mm to around 1000 mm. This indicates that aggregates with higher sphericity lead to shorter cracks, as their rounded shapes promote more uniform stress distribution and reduce localized stress concentrations. Crack volume also shows a clear downward trend, decreasing from $8\text{E-}4 \text{ mm}^3$ to approximately $5\text{E-}4 \text{ mm}^3$, further demonstrating the beneficial effect of spherical aggregates in mitigating crack formation and propagation. The average crack width fluctuates slightly between sphericity values of 0.5 and 0.8 but gradually decreases as sphericity approaches 1.0, suggesting that higher sphericity generally helps to maintain narrower cracks, although the effect is less pronounced than on crack length.

In Fig. III. 11 (b), the effects of elongation on crack characteristics are shown. As elongation increases from 1.0 to 2.0, crack length gradually rises from about 1000 mm to nearly 1200 mm, indicating that more elongated aggregates tend to produce longer cracks due to their anisotropic shape, which creates stress concentrations at their sharp edges. Crack volume also increases with higher elongation, suggesting that aggregates with greater elongation contribute to a larger total crack volume. This is attributed to the increased stress concentrations and reduced ability of elongated aggregates to accommodate shrinkage stresses. However, the average crack width increases only slightly, implying that elongation has a relatively minor effect on crack width compared to its impact on crack length and volume.

Fig. III. 11 (c) illustrates the effects of flatness on crack characteristics. As flatness increases from 1.0 to 2.0, crack length shows a gradual upward trend, rising from approximately 1000 mm to nearly 1400 mm, suggesting that flatter aggregates are associated with longer cracks, as their plate-like shape creates stress concentrations and promotes crack propagation. Crack volume also increases as flatness rises, going from about $5\text{E-}4 \text{ mm}^3$ to close to $6\text{E-}4 \text{ mm}^3$, indicating that flatter aggregates lead to a larger crack volume. However, the average crack width changes minimally, with only minor fluctuations, suggesting that flatness has a limited impact on crack width compared to its influence on crack length and volume.

In summary, sphericity has the most pronounced effect on controlling cracks, with higher sphericity effectively reducing crack length and volume, thereby enhancing concrete integrity during the drying process. Flatness and elongation also affect crack length and volume, though to a lesser extent, with flatness having a stronger influence than elongation. Both parameters exacerbate cracking due to their tendency to create stress concentrations

and anisotropic stress fields.

4.3 Discussion

To focus on how the shapes of crushed stone aggregates and gravel aggregates influence crack characteristics, Hakon Wadell's sphericity parameter HW_s is introduced. Wadell's sphericity is defined as the ratio of the surface area of a sphere with the same volume as the aggregate to the actual surface area of the aggregate:

$$HW_s = \frac{A_s}{A} \quad (\text{III. 35})$$

where A is the aggregate's surface area, and A_s is the surface area of a sphere with the same volume. The parameter HW_s ranges from 0 to 1, with a value of 1 representing a perfect sphere.

The relationship between the sphericity parameter HW_s and various crack characteristics is then analyzed. In Fig. III. 12(a), the crack length decreases significantly as HW_s increases from 0.8 to 0.9, with a steep decline from approximately 1600 mm to around 1200 mm. Beyond $HW_s = 0.9$, the crack length exhibits minor fluctuations but remains relatively stable, indicating that higher sphericity substantially reduces crack propagation. This reduction in crack length is attributed to the more uniform stress distribution provided by spherical aggregates, which mitigates localized stress concentrations and crack initiation. In Fig. III. 12(b), the crack width increases slightly up to $HW_s = 0.9$ and then stabilizes with minor fluctuations around a narrow range. This suggests that while the effect of sphericity on crack width is less pronounced than on crack length, aggregates with higher sphericity still maintain relatively narrower cracks. The stabilization of crack width at higher sphericity values further underscores the beneficial role of spherical aggregates in controlling development. Fig. III. 12(c) demonstrates that the crack volume exhibits a clear downward trend with increasing HW_s . This decrease in crack volume highlights the ability of spherical aggregates to minimize the overall damage caused by drying shrinkage, as they promote more uniform stress distribution and reduce the likelihood of crack formation and propagation.

Moreover, the results indicate that the influence of changes in the elongation and flatness of pebbles on crack characteristics is relatively small. This is primarily because variations in these two parameters have a minimal effect on the sphericity parameter (HW_s), resulting in limited changes in crack length, crack volume, and crack width. This further highlights the critical role of the sphericity parameter in describing the impact of aggregate shape on the crack characteristics of concrete.

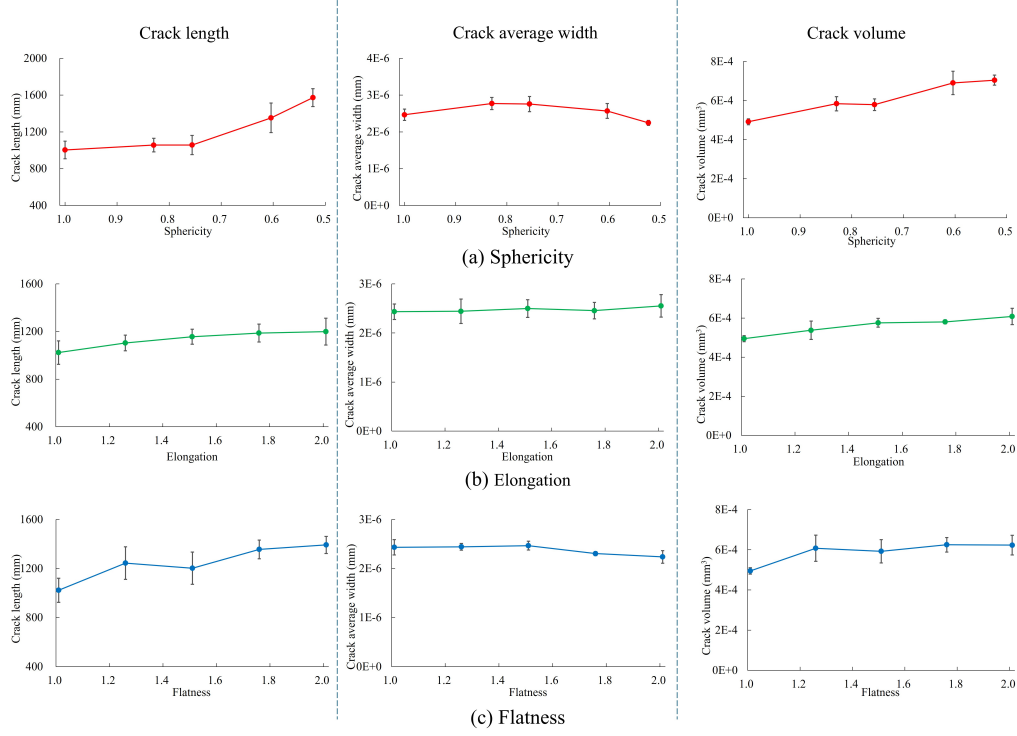


Figure III. 11: Crack information in samples with aggregates of varying shape: (a) Sphericity; (b) Elongation; (c) Flatness

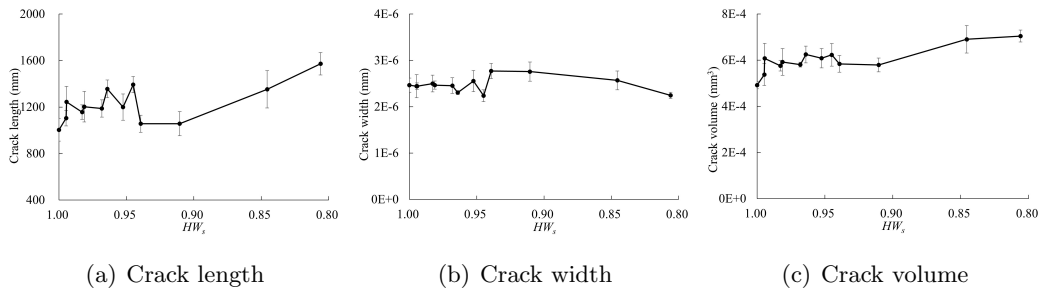


Figure III. 12: Crack information in samples with aggregates of varying HW_s

5 Conclusion

This study combines experimental characterization with a bond-based, fully coupled hydro-mechanical BB-PD model to investigate drying shrinkage-induced cracking in concrete at the meso-scale. The model is validated against experimental results, and concrete meso-structures incorporating aggregates with varying surface roughness and shapes are constructed to simulate the drying process. Based on this integrated experimental–numerical approach, the following key conclusions are drawn:

1. The peridynamic simulations show strong agreement with 3D crack segmentation results from X-ray tomography, both in crack volume and network morphology, validating the model’s effectiveness in linking ITZ properties and aggregate characteristics to macroscopic fracture behavior.
2. Aggregate shape plays a critical role in determining surface damage and crack propagation patterns in drying cementitious composites. Sphericity of aggregate improvements from 0.5 to 1.0 decreased crack length and volume by approximately 37.5%, indicating enhanced stress distribution. Conversely, elongation of aggregate increases from 1.0 to 2.0 resulted in a 20% growth in crack length, and flatness increases led to a 40% rise in crack length, both exacerbating crack formation due to anisotropic stress fields.
3. A detailed analysis of crack patterns associated with different aggregate shapes reveals that sphericity is the most influential parameter in controlling crack formation. Higher sphericity significantly reduces crack length and volume. While flatness and elongation also affect crack characteristics, their influence is comparatively weaker, with flatness exerting a stronger effect than elongation.

The obtained results highlight the critical role of aggregate surface roughness and geometry in mitigating drying shrinkage cracking and underscore the importance of aggregate selection in the design of durable concrete structures. Future research should explore the combined effects of aggregate composition, size, and shape under varying environmental conditions, such as fluctuations in humidity and temperature. Such investigations will contribute to the development of optimized concrete mixtures with enhanced resistance to cracking, ultimately advancing the durability and sustainability of concrete structures.

Chapter IV

A modified Peridynamic interface method for fracture analysis of concrete

1 Introduction

The Interfacial Transition Zone (ITZ) is a thin region surrounding coarse aggregates in concrete, typically ranging from 10 to 50 micrometers in thickness. Due to the wall effect and bleeding during casting, this zone exhibits higher porosity and a lower degree of hydration compared to the bulk cement paste. As a result, the ITZ is mechanically weaker and more brittle, often serving as the preferential path for microcrack initiation and propagation. Understanding and accurately modeling the ITZ is crucial for predicting the mechanical performance and fracture behavior of cementitious composites.

To capture the complex mechanical response of the ITZ, the Ordinary State-Based Peridynamic (OSB-PD) model is adopted. Unlike the Bond-Based formulation, which only allows isotropic pairwise interactions with limited material behavior, OSB-PD introduces vector-valued force and deformation states that account for the collective influence of all neighborhood. This framework enables the incorporation of heterogeneous material properties, stiffness mismatch, and direction-dependent interactions, which are essential for accurately simulating the ITZ. By using OSB-PD, it becomes possible to model interfacial damage, imperfect bonding, and localized failure mechanisms with improved physical fidelity, making it a powerful tool for investigating cracking phenomena at the meso-scale in concrete.

To address the limitations of conventional peridynamic formulations in modeling in-

terfacial behavior, a modified peridynamic interface method is developed. This approach introduces an imperfect interface representation within the OSB-PD framework to better capture the distinct mechanical properties and damage evolution of the ITZ. By adjusting the force state interactions across the interface and incorporating stiffness reduction or damage initiation criteria, the modified method allows for a more realistic simulation of debonding, crack deflection, and interfacial failure. This enhancement is particularly important for heterogeneous materials like concrete, where the ITZ governs the initiation and propagation of shrinkage-induced or mechanically driven cracks. The proposed method enables more accurate prediction of fracture processes at the meso-scale, bridging the gap between microstructural features and macroscopic mechanical response.

2 Modified peridynamic interface model

2.1 The ordinary state-based peridynamic model

The OSB-PD model is a nonlocal continuum mechanics framework that enables more general constitutive behavior than the Bond-Based Peridynamic (BB-PD) model. In OSB-PD, the internal forces between material points are determined by state variables, which depend on the collective deformation of all neighborhood points within a finite horizon. A "state" is a mathematical construct that characterizes how a material point interacts with its neighborhood, allowing the formulation of force and deformation as vector- or tensor-valued functions. Unlike BB-PD, which defines forces solely based on pairwise relative displacements and imposes restrictions such as a fixed Poisson's ratio, the OSB-PD model captures a wider range of material behaviors and complex fracture phenomena in heterogeneous materials.

$$\rho(\mathbf{x}_i) \ddot{\mathbf{u}}(\mathbf{x}_i, t) = \int_H \{ \underline{\mathbf{T}}[\mathbf{x}_i, t] \langle \mathbf{x}_j - \mathbf{x}_i \rangle - \underline{\mathbf{T}}[\mathbf{x}_j, t] \langle \mathbf{x}_i - \mathbf{x}_j \rangle \} dV + \mathbf{b}(\mathbf{x}_i, t) \quad (\text{IV. 1})$$

where ρ is the mass density, $\ddot{\mathbf{u}}$ is the acceleration quantity vector, $\mathbf{b}$ is a prescribed body force density; H is the neighborhood domain of the point $\mathbf{x}_i$; with the cut-off radius of nonlocal horizon δ . $\boldsymbol{\xi} = \mathbf{x}_j - \mathbf{x}_i$ is the bond vector as shown in Fig. IV. 1, $\underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle$ and $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ are the reference and deformed vectors of bond $\boldsymbol{\xi}$, and $\underline{\mathbf{T}}[\mathbf{x}_i, t]$ and $\underline{\mathbf{T}}[\mathbf{x}_j, t]$ are the force vector states of points $\mathbf{x}_i$ and $\mathbf{x}_j$. In the ordinary state-based peridynamic theory, the bond force vector can be expressed with the force scalar state t as:

$$\underline{\mathbf{T}}[\mathbf{x}_i, t]\langle\boldsymbol{\xi}\rangle = t\langle\boldsymbol{\xi}\rangle \frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|} \quad (\text{IV. 2})$$

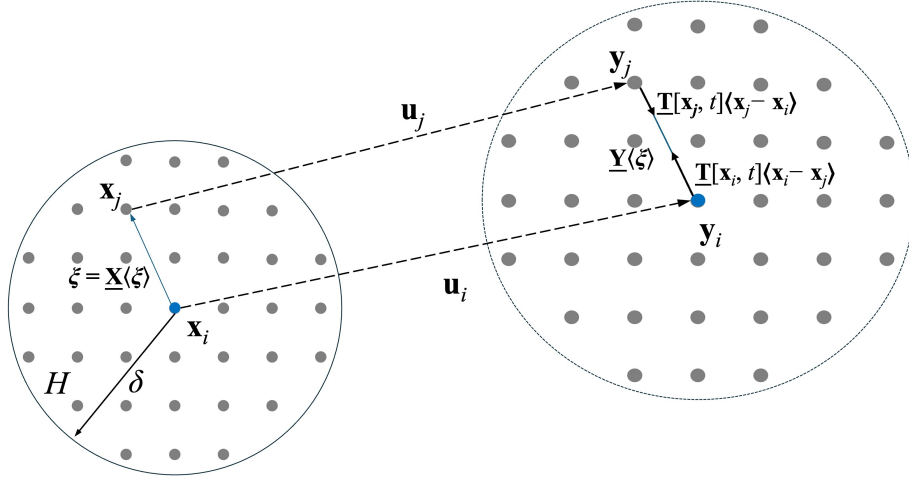


Figure IV. 1: The ordinary state-based peridynamic model

The hydro-mechanically coupled peridynamic constitutive model is defined as a linear peridynamic solid that accounts for the effect of pore fluid pressure on the deformation energy, whose elastic energy density W is expressed as

$$W = \frac{\kappa}{2}\Theta^2 + \frac{\alpha}{2}(\underline{\omega e}) \bullet e - \bar{\beta}\Theta p \quad (\text{IV. 3})$$

where κ , α and $\bar{\beta}$ are the peridynamic constants. After some rearrangement, the scalar force state $\underline{t}$ of the material points takes the form of:

$$\underline{t} = (\kappa\Theta - \bar{\beta}p)\nabla_{\underline{e}}\Theta + \alpha\underline{\omega e} \quad (\text{IV. 4})$$

where $\underline{\omega}$ is the influence function, p is fluid pore pressure. The pore-pressure field is computed using the unsaturated seepage algorithm introduced in Chapter III. And the peridynamic coupling coefficient $\bar{\beta}$ is taken identical to that used in Chapter III. The extension scalar state $\underline{e}$ is defined as: where $\underline{\omega}$ is the influence function; $\underline{e}$ is the extension scalar state can be expressed as:

$$\underline{e} = |\underline{Y}| - |\underline{X}| \quad \text{or} \quad \underline{e}(\underline{\xi}) = |\underline{Y}(\underline{\xi})| - |\underline{\xi}| \quad \forall \underline{\xi} \in H \quad (\text{IV. 5})$$

And Θ is the volume dilatation. $\nabla_{\underline{e}}\Theta$ is the Frechet derivative of Θ with respect to $\underline{e}$. Θ and $\nabla_{\underline{e}}\Theta$ are written as:

$$\Theta = \begin{cases} 3\frac{\underline{\omega x} \bullet \underline{e}}{q}; & \nabla_{\underline{e}}\Theta = 3\frac{\underline{\omega x}}{q}; & 3\text{D} \\ 2\frac{\underline{\omega x} \bullet \underline{e}}{q}; & \nabla_{\underline{e}}\Theta = 2\frac{\underline{\omega x}}{q}; & 2\text{D} \end{cases} \quad (\text{IV. 6})$$

where $\underline{x}$ is equal to bond length $|\underline{\xi}|$; q is the weighted volume that is defined as $\underline{\omega x} \bullet \underline{x}$, and the symbol $(\bullet)$ is the dot product of two states as $\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} = \int_H (\underline{\mathbf{A}} \underline{\mathbf{B}}) \langle \underline{\xi} \rangle dV$. κ and α are the constants related to the bulk modulus K and the shear modulus G . The relations among them in different cases can be expressed as follows (Silling et al., 2007; Zhang and Qiao, 2018):

$$\begin{aligned} \kappa &= K - \frac{5G}{3}; \quad \alpha = \frac{15G}{q}; \quad 3D \\ \kappa &= K - 2G; \quad \alpha = \frac{8G}{q}; \quad 2D \end{aligned} \quad (\text{IV. 7})$$

Unlike the BB-PD formulation, the OSB-PD model does not contain physical bonds between point pairs; the term bond is used only in a loose sense to represent the interaction potential between two material points (Foster et al., 2011). Nevertheless, the classical bond-stretching criterion remains applicable: when the deformation of the interaction between two points exceeds a prescribed critical stretch, that interaction is irreversibly broken. The stretch s of the bond is defined as:

$$s = \frac{|\underline{\mathbf{Y}}| - |\underline{\mathbf{X}}|}{|\underline{\mathbf{X}}|} \quad (\text{IV. 8})$$

Cracks initiate and propagate as many such broken interactions coalesce to form a surface. As shown in Fig. IV. 2, the energy density of $\mathbf{x}_i$ is lost due to the separation of H_r from the whole region H caused by the crack plane. The energy density loss W_r of $\mathbf{x}_i$ is

$$W_s = \frac{k}{2} \Theta_s^2 + \frac{\alpha}{2} \int_{H_s} \underline{\omega} \langle \underline{\xi} \rangle \underline{e} \langle \underline{\xi} \rangle \underline{e} \langle \underline{\xi} \rangle dV \quad (\text{IV. 9})$$

to compute the released energy at point $\mathbf{x}_i$, it is assumed that the bond stretch of all interaction vectors $\underline{\xi}$ crossing the crack surface reaches the critical stretch value s_0 . Under this assumption, the corresponding extension scalar is $\underline{e} = s_0 \underline{x}$. For 3D state-based peridynamic model, according to the definition of Θ in Eq. (IV. 6), the volume dilation caused by all broken bond is:

$$\Theta_s = 3 \frac{\underline{\omega x} \bullet \underline{e}}{q} = 3 \frac{\int_{H_s} \underline{\omega x}^2 s_0 dV}{\int_H \underline{\omega x}^2 dV} = 3\eta(z)s_0 \quad (\text{IV. 10})$$

where $\eta(z)$ is the the ratio of the volume weight from the points in the H_s domain to the volume weight from the points in the whole horizon, defined as:

$$\eta(z) = \frac{\int_{H_s} \underline{\omega x}^2 dV}{\int_H \underline{\omega x}^2 dV} = \frac{\int_{H_s} \underline{\omega x}^2 dV}{q} \quad (\text{IV. 11})$$

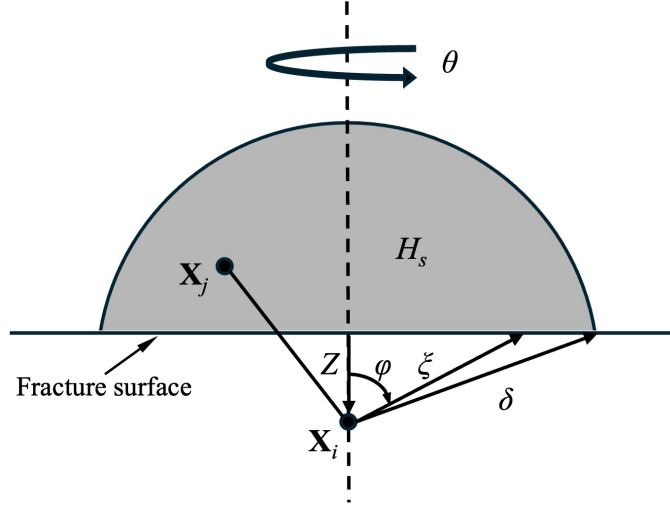


Figure IV. 2: General 3D model case to determine the critical bond value in peridynamic failure criterion

which is a function of the distance z from point $\mathbf{x}_i$ to the crack plane, since the reduced horizon H_s depends on z . Assuming that the bond stretch of all bonds crossing the crack surface reaches the critical value s_0 , Eq. (IV. 9) can be rewritten as

$$W_s = \frac{s_0^2}{2} (9\kappa\eta^2 + \alpha q\eta) \quad (\text{IV. 12})$$

Then, k and α are calculated by Eq. (IV. 7). The total released energy at unit area is equal to the critical energy release rate G_0 , which is expressed as

$$G_0 = 2 \int_0^\delta W_s dz \quad (\text{IV. 13})$$

According Eq. (IV. 12) and Eq. (IV. 13), the relations between the critical stretch S_0 and the critical energy release rate G_0 in the ordinary state-based peridynamics in the 3D can be given as:

$$s_0 = \sqrt{\frac{G_0}{9\kappa I_1 + \alpha q I_2}} \quad (\text{IV. 14})$$

in which $I_1 = \int_0^\delta \eta(z)^2 dz$ and $I_2 = \int_0^\delta \eta(z) dz$. It has been proven in [Zhang and Qiao \(2018\)](#) that the relations in Eq. (IV. 14) can be reduced to the bond-based version within the limitations of $\nu = 1/4$ in 3D and 2D plane strain cases and $\nu = 1/3$ in 2D plane stress cases when the influence function is chosen as $\omega(\xi) = \delta/\underline{x}(\xi)$. In this study, the influence function is chosen as gaussian form $\omega(\xi) = \exp[-(\underline{x}(\xi)/\delta)^2]$, which tends to give smoother results with less apparent ringing in the solution ([Aksoylu and Gazonas, 2020](#)). And I_1 and I_2 can be solved as

$$I_1 \approx 0.0645\delta; \quad I_2 \approx 0.2002\delta \quad (\text{IV. 15})$$

2.2 KGD Hydraulic Fracture Validation

To verify the reliability of the proposed hydro-mechanical coupled PD model for hydraulic fracture propagation problems, A storage-viscosity (M-vertex) KGD problem with crack propagation is constructed (Geertsma and Haafkens, 1979; Nguyen et al., 2017). The computational domain is a 10 m $\times$ 10 m homogeneous isotropic permeable medium. A horizontal pre-crack of length 0.05 m is preset at the center of the model. The pre-crack is represented by a bond-broken region, initially closed and driven to open and propagate solely by internal fluid injection.

The solid mechanics parameters are selected based on the reservoir rock properties adopted (Li et al., 2022a): Young's modulus $E = 17$ GPa, Poisson's ratio $\nu = 0.2$, fracture energy $G_f = 300$ N/m. The medium permeability is $k = 1.0 \times 10^{-15}$ m², Biot coefficient $\alpha = 0.9$, Biot modulus $Q_b = 6$ GPa, to reflect the poro-compressibility of low-permeability tight reservoirs. The fluid is Newtonian with viscosity $\mu_f = 0.1$ Pa $\cdot$ s. The discretization employs uniform PD nodes, with spacing Δx refined to 0.025 m, with horizon $\delta = 3.015$. And the PD model uses consistent material and fluid parameters.

Fluid injection is applied as a constant volumetric flux $Q = 1.0 \times 10^{-4}$ m²/s at the center of the pre-crack, corresponding to a line source under plane-strain unit thickness conditions, with time step $\Delta t = 0.001$ s for quasi-static evolution of fluid pressure and structural response.

For comparison with the classical storage-viscosity dominated M-vertex KGD analytical solution, three quantities are recorded over time: fracture length $l(t)$, fracture width $w(t)$, and injection point fluid pressure $p(t)$. The analytical solutions are:

$$\begin{aligned} l(t) &= 0.48 \left(\frac{GQ^3}{\mu_f(1-\nu)} \right)^{1/6} t^{2/3}, \\ w(t) &= 1.32 \left(\frac{\mu_f(1-\nu)Q^3}{G} \right)^{1/6} t^{1/3}, \\ p(t) &= 1.38 \left(\frac{G^3Q}{\mu_f(1-\nu)^3 l(t)^2} \right)^{1/4}, \end{aligned} \tag{IV. 16}$$

where $G = E/(2(1+\nu))$ is the shear modulus.

As shown in Fig. IV. 3, all numerical results are in good agreement with the corresponding analytical solutions. As illustrated in Fig. IV. 4, the PD model successfully captures crack initiation and propagation under fluid injection, demonstrating its capability to accurately simulate fluid-driven fracture processes.

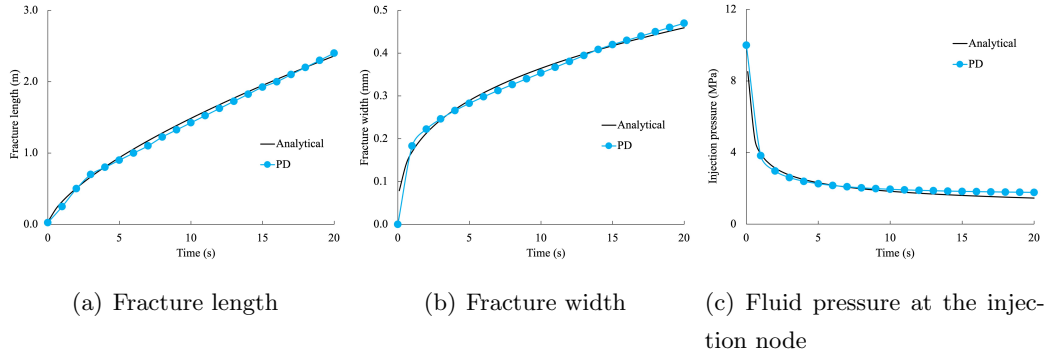


Figure IV. 3: Comparison of analytical solutions and numerical results with different internal length scale parameters of the KGD model

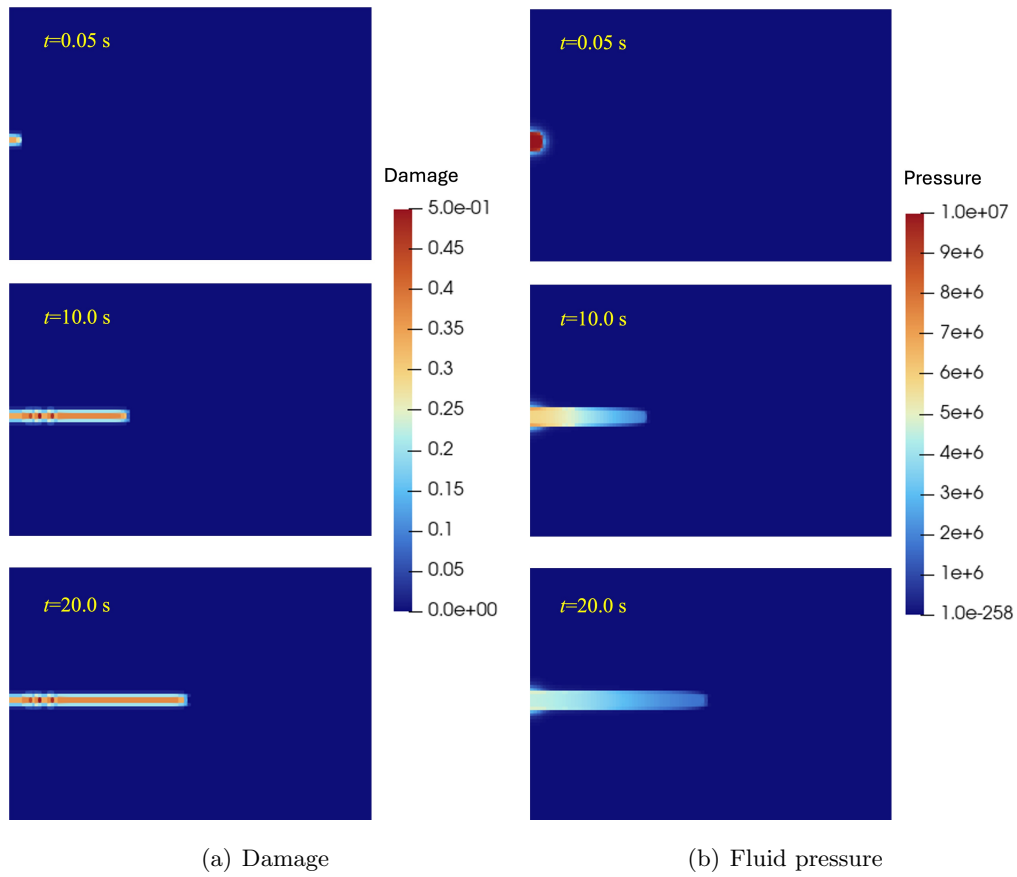


Figure IV. 4: Damage (a) and fluid pressure (b) evolutions of the KGD model in the 5.0 m x 3.0 m zone

2.3 The bond force of the OSB-PD interface bond

In the traditional peridynamic bimaterial model, the horizons of points located near the material interface extend across both material 1 and material 2 regions (see Fig. IV. 5). As a result, points belonging to different materials can interact through their connecting bonds, referred to as peridynamic interface bonds. Although the material interface is not explicitly defined in the model, internal forces can still be transmitted across the interface via these nonlocal bonds. In other words, while the force state at a point $\mathbf{x}_1$ is evaluated using the material parameters of material 1, its deformation state—characterized by the volume dilatation θ and the extension state $\underline{e}$ —is influenced by the deformation of all neighborhood points within its horizon, part of which lies within the material 2 domain.

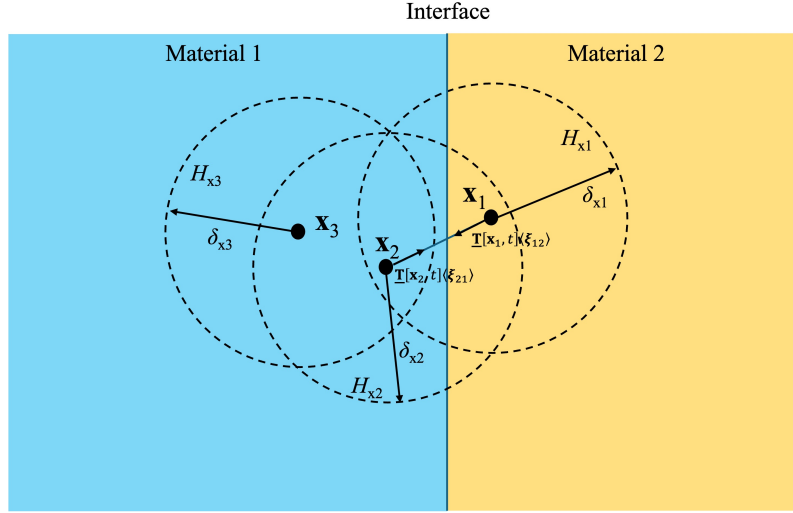


Figure IV. 5: Peridynamic bimaterial system

As shown in Fig. IV. 5, the bond force of point $\mathbf{x}_1$ effect by $\mathbf{x}_2$ through their connecting interface bond is given by:

$$\mathbf{f}[\mathbf{x}_1, t] \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle = \underline{\mathbf{T}}[\mathbf{x}_1, t] \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle - \underline{\mathbf{T}}[\mathbf{x}_2, t] \langle \mathbf{x}_1 - \mathbf{x}_2 \rangle \quad (\text{IV. 17})$$

Considering Eq. (IV. 2), Eq. (IV. 17) can be further expanded as:

$$\mathbf{f}[\mathbf{x}_1, t] \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle = (t[\mathbf{x}_1] \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle + t[\mathbf{x}_2] \langle \mathbf{x}_1 - \mathbf{x}_2 \rangle) \frac{\underline{\mathbf{Y}} \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle}{|\underline{\mathbf{Y}} \langle \mathbf{x}_2 - \mathbf{x}_1 \rangle|} \quad (\text{IV. 18})$$

where $t[\mathbf{x}_1]$ and $t[\mathbf{x}_2]$ are the force scalar states of points $\mathbf{x}_1$ and $\mathbf{x}_2$, which belong to material 1 and 2, respectively, and they can be calculated by Eq. (IV. 4).

Similarly, the bond force of point $\mathbf{x}_2$ effected by $\mathbf{x}_1$ is:

$$\mathbf{f}[\mathbf{x}_2, t]\langle \mathbf{x}_1 - \mathbf{x}_2 \rangle = (\underline{t}[\mathbf{x}_1]\langle \mathbf{x}_2 - \mathbf{x}_1 \rangle + \underline{t}[\mathbf{x}_2]\langle \mathbf{x}_1 - \mathbf{x}_2 \rangle) \frac{\underline{\mathbf{Y}}\langle \mathbf{x}_1 - \mathbf{x}_2 \rangle}{|\underline{\mathbf{Y}}\langle \mathbf{x}_1 - \mathbf{x}_2 \rangle|} = -\mathbf{f}[\mathbf{x}_1, t]\langle \mathbf{x}_2 - \mathbf{x}_1 \rangle \quad (\text{IV. 19})$$

Thus, the linear admissibility condition for the interaction force of the peridynamic interface bond is satisfied, which further ensures the fulfillment of the linear momentum balance in the bimaterial system. Additionally, due to the characteristics of the OSB-PD model described in Eq. (IV. 2), the balance of angular momentum is also inherently satisfied. Typically, considering the limitations on Poisson's ratio in the bond-based peridynamic formulation, and adopting a commonly used influence function $\underline{\omega} = \delta/|\boldsymbol{\xi}|$, the scalar force state $\underline{t}$ of points in material i can be reduced into:

$$\underline{t} = \frac{1}{2}c_i \underline{s} \quad (\text{IV. 20})$$

where $\underline{s}$ is the bond stretch scalar state defined as $\underline{s} = \underline{e}/|\boldsymbol{\xi}|$, and c_i is the peridynamic constant of material i in bond-based peridynamic model, which can be expressed as:

$$c_i = \begin{cases} \frac{18K_i}{\pi\delta^4}; & 3\text{D} \\ \frac{12K_i}{\pi\delta^3 S}; & 2\text{D} \\ \frac{2E_i}{h\delta^2}; & 1\text{D} \end{cases} \quad (\text{IV. 21})$$

where K_i and E_i are the bulk and elastic modulus of material i , respectively; S and h are the thickness and cross section for the 2D and 1D models, respectively. Then, the interaction force of the peridynamic interface bond can be rewritten as

$$\mathbf{f}[\mathbf{x}_1, t]\langle \mathbf{x}_2 - \mathbf{x}_1 \rangle = \frac{1}{2}(c_1 + c_2)\underline{s} \frac{\underline{\mathbf{Y}}\langle \mathbf{x}_2 - \mathbf{x}_1 \rangle}{|\underline{\mathbf{Y}}\langle \mathbf{x}_2 - \mathbf{x}_1 \rangle|} \quad (\text{IV. 22})$$

which is equal to the bond-based peridynamic interface model.

It can be observed that in the traditional OSB-PD model, the two-material interface problem is addressed by modifying the constitutive relation for bonds that span across materials with different properties. Each material point retains its own intrinsic elastic properties, such as bulk and shear moduli, and the interactions between points within the same material domain follow the standard OSB-PD formulation. For bonds crossing the material interface, effective material properties—typically defined as the arithmetic mean of the moduli from both sides—are employed to evaluate the force state. This approach enables continuity of interaction across the interface while maintaining material heterogeneity in the peridynamic framework.

However, this approach assumes a perfectly bonded interface and therefore cannot represent displacement or traction discontinuities across material boundaries. As a result, it fails to accurately capture interfacial debonding or sliding, which are prevalent in heterogeneous materials such as concrete. This limitation is particularly critical when modeling the ITZ—a thin, mechanically weaker region surrounding aggregates that often governs crack initiation and propagation. Due to its higher porosity and weaker bonding characteristics, the ITZ is prone to partial separation, interfacial slip, and localized failure under mechanical loading. These behaviors require an interface model that can differentiate between normal and tangential deformation components to determine whether failure is driven by tensile opening or shear sliding. The traditional OSB-PD formulations, which lack this capability, are thus insufficient for capturing the mode-specific fracture mechanisms occurring at such interfaces.

To overcome these limitations, and inspired by the work of [Zhang et al. \(2024\)](#), a modified three-dimensional peridynamic interface formulation is introduced in the following section. This model explicitly accounts for the mechanical response of imperfect interfaces by permitting displacement discontinuities and prescribing a traction–displacement jump relationship, thereby enabling accurate simulation of debonding, sliding, and mixed-mode fracture within the ITZ at the mesoscale.

2.4 Imperfect interface in peridynamics

For the imperfect interface, as illustrated in Fig. IV. 6, displacements are discontinuous across the interface, while traction vectors remain continuous. In the two-dimensional (2D) case, the traction vectors are linearly related to the displacement jumps across the interface ([Zhong et al., 2009](#)).

$$T_n^1 = T_n^2 = D_n (U_n^1 - U_n^2), \quad T_t^1 = T_t^2 = D_t (U_t^1 - U_t^2) \quad (\text{IV. 23})$$

where T and U are the interface tractions and displacements, respectively. The superscripts 1 and 2 denote quantities on side 1 and side 2 of the interface, while the subscripts n and t correspond to the normal and tangential directions defined in a local orthogonal coordinate system on the interface. The parameters D_n and D_t are independent spring-like interface stiffnesses that govern the resistance to separation and sliding, respectively. When D_n and D_t tend to infinity, the interface behaves as a perfect bond, enforcing continuity of displacement across the interface. In contrast, when D_n and D_t approach zero, the interface is effectively debonded, allowing complete displacement discontinuity.

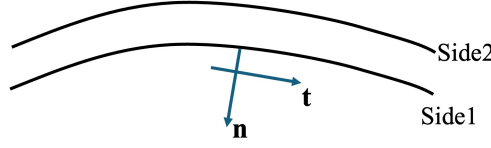


Figure IV. 6: The imperfect interface between two sides and its normal vector

2.4.1 Formation of interface

The material interface region in the discrete PD model is illustrated in Fig. IV. 7. Peridynamic nodes located nearest to the imperfect interface are designated as interface nodes, and two rows of such nodes are evenly distributed on either side of the interface. For example, an interface node $\mathbf{x}_i$ is connected to nodes in its interface neighborhood set H_{ic} , located within the interface horizon δ_c defined around it.

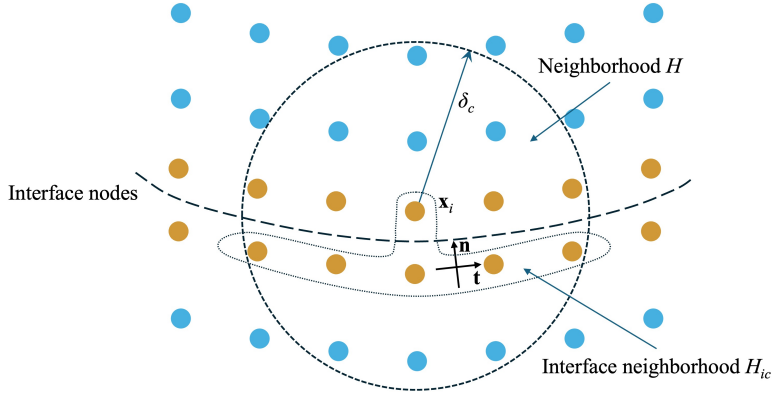


Figure IV. 7: Peridynamic imperfect interface model

The interface nodes across the interface are connected by peridynamic interface bonds. For example, as shown in Fig. IV. 8, interface nodes $\mathbf{x}_i$ and $\mathbf{x}_k$ are connected through a bond $\bar{\xi}_{ik}$, where the overline notation is used to distinguish these interface bonds from the original peridynamic bonds. In the deformed state, the peridynamic normal and tangential interface bond forces can be expressed, respectively, as:

$$\begin{aligned}\underline{\mathbf{f}}_n\langle\bar{\xi}_{ik}\rangle &= c_n\omega\langle\bar{\xi}_{ik}\rangle\underline{\Delta\mathbf{u}}_n\langle\bar{\xi}_{ik}\rangle\mathbf{n} \\ \underline{\mathbf{f}}_t\langle\bar{\xi}_{ik}\rangle &= c_t\omega\langle\bar{\xi}_{ik}\rangle\underline{\Delta\mathbf{u}}_t\langle\bar{\xi}_{ik}\rangle\mathbf{t}\end{aligned}\tag{IV. 24}$$

where ω is the influence function, c_n and c_t are the normal and tangential micromodulus for the peridynamic interface bond, $\mathbf{n}$ and $\mathbf{t}$ are the unit normal and tangential vectors of the interface surface. $\underline{\Delta\mathbf{u}}_n$ and $\underline{\Delta\mathbf{u}}_t$ are the normal and tangential displacement differences,

which can be expressed in terms of the displacements of the interface nodes as:

$$\underline{\Delta \mathbf{u}}_n \langle \bar{\xi}_{ik} \rangle = \mathbf{u}_n^i - \mathbf{u}_n^k, \quad \underline{\Delta \mathbf{u}}_t \langle \bar{\xi}_{ik} \rangle = \mathbf{u}_t^i - \mathbf{u}_t^k \quad (\text{IV. 25})$$

In the 3D rectangular coordinate system, the normal and tangential displacement differences, denoted as $\underline{\Delta \mathbf{u}}_n$ and $\underline{\Delta \mathbf{u}}_t$, respectively, can be computed as:

$$\underline{\Delta \mathbf{u}}_n = \underline{\Delta \mathbf{u}}_x n_x + \underline{\Delta \mathbf{u}}_y n_y + \underline{\Delta \mathbf{u}}_z n_z, \quad \underline{\Delta \mathbf{u}}_t = \underline{\Delta \mathbf{u}}_x t_x + \underline{\Delta \mathbf{u}}_y t_y + \underline{\Delta \mathbf{u}}_z t_z \quad (\text{IV. 26})$$

where $\underline{\Delta \mathbf{u}}_x, \underline{\Delta \mathbf{u}}_y$ and $\underline{\Delta \mathbf{u}}_z$ are the x, y and z directional displacement differences of nodes i and k , $\mathbf{n} = (n_x, n_y, n_z)$ and $\mathbf{t} = (t_x, t_y, t_z)$ are the unit normal and tangential vectors of the interface surface in Fig. IV. 8. With the peridynamic normal and tangential interface bond forces in Eqs. (IV. 24), the x, y and z directional interface bond forces can be expressed as:

$$\underline{\mathbf{f}}_x = \underline{\mathbf{f}}_n n_x + \underline{\mathbf{f}}_t t_x, \quad \underline{\mathbf{f}}_y = \underline{\mathbf{f}}_n n_y + \underline{\mathbf{f}}_t t_y, \quad \underline{\mathbf{f}}_z = \underline{\mathbf{f}}_n n_z + \underline{\mathbf{f}}_t t_z \quad (\text{IV. 27})$$

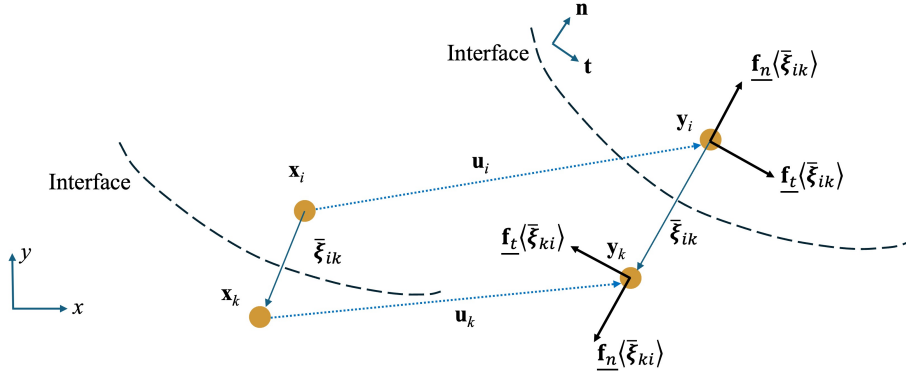


Figure IV. 8: Peridynamic imperfect interface bond forces between two interface nodes.

2.4.2 Interface bond micromodulus

In the 3D case, assuming uniform displacement differences at the interface, denoted as $\underline{\Delta \mathbf{u}}_n$ and $\underline{\Delta \mathbf{u}}_t$, the normal and tangential traction vectors are given by:

$$\mathbf{V}_n = D_n \underline{\Delta \mathbf{u}}_n, \quad \mathbf{V}_t = D_t \underline{\Delta \mathbf{u}}_t \quad (\text{IV. 28})$$

The interface bond forces in the interface area ds can be calculated as:

$$\mathbf{F}_n = D_n \underline{\Delta \mathbf{u}}_n ds, \quad \mathbf{F}_t = D_t \underline{\Delta \mathbf{u}}_t ds \quad (\text{IV. 29})$$

In the peridynamic imperfect interface model, the total normal and tangential interface forces over an interface area ds can be computed using the bond forces defined in Eqs. (IV. 24), as follows:

$$F_n = 2 \sum_{H_{ic}} c_n \omega \Delta \mathbf{u}_n V_i V_k, \quad F_t = 2 \sum_{H_{ic}} c_t \omega \Delta \mathbf{u}_t V_i V_k \quad (\text{IV. 30})$$

By comparing the interface forces obtained in Eq. (IV. 30) with those in Eq. (IV. 29), the peridynamic interface micromodulus can be derived as:

$$c_n = \frac{D_n}{2 \Delta x_i \sum_{H_{ic}} \omega V_k}, \quad c_t = \frac{D_t}{2 \Delta x_i \sum_{H_{ic}} \omega V_k} \quad (\text{IV. 31})$$

where Δx_i is the mesh size of point $\mathbf{x}_i$. Then, the interface bond micromodulus c_n and c_t can be computed in Eq. (IV. 31) with the interface stiffness parameters D_n and D_t , the typical mesh size and interface neighborhood H_{ic} . Under compressive loading conditions, the normal displacement across the interface typically remains continuous, indicating a mechanically perfect bond in the normal direction. To accurately capture this behavior within the peridynamic interface formulation, the normal interface micromodulus c_n is assigned an infinite value to enforce the constraint of displacement continuity under compression. Accordingly, the micromodulus c_n is defined as a function of the deformation state: when the interface bond is subjected to compression ($\Delta u_n < 0$), an infinite value c_n is imposed; in contrast, when the bond is under tension ($\Delta u_n > 0$), the normal micromodulus defined in Eq. (IV. 31) is adopted.

2.5 Imperfect interface fracture in peridynamics

To model fracture behavior at the ITZ in concrete, an extended critical bond energy density-based criterion is proposed for analyzing failure of interface bonds within the peridynamic imperfect interface framework. This criterion accounts for mixed-mode fracture mechanisms, which are particularly relevant for the ITZ due to its heterogeneous microstructure and weak bonding characteristics.

In the peridynamic interface model, considering the property of interface bond force, the interface bond energy density in normal and tangential directions can be expressed as:

$$\begin{aligned} W_n \langle \bar{\xi}_{ik} \rangle &= \frac{1}{2} c_n \omega \langle \bar{\xi}_{ik} \rangle (\Delta \mathbf{u}_n \langle \bar{\xi}_{ik} \rangle)^2 \\ W_t \langle \bar{\xi}_{ik} \rangle &= \frac{1}{2} c_t \omega \langle \bar{\xi}_{ik} \rangle (\Delta \mathbf{u}_t \langle \bar{\xi}_{ik} \rangle)^2 \end{aligned} \quad (\text{IV. 32})$$

where c_n and c_t are the interface micromodulus in Eq. (IV. 31).

The critical interface bond energy densities, W_n^c and W_t^c , are defined to predict the failure of interface bonds. Based on the fracture energy equivalence principle outlined in previous research of [Zhang and Qiao \(2019\)](#), the total energy released by broken bonds per unit area of the interface crack is assumed to be equal to the interfacial fracture toughness. Accordingly, the values of and can be determined as follows:

$$W_n^c = \frac{G_{nc}}{2\Delta x_i \sum_{H_{ic}} V_k}, \quad W_t^c = \frac{G_{tc}}{2\Delta x_i \sum_{H_{ic}} V_k} \quad (\text{IV. 33})$$

where G_{nc} and G_{tc} are the mode I and mode II interfacial critical energy release rates, respectively.

Similar to the Power law fracture criterion ([Ryoji et al., 1994](#)) in fracture mechanics, the mixed mode bond failure criterion is presented for interface fracture:

$$\left(\frac{W_n \langle \bar{\xi}_{ik} \rangle}{W_n^c} \right) + \left(\frac{W_t \langle \bar{\xi}_{ik} \rangle}{W_t^c} \right) > 1 \quad (\text{IV. 34})$$

For each interface bond, when the failure criterion given in Eq. (IV. 34) is satisfied, the bond is irreversibly broken, meaning it can no longer sustain any force in either the normal or tangential direction. The bond is deleted from subsequent force and energy calculations in the peridynamic formulation. This irreversible damage mechanism enables the model to simulate the progressive initiation and propagation of mixed-mode interface cracks under complex loading conditions.

2.6 Numerical implementation

In the peridynamic numerical model with an imperfect interface, the equation of motion for a peridynamic node $\mathbf{x}_i$ can be expressed as:

$$\rho(\mathbf{x}_i) \ddot{\mathbf{u}}(\mathbf{x}_i, t) = \sum_{j \in H} \{ \underline{\mathbf{T}}[\mathbf{x}_i, t] \langle \mathbf{x}_j - \mathbf{x}_i \rangle - \underline{\mathbf{T}}[\mathbf{x}_j, t] \langle \mathbf{x}_i - \mathbf{x}_j \rangle \} V_j + \mathbf{F}_i + \mathbf{b}(\mathbf{x}_i, t) \quad (\text{IV. 35})$$

where ρ is the density of node $\mathbf{x}_i$, $\mathbf{x}_j$ is the neighborhood node of $\mathbf{x}_i$ in its neighborhood H . As shown in Fig. IV. 7, the neighborhood of the interface node is not a complete circle, as it is truncated by the interface line (outlined by the dotted line). The OSB-PD model is considered for the force vector states computation. The $\mathbf{b}(\mathbf{x}_i, t)$ is the body force density. For the interface nodes, $\mathbf{F}_i$ denotes the interface force density, which can be expressed as:

$$\mathbf{F}_i = \sum_{k \in H_{ic}} \{ \underline{\mathbf{f}}_n \langle \bar{\xi}_{ik} \rangle + \underline{\mathbf{f}}_t \langle \bar{\xi}_{ik} \rangle - \underline{\mathbf{f}}_n \langle \bar{\xi}_{ki} \rangle - \underline{\mathbf{f}}_t \langle \bar{\xi}_{ki} \rangle \} V_k \quad (\text{IV. 36})$$

where $\underline{\mathbf{f}}_n$ and $\underline{\mathbf{f}}_t$ are normal and tangential interface bond forces in Eq (IV. 24). $\bar{\xi}_{ik} = \mathbf{x}_k - \mathbf{x}_i$ is the bond vector between interface nodes $\mathbf{x}_i$ and $\mathbf{x}_k$. If the node is not in H_{ic} , $\mathbf{F}_i = 0$.

Additionally, it is evident that there is no overlapping node between the neighborhood H and the interface neighborhood H_{ic} , as they lie on opposite sides of the interface. Furthermore, interactions between non-interface particles do not occur across the interface.

2.6.1 Interface normal vector caculating

In the concrete mesoscale modeling, the normal vectors of the ITZ, treated as imperfect interfaces, evolve during loading due to overall deformation of the material. For cases involving deformations—such as those induced by shrinkage or mechanical loading—it becomes essential to update these interface normal vectors dynamically within the peridynamic interface model to accurately capture the evolving interface behavior.

For a peridynamic interface node $\mathbf{x}_i$, the interface normal vector in the deformed configuration can be computed based on the deformation states of its surrounding nodes within its neighborhood horizon H_i . In this deformed state, the weighted mass of the peridynamic interface node $\mathbf{x}_i$ can be defined as

$$q_i = \rho_i \underline{y} \bullet \underline{y} = \sum_{j \in H} \rho_i(\underline{y}\underline{y}) \langle \xi_{ij} \rangle V_j \quad (\text{IV. 37})$$

where ρ_i is the density of node $\mathbf{x}_i$, $\mathbf{x}_j$ is the neighborhood node of $\mathbf{x}_i$ in H_i , $\underline{y}$ is the deformation scalar state that is caculated as $|\underline{\mathbf{Y}}|$. Thus, the unit outward normal vector of the interface node $\mathbf{x}_i$ in the deformed configuration can be obtained by computing the gradient of its weighted mass distribution. It is defined as:

$$\mathbf{n}_i = -\frac{q_{i,I}}{|q_{i,I}|} = -\frac{\sum_{j \in H} \rho_i(\underline{y}\underline{y}) \langle \xi_{ij} \rangle_I V_j}{|\sum_{j \in H} \rho_i(\underline{y}\underline{y}) \langle \xi_{ij} \rangle_I V_j|} = -\frac{\sum_{j \in H} (y_{jI} - y_{iI}) V_j}{|\sum_{j \in H} (y_{jI} - y_{iI}) V_j|} \quad (\text{IV. 38})$$

where $q_{i,I}$ denotes the partial derivative of q_i in the I -th direction, and y_{jI} represents the I -th component of the deformed position vector $\mathbf{y}_j$. With refined spatial discretization, Eq. (IV. 38) can be effectively used to compute the normal vectors of interface nodes, not only for flat interfaces but also for smoothly curved interfaces. However, this method is not applicable in cases where the interface exhibits sharp corners or branching features, due to the discontinuity or ambiguity in the definition of a unique normal direction in such regions.

2.6.2 Computational framework for the peridynamic imperfect interface model

The flowchart of the peridynamic imperfect interface fracture analysis is presented in Fig. IV. 9. For imperfect interface modeling, interface nodes are first identified, and the peridynamic normal and tangential bond forces are computed using Eq. (IV. 24) For

fracture analysis, the mixed-mode bond failure criterion defined in Eq. (IV. 34) is applied, where the corresponding bond energy densities are evaluated using Eq. (IV. 32), and the critical energy thresholds are specified in Eq. (IV. 33).

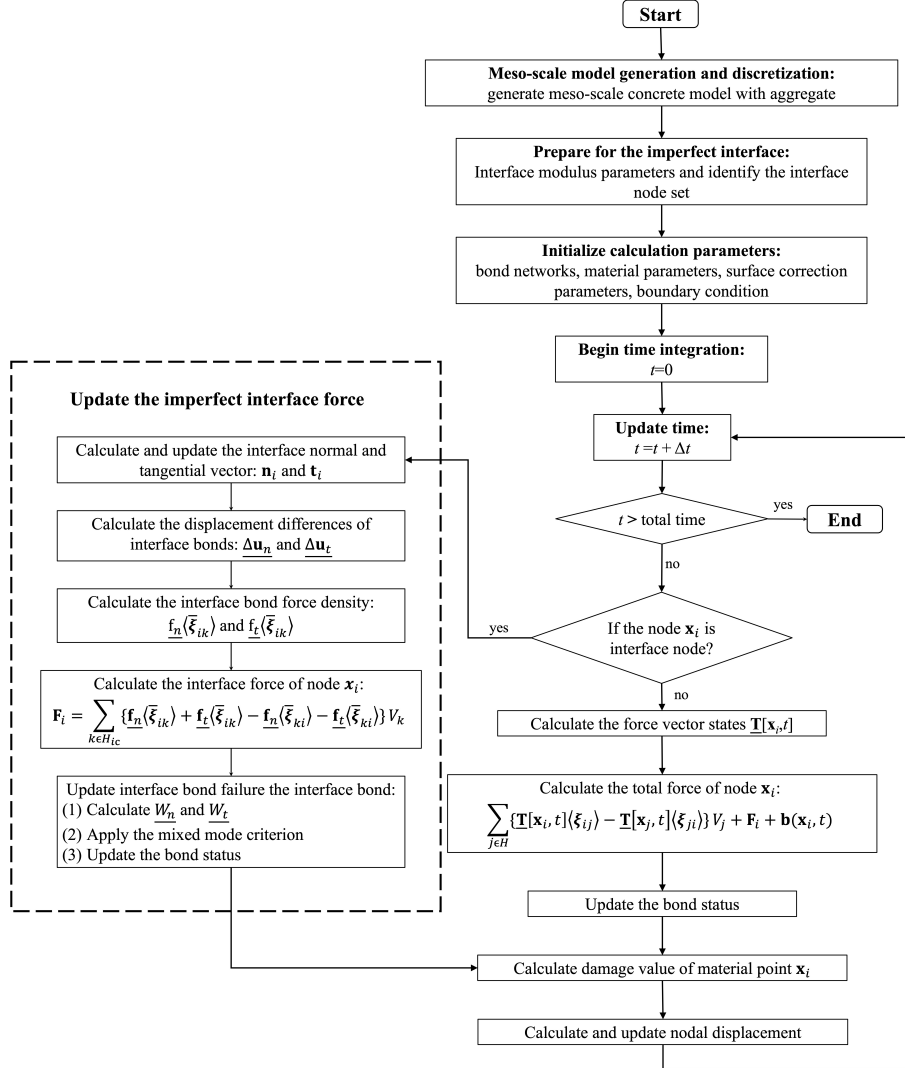


Figure IV. 9: The flowchart of interface fracture analysis in peridynamics

In this way, a imperfect interface OSB-PD model is established. Unlike the original perfect interface formulation discussed earlier, the proposed model explicitly incorporates displacement discontinuities across the interface. When the normal and tangential micro-modulus c_n and c_t tend to infinity, the relative displacement across the interface vanishes, and the imperfect interface degenerates into a perfect interface.

3 Model Validation Example

In this section, two examples, two plates bonded with imperfect interface and crack diversion with an imperfect interface are analyzed for the interface model verification and application.

3.1 Two plates bonded with imperfect interface

First, a benchmark problem involving two elastic plates bonded by a horizontal imperfect interface is analyzed. The geometric dimensions and boundary conditions are illustrated in Fig. IV. 10. The two plates are composed of different elastic materials, as specified in Table IV. 1. To investigate the influence of interface behavior, various values of the normal and tangential interface stiffness parameters D_n and D_t are considered.

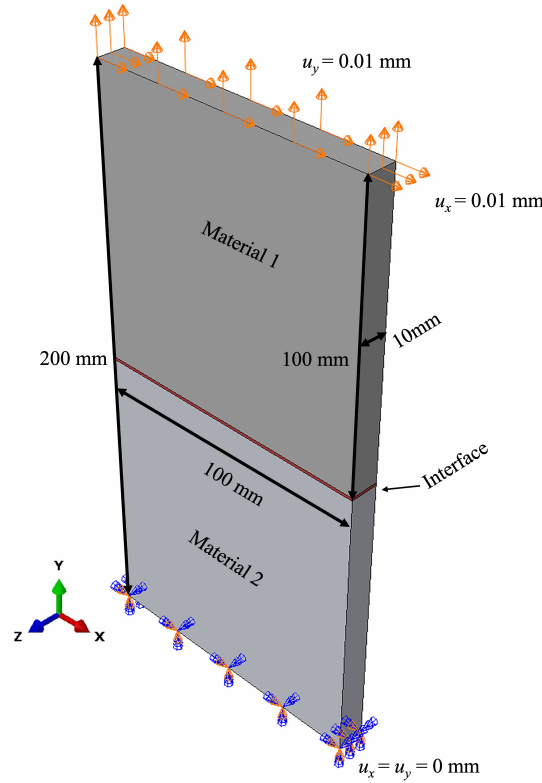


Figure IV. 10: Two plates bonded with imperfect interface and boundary condition

In the peridynamic numerical model, a uniform mesh size of $\Delta x = 1$ mm is employed. The Adaptive Dynamic Relaxation (ADR) method is utilized to obtain the equilibrium solution. For the interface analysis, the peridynamic model proposed in this section is implemented, with the interface horizon set as $\delta_c = \delta = 3.015\Delta x$. To verify the accuracy

Table IV. 1: Material parameters for verification simulation

Parameters	Material 1	Material 2
Elastic modulus E (GPa)	200	100
Poisson's ratio ν	0.3	0.3
Density ρ (kg/m ³)	7900	7900

of the peridynamic simulation, a comparative analysis is conducted using a finite element model (FEM) that simulates the interface behavior using a cohesive zone model. The FEM model shares the same geometry, mesh size, and boundary conditions as the peridynamic model to ensure consistency and comparability.

The displacement distributions of the two plates with an imperfect interface are presented in Figs. IV. 11 and IV. 12, in witch interface parameters of $D_t = D_n = 1000\text{MPa/mm}$ are used. As shown in Figures IV. 11 and IV. 12, the displacements in the x and y directions exhibit discontinuities across the imperfect interface, as expected. The results obtained from the peridynamic model are generally consistent with the FEM results. Minor discrepancies may arise due to differences in post-processing procedures, as well as variations in finite element mesh discretization and the peridynamic point cloud distribution.

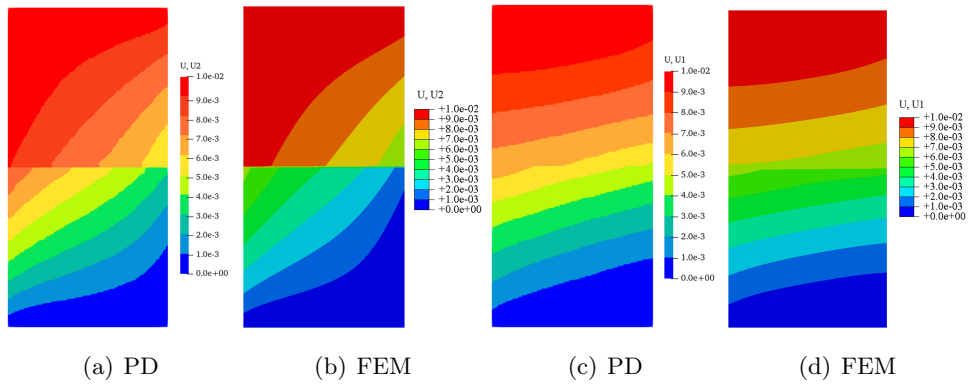


Figure IV. 11: Comparison of PD and FEM displacement distributions (mm). U1 represents the displacement along the x -direction, and U2 represents the displacement along the y -direction

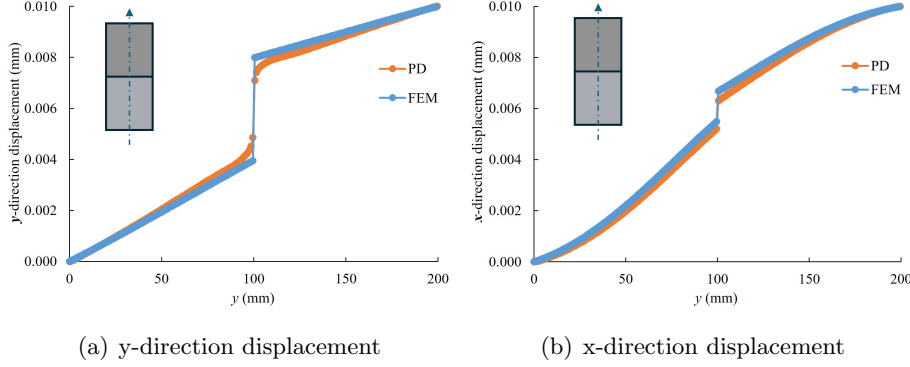


Figure IV. 12: Displacement distributions along the center line

Different values of the interface stiffness parameters D_t and D_n are used to model the imperfect interface, and the corresponding x - and y -directional displacements along the middle line are shown in Fig. IV. 13. As illustrated, larger values of D_t and D_n lead to smaller displacement jumps across the interface. When these parameters exceed 10000 MPa/mm, the displacement discontinuities become negligible, and the interface behavior closely approximates that of a perfectly bonded interface. In contrast, when D_t and D_n are below 10 MPa/mm, significant displacement jumps are observed, indicating that the interface is nearly fully separated.

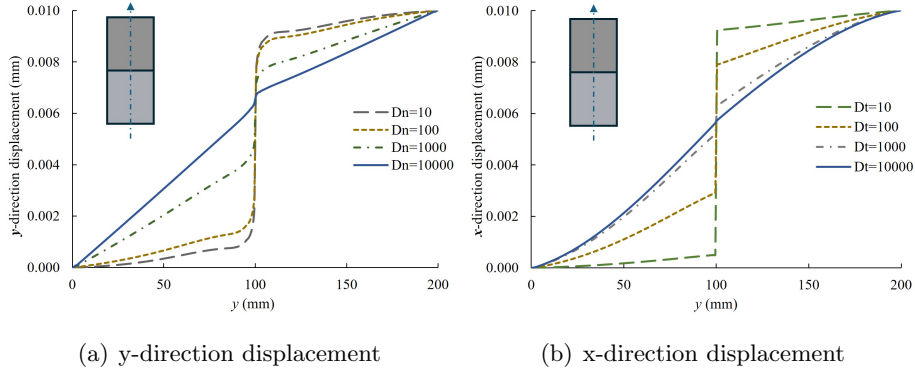


Figure IV. 13: Displacement distributions along the center line with the different interface stiffness parameters D_n and D_t

3.2 Crack diversions with an imperfect interface

A plate containing a preset crack and an imperfect interface is analyzed to study crack-interface interactions, as shown in Fig. IV. 14. The material parameters used are $E=200$ GPa, $\nu=0.3$ and $\rho=7900$ kg/m³. A predefined crack is located on the left side of

the plate, and the material critical energy release rate $G_0 = 30 \text{ J/m}^2$ is considered for crack prediction. An oblique imperfect interface is introduced, characterized by interface stiffness parameters and $D_t = D_n = 1000 \text{ MPa/mm}$. Various values of interface critical energy release rates are considered to evaluate their influence on crack–interface interaction.

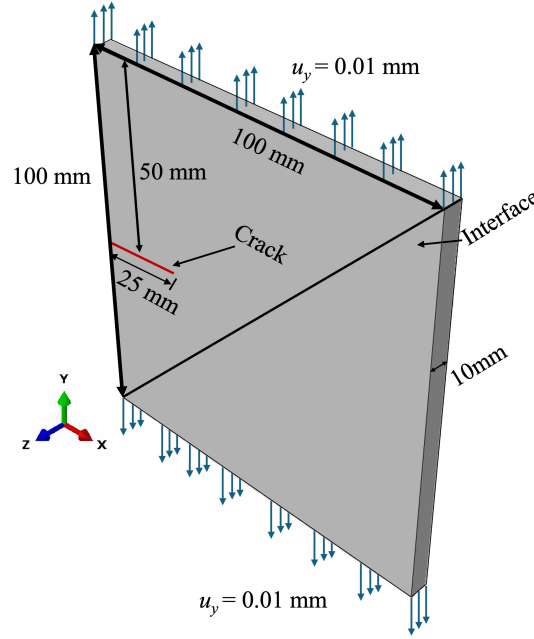


Figure IV. 14: Two plates bonded with imperfect interface and boundary condition

When a increasing displacement is applied to the plate, the resulting crack paths are illustrated in Fig. IV. 15. In this case, the interface fracture critical critical energy release rates are set as $G_{nc} = G_{tc} = 30 \text{ J/m}^2$. Under displacement loading, the crack initiates and propagates from the crack tip (see Fig. IV. 15 (a)). Due to the asymmetric arrangement of the imperfect interfaces, the crack follows a curved trajectory. Upon reaching the interface (see Fig. IV. 15 (b)), the crack deflects and propagates along the interface until it reaches the right boundary (see Fig. IV. 15 (c)).

To investigate the influence of interface parameters on crack propagation behavior, two key aspects were examined: the critical energy release rate and the interfacial stiffness parameters. Fig. IV. 16 illustrates the final crack paths in the plate with varying interfacial critical energy release rates ($G_{nc} = G_{tc} = 10, 20, \text{ and } 30 \text{ J/m}^2$). It can be observed that when G_c is relatively low (see Fig. IV. 16 (a)), the crack tends to propagate along the interface due to its low resistance to fracture. As G_c increases to 20 J/m^2 (see Fig. IV. 16 (b)), partial deflection into the bulk material occurs, but the interface still governs a significant portion of the crack path. When G_c reaches 30 J/m^2 (see Fig. IV. 16 (c)), the

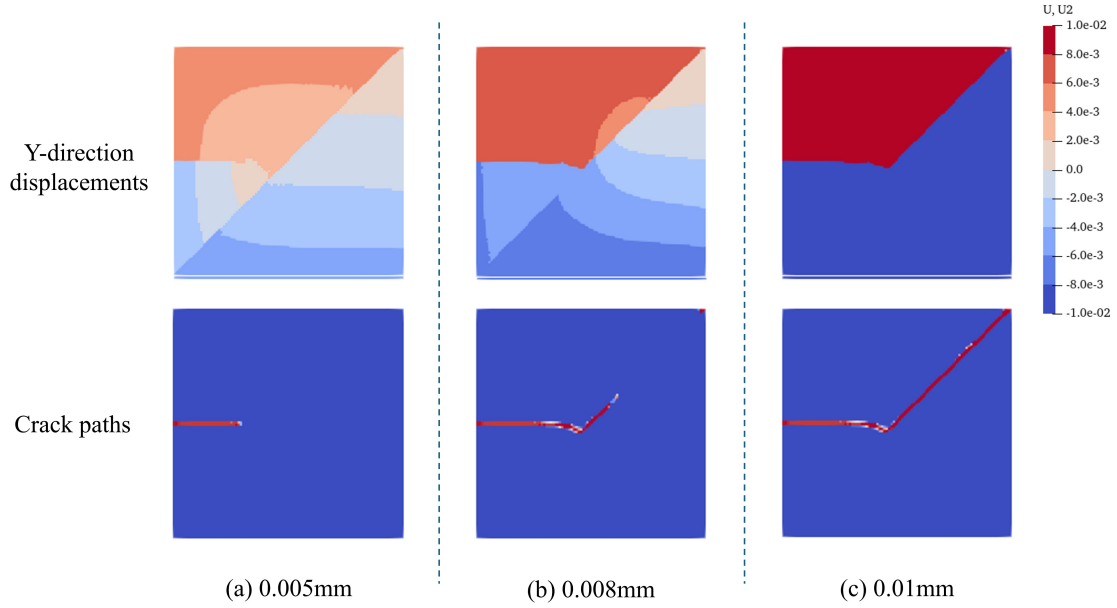


Figure IV. 15: Distributions of Y-displacements (mm) and crack paths of the plate at different displacement loads.

crack is fully deflected into the bulk material, bypassing the interface.

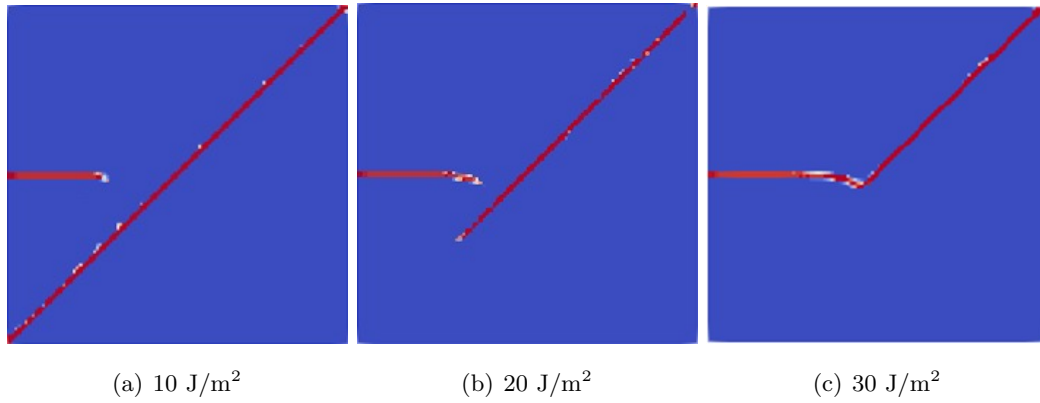


Figure IV. 16: Final crack paths of the plate with different interface critical energy release rates.

Fig. IV. 17 presents the final crack paths for three different values of the normal and tangential interfacial stiffness parameters ($D_n = D_t = 100, 1000, \text{ and } 10000 \text{ MPa/mm}$). When the interface stiffness is relatively low (see Fig. IV. 17 (a)), large displacement discontinuities develop across the interface due to its high compliance. This weak cou-

pling reduces stress transfer across the interface, resulting in stress relaxation near the crack tip and suppressing crack propagation or deflection. As the stiffness increases to 1000 MPa/mm (see Fig. IV. 17 (b)), the crack is able to deflect and propagate along the interface, indicating a balance between energy dissipation and stress continuity. When the interface becomes very stiffness ($D_n = D_t = 10000$ MPa/mm, see Fig. IV. 17 (c)), the interface behaves nearly as a perfect bond, forcing the crack to penetrate through the interface and continue into the adjacent material. These results demonstrate that interfacial stiffness plays a critical role in determining whether a crack is arrested, deflected, or penetrates the interface—complementing the influence of interfacial fracture toughness discussed previously.

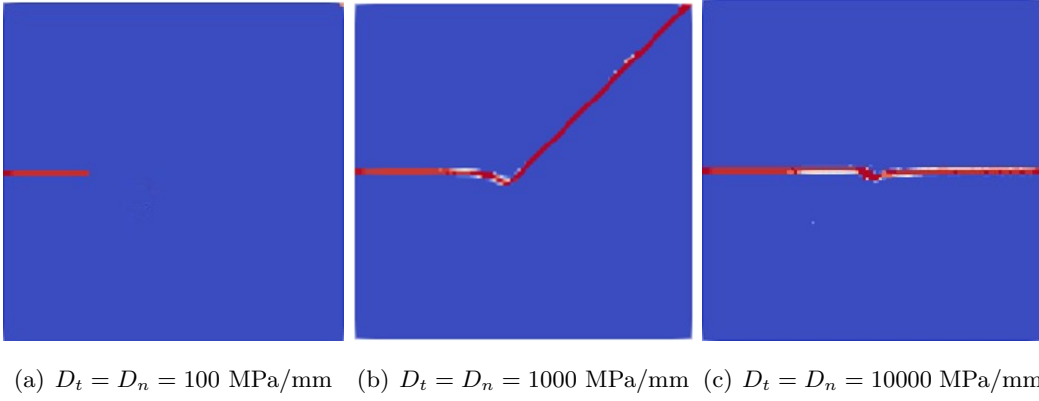


Figure IV. 17: Final crack paths of the plate with different interface stiffness parameters.

4 Comparison with bond-based PD in concrete shrinkage cracking simulation

To further validate the proposed imperfect interface model under realistic mesoscopic conditions, a comparative simulation was conducted on a three-dimensional concrete cylindrical specimen subjected to drying shrinkage. Both the proposed interface ordinary state-based peridynamics (IOSB-PD) model and the bond-based peridynamic (BB-PD) model were applied to the same mesostructure containing mortar matrix and randomly distributed spherical aggregates with a diameter of 2 mm. The geometric dimensions of the specimen are $\Phi 8 \text{ mm} \times 15 \text{ mm}$, with an aggregate volume fraction of approximately 40%.

In the bond-based PD model, the aggregate and mortar phases are connected by weaker bonds, whose micro-modulus and critical stretch are reduced to 50% of those of the mortar

matrix to represent a simplified weak interfacial behavior, while all other parameters and the hydraulic conditions are kept identical to the previous simulation setup. In contrast, in the present imperfect IOSB-PD model, the interface bonds are explicitly defined with distinct normal and tangential stiffness parameters, with $D_n = D_t = 1000$ MPa/mm. The corresponding interface fracture energies are set to $G_{nc} = 0.5 G_m$ and $G_{tc} = 0.7 G_m$, where G_m denotes the fracture energy of the mortar matrix. These values distinguish the tensile (Mode I) and shear (Mode II) failure modes of the interface, reflecting the lower resistance of the ITZ under normal tension compared with shear.

As illustrated in Fig. IV. 18, the IOSB-PD model reproduces realistic crack patterns with clear deflection and branching along aggregate surfaces, forming a connected but physically reasonable three-dimensional crack network. In contrast, the bond-based PD (BB-PD) model, in which ITZ is represented only by weakened bonds with 50% of the matrix strength, fails to capture the actual debonding behavior. Since all bonds in the BB-PD formulation respond isotropically and no explicit distinction is made between normal and tangential directions, cracks propagate almost straight through the matrix and appear excessively dense and diffused across the sample. This over-prediction of cracking is a direct consequence of the simplified treatment of the ITZ, which leads to underestimated stress localization and unrealistic damage accumulation. By contrast, the IOSB-PD model, through explicit interfacial stiffness and fracture energy parameters (D_n , D_t , G_{nc} , G_{tc}), allows for partial separation and shear slip along the ITZ, resulting in more physically consistent crack spacing and tortuous paths that better match experimental observations.

Overall, this comparative study demonstrates that the proposed interface model provides a more physically realistic description of ITZ debonding and stress redistribution in heterogeneous cementitious composites, bridging the gap between mesoscale structure and macroscopic fracture behavior under drying conditions.

5 Conclusion

In this chapter, a modified peridynamic interface method was proposed to model the fracture behavior of heterogeneous materials such as concrete, with a particular focus on the ITZ. Building upon the OSB-PD framework, the proposed approach introduces an imperfect interface representation that captures displacement discontinuities and enables the simulation of mixed-mode fracture phenomena across weakly bonded interfaces.

A interface formulation was developed by incorporating independent normal and tan-

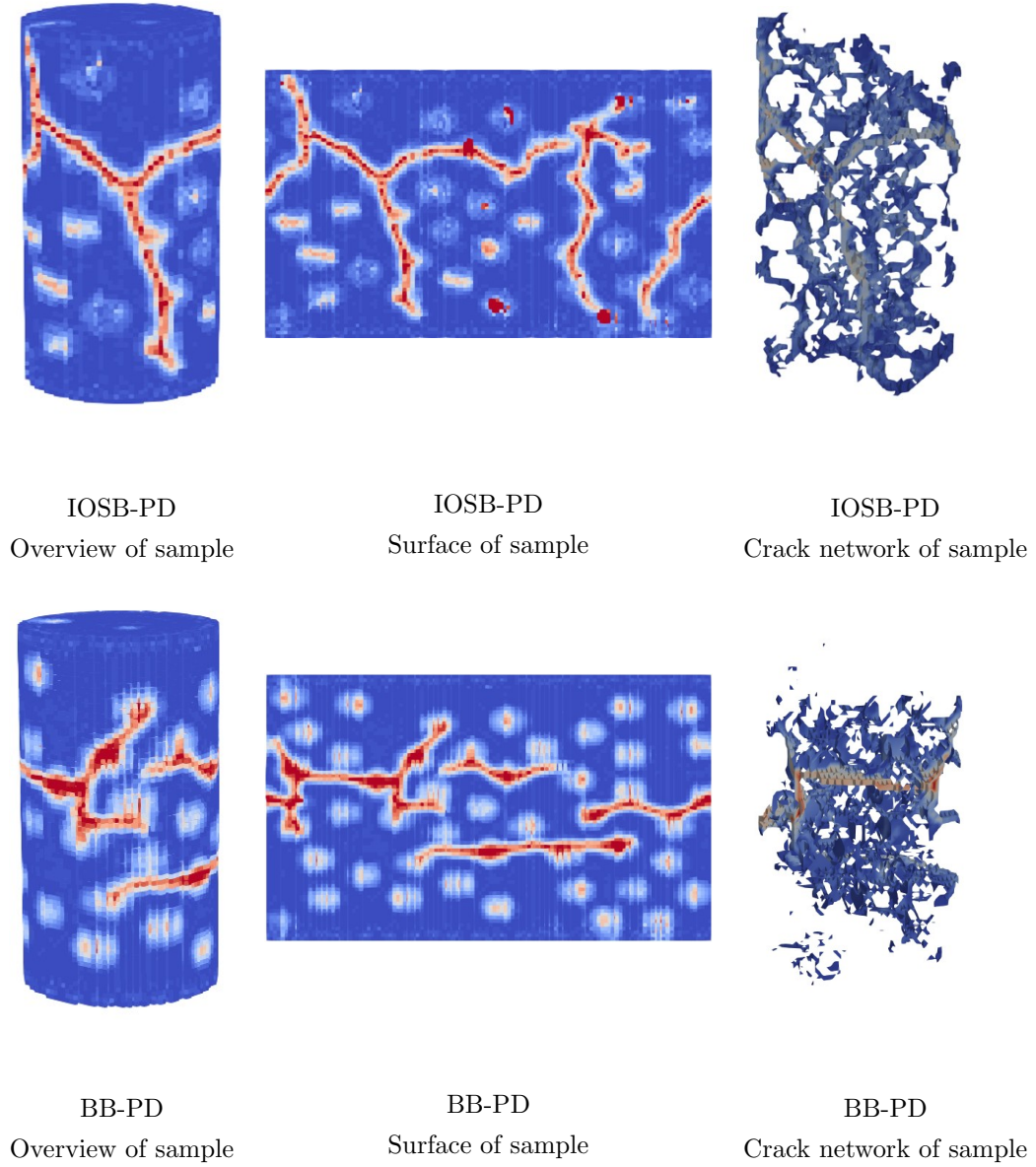


Figure IV. 18: Comparison of shrinkage-induced crack patterns predicted by the IOSB-PD and BB-PD models

gential stiffness parameters into the peridynamic bond force model. A mixed-mode energy-based failure criterion was also introduced to govern the progressive debonding and sliding behavior of interface bonds under complex loading conditions. The implementation accounts for evolving interface normals in deformed configurations, enhancing the model's capability to track interface evolution in mesoscale simulations.

Validation examples demonstrated that the proposed interface model accurately captures displacement jumps across imperfect interfaces and effectively simulates crack deflection, penetration, and arrest behaviors. Parametric studies further highlighted the role of interfacial stiffness and critical energy release rates in determining crack–interface interaction mechanisms. Notably, low interface toughness promotes interfacial crack propagation, while high stiffness conditions lead to crack penetration into the bulk material.

Furthermore, the comparative simulation of drying-shrinkage-induced cracking in a mesoscale concrete confirmed the effectiveness of the proposed IOSB-PD model. Compared with the BB-PD formulation, in which the ITZ is merely represented by weakened bonds, the IOSB-PD model explicitly accounts for the normal and tangential mechanical responses of the interface. As a result, it successfully reproduces realistic interfacial debonding, crack deflection, and three-dimensional crack network formation consistent with experimental observations, avoiding the excessively dense and diffused cracks predicted by the BB-PD model.

Overall, the developed peridynamic imperfect interface model provides a robust and physically consistent framework for analyzing interface-dominated fracture in concrete and other composite materials, bridging the gap between mesostructural heterogeneity and macroscopic fracture behavior.

Chapter V

Numerical Analysis of Interfacial Transition Zone Properties on Drying-Induced Cracking in Concrete

1 Introduction

The previous chapter investigated the influence of aggregate geometry on drying-induced cracking in concrete using a mesoscale peridynamic framework. The results revealed that aggregate shape significantly affects stress localization and crack deflection, thus governing the initiation and evolution of shrinkage-induced fractures. Building upon these findings, the present chapter shifts the focus to the mechanical characteristics of the interfacial transition zone (ITZ), which critically mediate stress transfer between the aggregate and matrix. Variations in ITZ stiffness and fracture energy are introduced to represent different interfacial bonding conditions that may arise from changes in inclusion surface roughness.

A comprehensive parametric study is performed using the modified peridynamic interface model, where these interfacial parameters are systematically varied to quantify their influence on crack initiation and propagation. The numerical results are finally compared with corresponding experimental observations, demonstrating the model's capability to capture the governing role of ITZ properties in the fracture evolution of cementitious composites.

2 Effects of ITZ properties on concrete drying shrinkage cracks

Understanding the role of interfacial mechanical parameters is essential for predicting and controlling crack evolution in cementitious composites subjected to drying shrinkage. While aggregate shape and spatial distribution influence stress localization and crack deflection, the mechanical behavior of the ITZ governs the local failure mode—either by interfacial debonding or by crack penetration into the matrix. To quantitatively assess the role of these interfacial properties, a series of mesoscale peridynamic simulations were conducted, explicitly resolving the aggregates, cement matrix, and ITZ.

The simulation configuration is consistent with the previous model. The computational domain is a cylindrical specimen with a diameter of 9 mm and a height of 18 mm. Aggregates are modeled as spherical inclusions with a diameter of 3 mm, occupying 40% of the specimen volume. As shown in Fig. V. 1, the ITZ is explicitly defined as the region surrounding each aggregate, bounded by interface nodes located between the aggregate and the surrounding matrix. The material properties of each interface node correspond to the phase (aggregate or matrix) to which the node belongs.

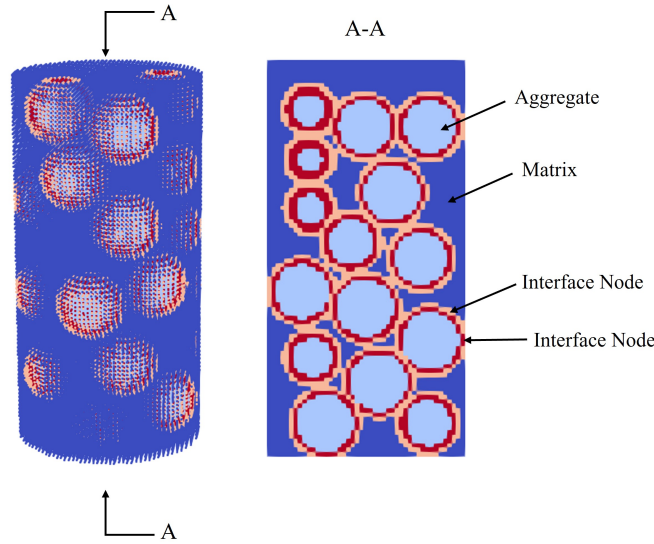


Figure V. 1: The meso-scale model used in this simulation

The model is discretized using a uniform grid with a spacing of $\Delta x = 0.2$ mm, resulting in 197,088 material points. The peridynamic horizon is set to $\delta = 3.015\Delta x$, and the time step for the diffusion equation is $\Delta t = 0.4$ s. Aggregates are assumed to be linear elastic

and impermeable, with drying shrinkage applied only to the cement matrix and ITZ.

The material parameters used in the simulations are summarized in Table V. 1. Hydraulic parameters are consistent with those in the mesoscale model described in Chapter III. To examine the influence of ITZ mechanical behavior on drying-induced cracking, four key parameters were varied systematically: the normal stiffness D_n , tangential stiffness D_t , normal fracture energy G_{nc} , and tangential fracture energy G_{tc} . These parameters were independently adjusted over representative ranges, with $D_t = 1000$ MPa/mm, $D_n = 1000$ MPa/mm, $G_{nc} = 0.02$ N/mm, and $G_{tc} = 0.02$ N/mm taken as baseline values (Table V. 1). All other material and geometric properties were kept constant. This approach enables isolation of each parameter's contribution to crack initiation, propagation, and overall damage evolution under shrinkage-induced stresses.

Table V. 1: Material parameters used in the parametric analysis simulations

Parameters	Cement Paste	Aggregate	ITZ
Elastic modulus E (GPa)	15	68	-
Poisson's ratio ν	0.30	0.25	-
Energy release rate G_0 (N/mm)	0.03	0.50	-
D_n (MPa/mm)	-	-	100–1000
D_t (MPa/mm)	-	-	100–1000
G_{nc} (N/mm)	-	-	0.005–0.03
G_{tc} (N/mm)	-	-	0.005–0.03

2.1 The tangential stiffness D_t

The effect of tangential stiffness D_t was studied for values of 100, 300, 600, and 1000 MPa/mm. Fig. V. 2 illustrates the influence of tangential stiffness D_t on the spatial distribution of cracks in specimens containing aggregates. As D_t decreases, the crack network evolves from sparse, localized cracks to more connected and extensive fracture paths. At higher D_t values, cracks remain relatively short and isolated, with limited opening widths. In contrast, lower D_t values lead to partial crack coalescence and an increase in crack width, particularly along the interfacial transition zones. At the lowest D_t , several cracks become continuous across the specimen, forming interconnected damage zones with wider openings. This trend indicates that reduced tangential stiffness promotes both crack

propagation and opening, thereby accelerating damage evolution under shrinkage-induced stresses.

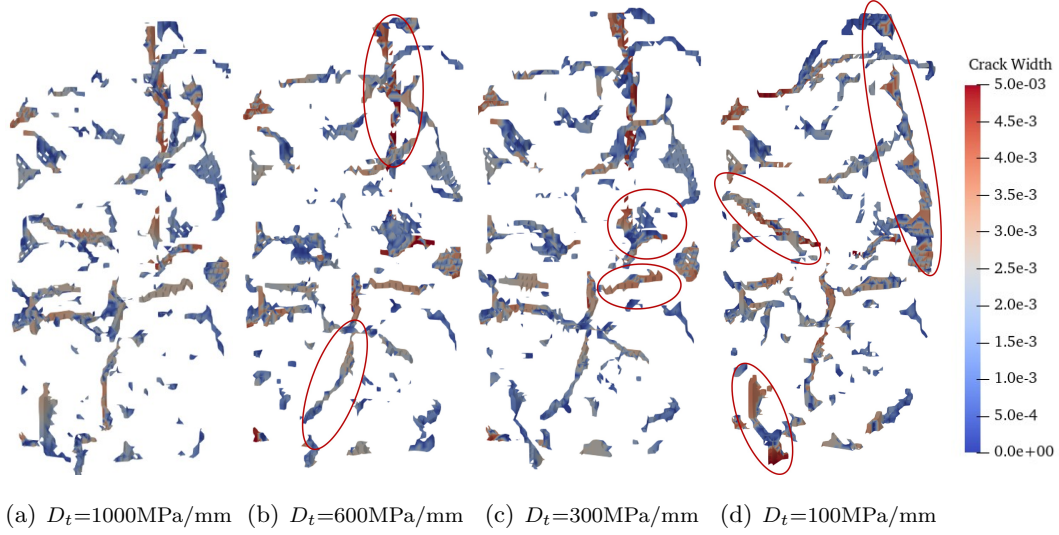


Figure V. 2: Distribution of crack in samples with aggregate of varying tangential stiffness D_t

As shown in Fig. V. 3, a reduction in the tangential stiffness D_t results in an increase in crack width, crack volume, and total crack length. When D_t decreases from 1000 to 100 MPa/mm, the average crack width rises from 1.84×10^{-3} mm to 2.07×10^{-3} mm, an increase of approximately 12.5%. Crack volume grows from 0.237 mm^3 to 0.297 mm^3 , corresponding to a 25.3% increase, with the largest increment observed between $D_t = 300$ and $D_t = 100$. The most pronounced change is seen in crack length, which increases from 479 mm to 569 mm, a 18.8% rise, indicating that reduced tangential stiffness significantly enhances crack network connectivity and promotes fracture path extension.

2.2 The normal stiffness D_n

As shown in Fig. V. 4, variations in the normal stiffness D_n markedly influence the spatial distribution and morphology of cracks. At higher D_n values (e.g., $D_n = 1000 \text{ MPa/mm}$), cracks are relatively narrow and less connected, with most fractures localized around the ITZ and limited penetration into the matrix. As D_n decreases to 600 and 300 MPa/mm, the number of through-going cracks increases, and several fracture segments coalesce into longer and more continuous crack paths. This trend is accompanied by localized widening of certain crack regions, indicating enhanced normal separation across the interface. When D_n is reduced to 100 MPa/mm, cracks become more widely

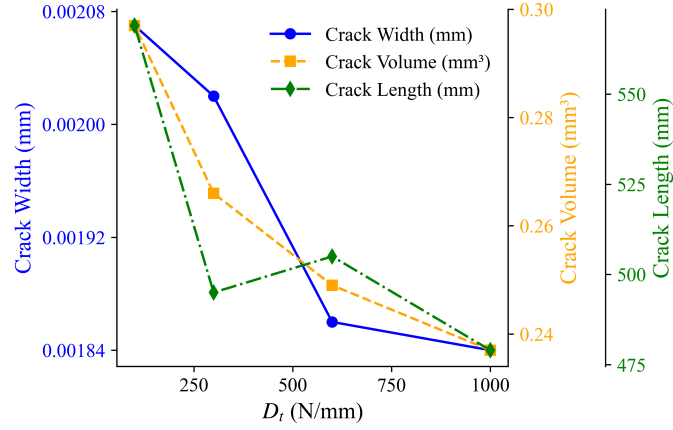
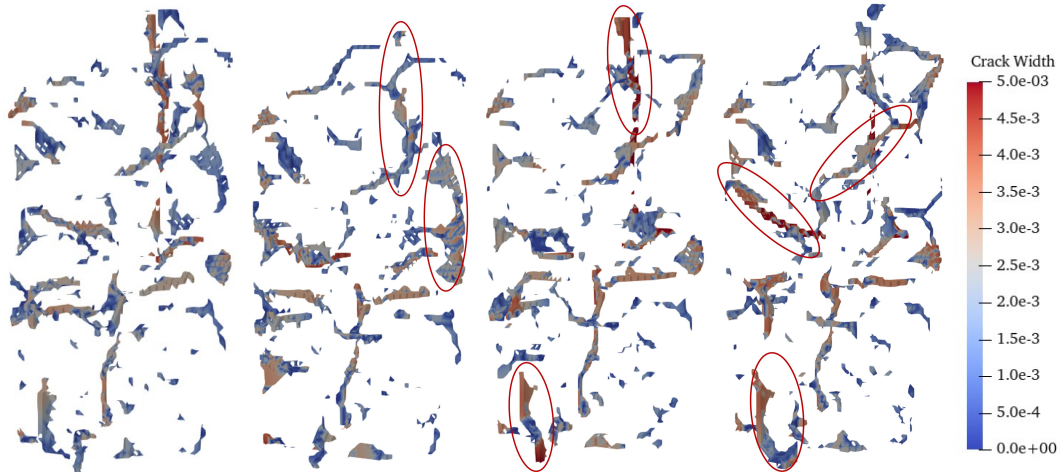


Figure V. 3: Effect of tangential stiffness D_t on crack characteristics

distributed throughout the matrix, with a higher degree of connectivity between individual crack branches, suggesting that low normal stiffness promotes more extensive crack propagation and network formation under shrinkage-induced stresses.



(a) $D_n=1000\text{MPa/mm}$ (b) $D_n=600\text{MPa/mm}$ (c) $D_n=300\text{MPa/mm}$ (d) $D_n=100\text{MPa/mm}$

Figure V. 4: Distribution of crack in samples with aggregate of varying normal stiffness D_n

As shown in Fig. V. 5, a reduction in the normal stiffness D_n also leads to a clear increase in all three crack metrics. As D_n decreases from 1000 to 100 MPa/mm, the average crack width grows from 1.84×10^{-3} mm to 2.15×10^{-3} mm, corresponding to an increase of approximately 16.8%. Crack volume exhibits the most pronounced change, increasing from 0.237 mm^3 to 0.312 mm^3 (31.6% growth). Crack length rises from 479 mm

to 545 mm, marking a 13.8% increase, and shows a local maximum of 503 mm at $D_n = 600$, likely due to enhanced connectivity within the crack network.

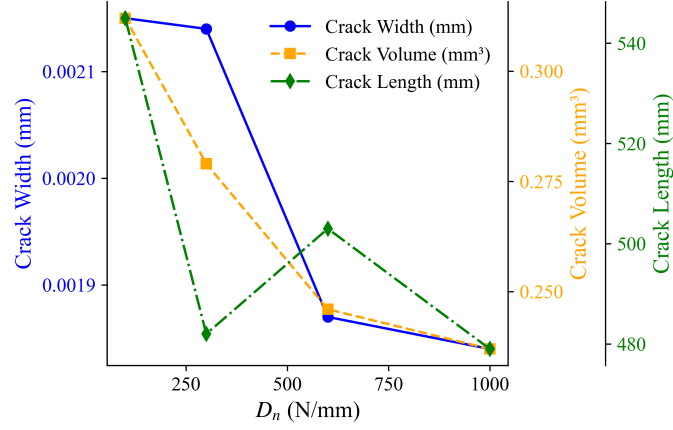


Figure V. 5: Effect of normal stiffness D_n on crack characteristics

While both D_n and D_t reductions cause crack widening, volumetric growth, and longer fracture paths, their relative influence differs. Variations in D_n have a stronger impact on crack volume, highlighting its direct role in controlling normal opening displacement and mode-I fracture behavior. In contrast, changes in D_t more substantially affect crack length, particularly at lower stiffness values, reflecting its greater influence on crack coalescence and mixed-mode fracture propagation. Overall, D_n predominantly governs the magnitude of crack opening, whereas D_t plays a more critical role in shaping crack path connectivity and the development of an interconnected fracture network.

2.3 The tangential fracture energy G_{tc}

The effect of tangential fracture energy G_{tc} was examined for values of 0.005, 0.01, 0.02, and 0.03 N/mm. As illustrated in Fig. V. 6, the influence of G_{tc} on crack morphology exhibits a distinct threshold effect. For relatively high values (e.g., $G_{tc} = 0.03$, 0.02, and 0.01 N/mm), the spatial distribution and connectivity of cracks remain relatively stable. In these cases, cracks are primarily confined to the ITZs, and most fracture paths remain discrete and unconnected. While a gradual increase in crack length is observed as G_{tc} decreases, the overall crack topology and density are not significantly altered.

However, when G_{tc} is further reduced to 0.005 N/mm, a dramatic transition in fracture behavior occurs. The system evolves into a highly damaged state characterized by an extensive and densely connected crack network that penetrates both the ITZs and surrounding cement matrix. This sharp shift suggests the existence of a critical energy

threshold, below which the interface can no longer resist shear-driven failure. As a result, large-scale shear debonding and crack coalescence are activated, promoting widespread damage. Interestingly, despite this extensive cracking, the average crack width decreases, as indicated by the dominance of blue regions in the crack-width colormap. This trend implies that under severely reduced tangential fracture energy, crack multiplication becomes the primary damage mechanism, outweighing individual crack opening.

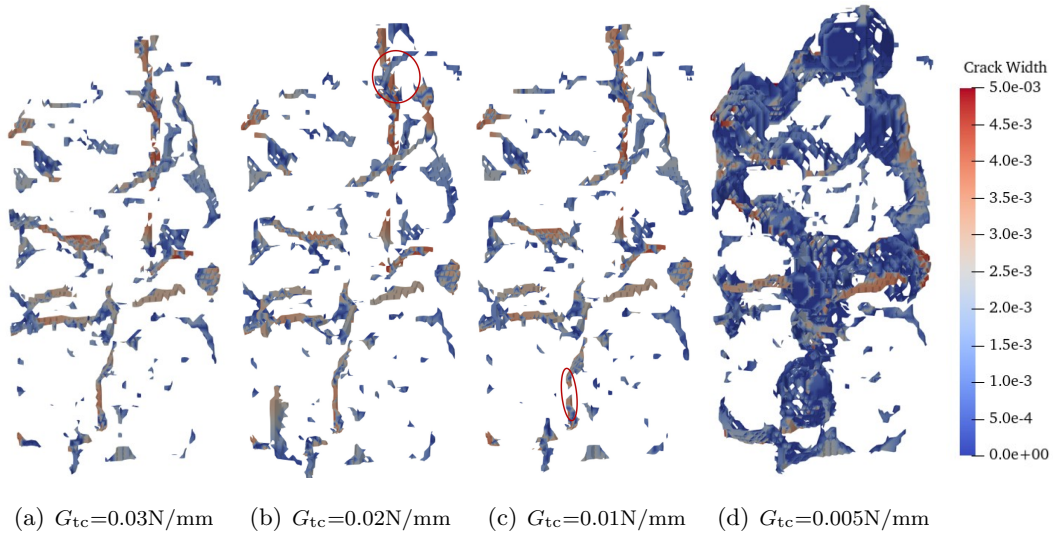


Figure V. 6: Crack patterns in specimens with varying tangential fracture energy G_{tc}

As shown in Fig. V. 7, reducing G_{tc} from 0.03 to 0.005 N/mm results in a slight decrease in average crack width, from 1.85×10^{-3} to 1.60×10^{-3} mm (13.5% reduction). However, the total crack volume increases substantially from 0.241 mm^3 to 0.435 mm^3 , corresponding to an 80.5% increase. This dramatic growth is primarily driven by the total crack length, which rises from 484 mm to 1940 mm—a fourfold increase. These results further support the notion that G_{tc} acts as a controlling parameter in shear-induced damage, with a distinct threshold below which extensive crack branching and matrix penetration dominate the fracture process.

2.4 The normal fracture energy G_{nc}

As shown in Fig. V. 8, the effect of the normal fracture energy G_{nc} on crack morphology was investigated for values of 0.005, 0.01, 0.02, and 0.03 N/mm. A clear threshold behavior is observed in the spatial distribution of cracks with decreasing G_{nc} . When G_{nc} is relatively high (i.e., 0.03 and 0.02 N/mm), the variation in crack patterns remains limited. As G_{nc} decreases to 0.01 N/mm, a slight increase in crack connectivity and total length can be

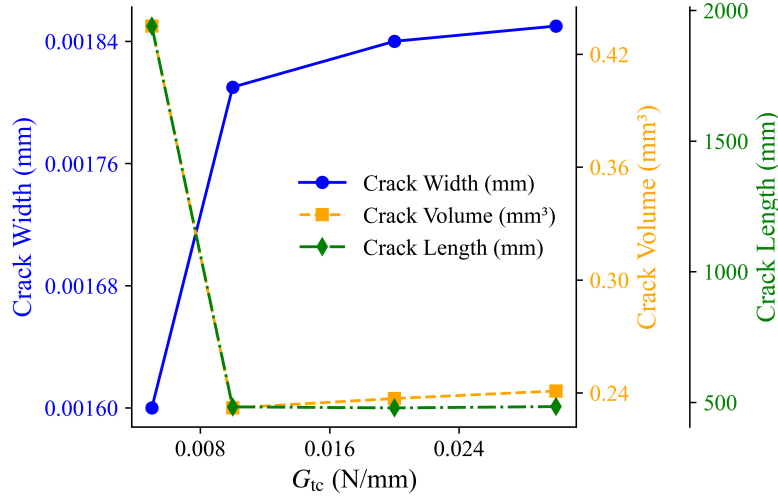


Figure V. 7: Effect of tangential fracture energy G_{tc} on crack characteristics

observed. Cracks tend to propagate more extensively along the ITZ, with some penetrating into the cement matrix. However, the overall topology still retains a moderate degree of localization.

A pronounced transition occurs when G_{nc} is further reduced to 0.005 N/mm. In this case, the fracture pattern changes drastically, with a large number of microcracks forming within the ITZ regions. This leads to a high-density fracture network in the specimen. As seen in Fig. V. 8 (d), although the crack density increases significantly, the average crack width remains low. This indicates that the sharp increase in crack volume at low G_{nc} is primarily attributed to the multiplication of fine cracks rather than the widening of existing ones, and that the formation of wider cracks is suppressed.

As shown in Fig. V. 9, a reduction in the normal fracture energy G_{nc} significantly alters the crack characteristics in concrete. When G_{nc} decreases from 0.03 to 0.005 N/mm, the average crack width drops markedly from 1.87×10^{-3} mm to 5.87×10^{-4} mm, representing a reduction of approximately 68.6%. In contrast, the crack volume declines from 0.244 mm³ to 0.130 mm³, while the total crack length increases dramatically from 479.5 mm to 3258.3 mm. This divergence indicates that the reduction in G_{nc} significantly lowers the tensile fracture resistance of the interfacial zones, promoting the initiation of numerous microcracks and forming a highly connected and extended crack network. Despite the narrowing of individual crack openings, the sharp increase in total crack length leads to a widespread damage pattern that reflects the brittle nature of the ITZ under low fracture energy conditions.

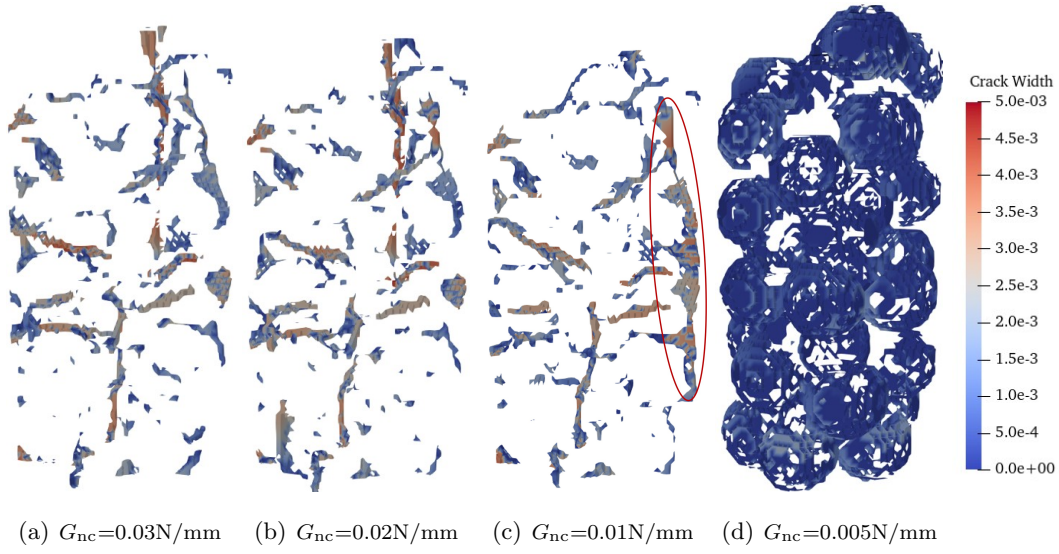


Figure V. 8: Distribution of crack in samples with aggregate of varying normal fracture energy G_{nc}

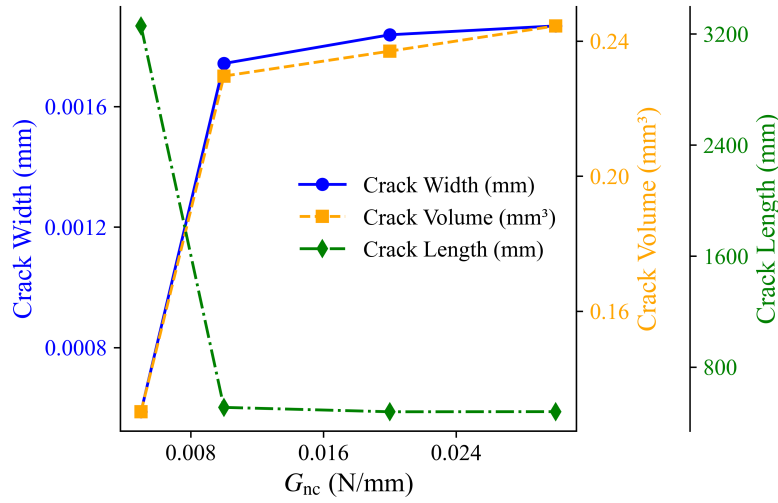


Figure V. 9: Effect of normal fracture energy G_{nc} on crack characteristics

Given the observed threshold effects in both normal (G_{nc}) and tangential (G_{tc}) fracture energies, additional simulations were performed with intermediate values in the range of 0.006–0.009 N/mm (Fig. V. 10). This supplementary analysis provided a finer resolution of the transition zone between the high- and low-fracture-energy regimes. The updated results reveal that the most pronounced variations in crack width, volume, and length are concentrated within this narrow range, with crack morphology evolving more gradually

outside of it. These observations confirm the existence of critical fracture energy levels that govern the transition from localized to highly connected crack networks. Building upon this refined understanding, a comparative analysis of G_{nc} and G_{tc} reveals that, although both parameters govern the fracture resistance of the ITZ, their influence on crack evolution exhibits distinct characteristics.

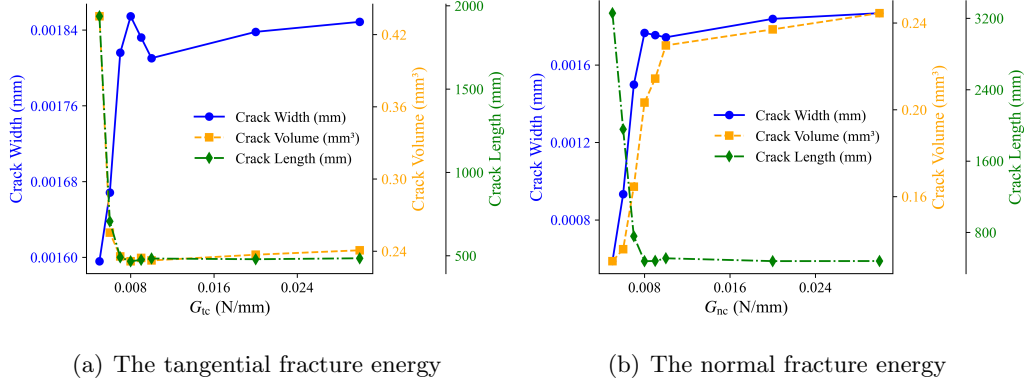


Figure V. 10: Effect of fracture energy G_{tc} and G_{nc} on crack characteristics, including supplementary data in the range 0.006–0.009 N/mm

A reduction in G_{nc} primarily promotes mode I debonding along the interface, leading to the formation of a dense network of narrow, highly interconnected cracks concentrated around the aggregates. The damage pattern remains largely confined to the ITZ, with limited crack opening but extensive connectivity. In contrast, reducing G_{tc} facilitates shear-induced crack propagation, characterized by more pronounced branching and sliding. This results in a more spatially extended crack network that penetrates both the ITZ and surrounding matrix. While cracks under lower G_{tc} may appear less connected than those under reduced G_{nc} , they tend to exhibit greater morphological complexity and wider openings. Overall, the fracture mode associated with G_{nc} reduction is dominated by interfacial microcracking, whereas G_{tc} reduction leads to a mixed-mode fracture process with increased crack dispersion and matrix involvement.

2.5 Discussion

To quantitatively assess the influence of key interfacial parameters on the fracture behavior of cementitious composites, a global sensitivity analysis was conducted using the Sobol method. This approach is particularly suitable for non-linear, multivariable models, and enables a systematic evaluation of how each input parameter contributes to variations in model outputs, both individually and through interaction effects.

In this study, four parameters were considered: the normal and tangential stiffnesses (D_n , D_t), and the normal and tangential fracture energies (G_{nc} , G_{tc}). The outputs of interest included average crack width, total crack volume, and crack path length. The Sobol method focuses on the total effect index (S_T). The S_T index quantifies the overall contribution of each input parameter to the output variance, including both its individual influence and its interactions with other parameters.

Previous analyses revealed that both normal (G_{nc}) and tangential (G_{tc}) interfacial fracture energies exhibit clear threshold effects in governing crack development. Specifically, a critical transition was observed around $G_{nc}, G_{tc} \approx 0.008$ N/mm, where crack morphology, connectivity, and extent change significantly. To further investigate the underlying mechanisms and quantify the influence of interfacial parameters in both fracture regimes, a global sensitivity analysis was conducted using the total effect index (S_T) from Sobol's method. The analysis was performed separately for the low-energy (≤ 0.008 N/mm) and high-energy (> 0.008 N/mm) regimes, using three results—crack width, volume, and length—to represent different aspects of fracture behavior.

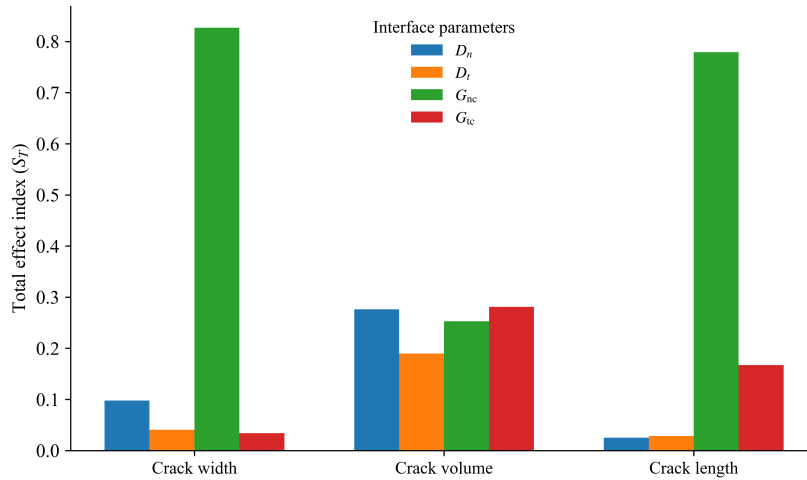


Figure V. 11: Total Sobol effect indices (S_T) for crack width, volume, and length in the low fracture energy regime ($G_{nc}, G_{tc} \leq 0.008$ N/mm)

As shown in Fig. V. 11, which presents the sensitivity indices in the low-energy regime ($G_{nc}, G_{tc} \leq 0.008$ N/mm), the total effect index S_T indicates that the normal fracture energy G_{nc} overwhelmingly governs crack width and length, with values exceeding 0.8. This result confirms that, in weak interfaces, crack evolution is highly sensitive to the magnitude of the available normal fracture energy. The interfacial damage remains concentrated, and the capacity of the interface to resist opening or sliding is the dominant

factor influencing crack connectivity and propagation. For crack volume, the total effect indices of the four parameters exhibit a relatively balanced distribution, suggesting a coupled regulatory mechanism in which both fracture energy parameters (G_{nc} , G_{tc}) and stiffness parameters (D_n , D_t) jointly govern the extent of volumetric cracking.

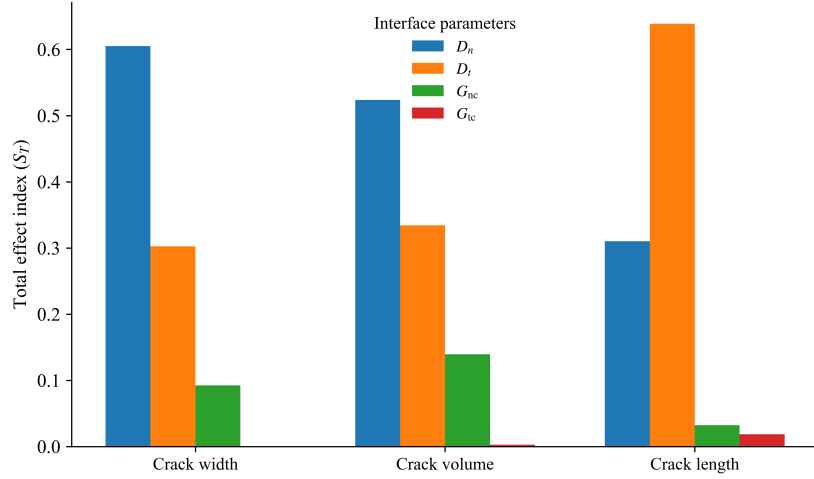


Figure V. 12: Total Sobol effect indices (S_T) for crack width, volume, and length in the high fracture energy regime ($G_{nc}, G_{tc} > 0.008$ N/mm)

In contrast, Fig. V. 12 shows the results for the high-energy regime ($G_{nc}, G_{tc} > 0.008$ N/mm). Here, the influence of fracture energy parameters diminishes notably, while the stiffness parameters—especially the tangential stiffness D_t —become the primary drivers of crack volume and length, with S_T reaching up to 0.65. This shift suggests that once the fracture energy surpasses the critical threshold, the fracture process becomes less constrained by energy limitations and more dependent on mechanical constraints. In this regime, stiffness dictates the spatial distribution and growth pattern of cracks, particularly through its control of interfacial sliding and separation resistance.

3 Simulation results of the effect of aggregate surface roughness on cracking

Previous experimental observations and analyses of interfacial parameters have shown that aggregate surface roughness plays a decisive role in crack development in concrete subjected to drying shrinkage (see Chapter II). Smooth inclusions tend to weaken the interfacial bond, leading to more severe and interconnected crack networks. These results underline the importance of interface strength as a key factor in crack evolution. Ac-

cordingly, in the numerical simulations, interface strength parameters are introduced to represent the bonding quality associated with different levels of surface roughness.

To ensure consistency and enable direct comparison with experimental results, the numerical model is constructed with the same geometrical dimensions as the experimental specimens. Specifically, a cylindrical concrete sample with a diameter of 8 mm and a height of 15 mm is modeled, matching the physical specimens used in the drying shrinkage tests. The internal meso-structure, including aggregate size, volume fraction, and spatial distribution, is also designed to reflect the experimental configuration. The model is discretized using a uniform grid spacing of $\Delta x = 0.2$ mm. Based on the preceding parameter analysis, the effects of surface roughness can be incorporated by modifying the interfacial parameters: rough aggregate surfaces are represented by stronger bonding properties to account for enhanced mechanical interlocking, whereas smoother surfaces are modeled with weaker interfacial parameters, as summarized in Table V. 2. These parameters enables the numerical model to reproduce the experimentally observed differences in cracking behavior associated with varying aggregate surface roughness.

Table V. 2: Material parameters used in the interface model

Parameters	Cement Paste	Aggregate	Rough ITZ	Smooth ITZ
Elastic modulus E (GPa)	15	68	-	-
Poisson's ratio ν	0.30	0.25	-	-
Energy release rate G_0 (N/mm)	0.03	0.50	-	-
D_n (MPa/mm)	-	-	1000	300
D_t (MPa/mm)	-	-	1000	300
G_{nc} (N/mm)	-	-	0.02	0.007
G_{tc} (N/mm)	-	-	0.02	0.007

Fig. V. 13 presents a comparative analysis of experimental observations and PD simulation results for specimens incorporating rough (Gl-R) and smooth (Gl-S) aggregate surfaces at the end of the first drying step. The surfaces of the samples illustrate the crack patterns predicted by PD simulations, revealing clear differences between specimens with rough and smooth aggregate surfaces. In the Gl-R case, a relatively continuous surface crack network develops, but the cracks remain narrow, reflecting the enhanced bonding and mechanical interlocking associated with rough aggregates. By contrast, the

GI-S specimen exhibits only two dominant surface cracks with significantly larger widths. The corresponding 3D crack networks further confirm this trend: the GI-R specimen is characterized by less connected fracture paths, whereas the GI-S specimen develops highly interconnected crack structures that extend throughout the matrix. These combined results indicate that smoother aggregates promote the formation of a greater number of interfacial cracks, leading to extensive crack coalescence. Overall, the strong agreement between experimental and numerical findings demonstrates that aggregate surface roughness exerts a decisive influence on crack initiation, connectivity, and propagation under drying shrinkage conditions.

These experimental and numerical results consistently demonstrate that aggregate surface roughness exerts a decisive influence on the initiation and propagation of shrinkage-induced cracks in cementitious composites. Rough aggregate surfaces enhance mechanical interlocking at the cement–aggregate interface, leading to stronger ITZ bonding and the development of relatively wider but less connected cracks within the surrounding matrix. In contrast, smooth aggregate surfaces weaken the ITZ, resulting in the formation of narrow interfacial cracks that are highly continuous and prone to coalescence into interconnected networks. The strong agreement between experimental observations and PD simulations highlights the capability of the proposed model to reliably capture the role of surface roughness in crack evolution.

4 Conclusion

This chapter investigated the role of inclusion surface characteristics on drying shrinkage-induced cracking in concrete using a mesoscale peridynamic framework with an imperfect interface formulation. By systematically varying the stiffness and fracture energy parameters of the ITZ, the study quantified how surface roughness—represented through interfacial mechanical properties—governs crack initiation, propagation, and network development. The main conclusions can be summarized as follows:

1. Reductions in normal stiffness (D_n) and tangential stiffness (D_t) promote wider cracks, larger crack volumes, and longer fracture paths. D_n primarily controls crack opening (mode I behavior), whereas D_t exerts a stronger influence on crack connectivity and mixed-mode propagation.
2. Both normal (G_{nc}) and tangential (G_{tc}) fracture energies exhibit pronounced threshold effects. Below a critical value of approximately 0.008 N/mm, fracture behavior

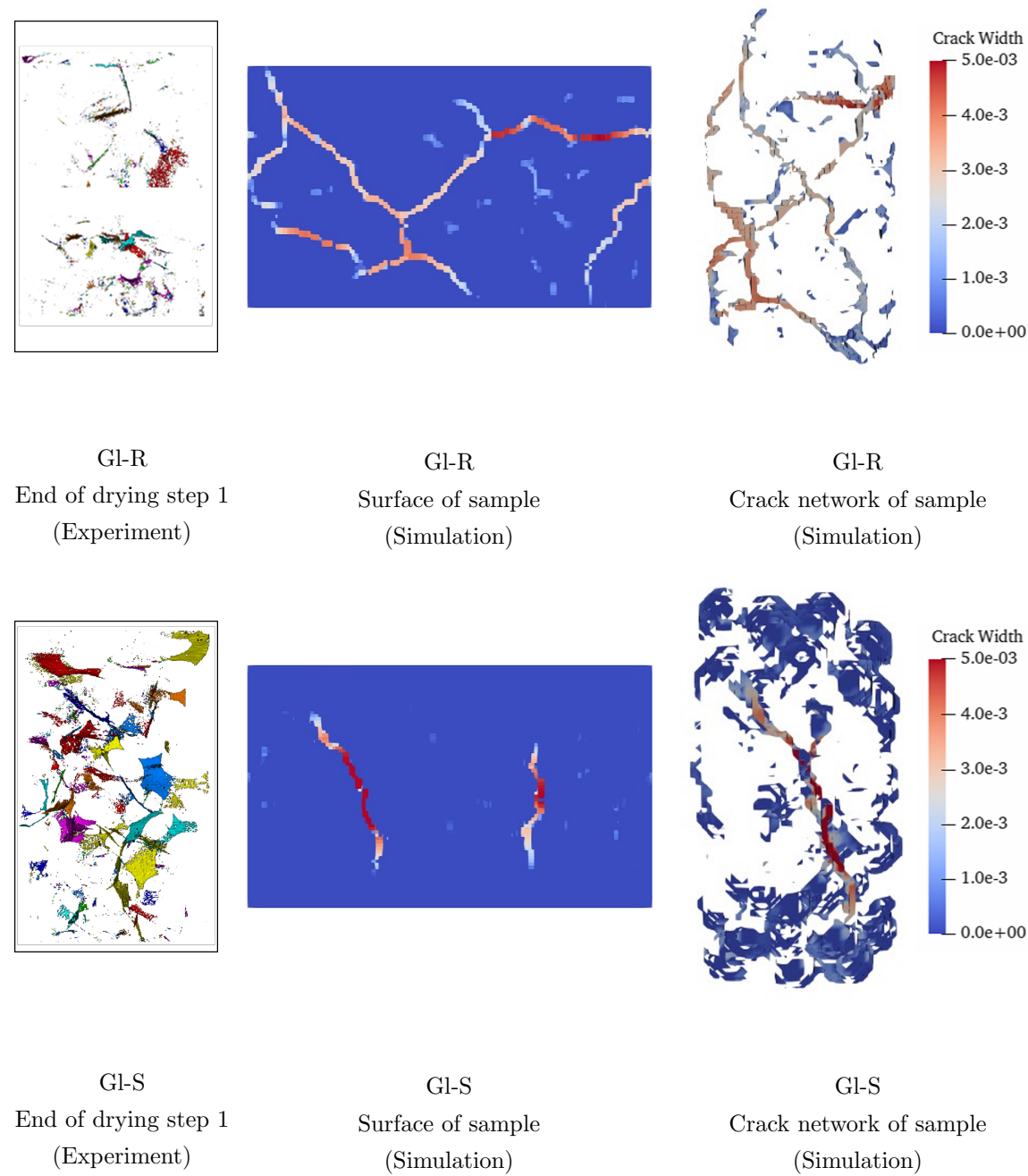


Figure V. 13: Experimental and simulated crack patterns for rough and smooth aggregate surfaces

transitions from localized interfacial cracking to highly connected networks of microcracks, with G_{nc} driving tensile debonding and G_{tc} facilitating shear-induced branching and matrix penetration.

3. Global sensitivity analysis shows that in the low-fracture-energy regime, crack evolution is dominated by G_{nc} , highlighting the key role of interfacial toughness in weak ITZs. In contrast, in the high-fracture-energy regime, fracture energy becomes less influential, and stiffness parameters—particularly D_t —emerge as the primary factors regulating crack growth and volumetric damage.
4. Experimental and numerical results demonstrate that aggregate surface roughness strongly governs drying shrinkage cracking. Smooth aggregates weaken the ITZ, leading to the formation of narrow but highly continuous interfacial cracks, whereas rough surfaces strengthen interfacial bonding, resulting in wider but less connected cracks within the matrix.

Overall, the findings confirm that inclusion surface characteristics critically influence drying shrinkage cracking through their effect on interfacial mechanical parameters. These insights provide a mechanistic understanding of how surface roughness modulates fracture resistance in cementitious composites and offer guidance for tailoring aggregate–matrix interactions to improve the durability and cracking resistance of concrete.

Chapter VI

Conclusions and Perspectives

As demonstrated in the preceding chapters, this thesis has addressed fundamental questions regarding the mechanisms, influencing factors, and predictive modeling of drying shrinkage-induced cracking in concrete. By combining mesoscale peridynamic modeling, parametric studies, and mechanistic analysis, a unified framework has been developed to link microstructural heterogeneity with macroscopic fracture behavior. The following sections summarize the principal findings and contributions of this work and outline prospective research directions aimed at advancing both the understanding and mitigation of cracking phenomena in durable concrete structures.

1 Conclusions

The main outcomes and implications of the present work are summarized in this section. The mechanisms of drying shrinkage-induced cracking in concrete were investigated through mesoscale peridynamic (PD) modeling that integrated theoretical development, numerical implementation, and mechanistic interpretation. The proposed frameworks have deepened the understanding of the relationship between microstructural heterogeneity and fracture processes and have provided predictive tools for designing more durable cementitious materials. The main scientific contributions and insights are summarized below.

A coupled hydro-mechanical bond-based peridynamic (BB-PD) framework was developed to describe the multiphysical coupling between pore pressure evolution and fracture propagation during the drying process. Crack initiation, growth, and coalescence under nonuniform moisture gradients were successfully reproduced, thereby providing a robust mechanistic platform for simulating shrinkage-induced cracking in cementitious composites. This framework effectively bridged microscale moisture transport phenomena with

mesoscale fracture processes, offering a physically consistent foundation for predictive modeling of drying-induced damage.

The influence of aggregate morphology on shrinkage cracking was investigated using mesoscale concrete models that explicitly incorporated aggregates of different shapes, including spherical, elongated, and flat inclusions. Numerical simulations revealed that aggregate geometry critically affects stress redistribution, strain localization, and crack morphology. Increased aggregate sphericity was found to reduce crack length and volume by promoting isotropic stress fields, whereas elongated and flat aggregates intensified anisotropy and facilitated the formation of preferential cracking paths. These findings identified aggregate shape as a key design variable for improving cracking resistance and long-term durability in concrete.

To more accurately represent heterogeneous interfaces, a novel three-dimensional imperfect peridynamic interface formulation was proposed. This model introduced independent normal and tangential stiffnesses as well as fracture energy parameters, enabling realistic simulation of debonding, sliding, and mixed-mode fracture processes. The transition from interfacial to matrix cracking and the threshold effects of interfacial toughness and stiffness on fracture propagation were successfully captured. These developments overcame the limitations of existing peridynamic interface representations and provided a generalized, physically interpretable framework for interfacial failure analysis.

Mechanistic analyses of the interfacial transition zone (ITZ) demonstrated that inclusion surface characteristics significantly influence crack initiation and propagation under drying shrinkage. Weak ITZs with low fracture energy were observed to promote crack localization and interfacial debonding, while stronger interfaces favored crack penetration into the bulk matrix. These results clarified the competing roles of interfacial toughness and stiffness in determining fracture path selection, thereby enhancing understanding of ITZ-controlled damage evolution in heterogeneous cementitious materials.

Overall, this thesis has demonstrated that aggregate geometry and ITZ properties jointly control the mesoscale cracking behavior of drying concrete. The proposed peridynamic formulations have bridged the gap between microstructural heterogeneity and macroscopic fracture responses, providing a predictive and physically grounded framework for assessing shrinkage-induced damage. Beyond methodological innovation, the findings contribute valuable guidance for the optimization of aggregate selection, ITZ engineering, and mixture design strategies toward more durable and sustainable concretes.

2 Perspectives

The developments presented in this thesis have established a rigorous theoretical and computational foundation for understanding and modeling drying shrinkage-induced cracking in cementitious materials. Building on these achievements, two major research directions are proposed for future work: (1) the extension of the peridynamic (PD) approach toward the durability and sustainability of conventional and low-carbon cementitious materials, accounting for the various coupled physical and chemical processes that govern degradation; and (2) the application of the PD framework to explore the dynamic behavior of concrete materials and structures subjected to extreme mechanical loading, such as projectile penetration and impact events.

2.1 Durability and Sustainability of Cementitious Materials

Peridynamics, with its nonlocal formulation and inherent ability to represent discontinuities, provides a powerful framework for studying the multiphysics deterioration of cementitious materials. Unlike classical continuum models, PD can describe the initiation and propagation of complex cracking networks and their interactions with moisture, heat, and chemical fields. This capability makes it ideally suited for the mechanistic modeling of durability-related phenomena in both conventional and emerging low-carbon concretes.

Future developments should first aim to extend the current hydro-mechanical PD framework into a fully coupled thermo-hydro-mechanical (THM) model. Such an extension would enable the simultaneous simulation of drying, thermal gradients, and freeze-thaw cycles under realistic environmental conditions. Within this framework, the progressive evolution of transport and mechanical properties—particularly permeability, diffusivity, and stiffness within the interfacial transition zone (ITZ)—should be explicitly modeled as functions of microcracking. These couplings are critical for predicting moisture redistribution, damage localization, and the onset of durability loss. Moreover, incorporating temperature-dependent transport properties and phase changes of pore water would significantly enhance the predictive capability for long-term performance and service life.

A second promising direction involves coupling the PD approach with advanced fluid and mass transport solvers, such as the Lattice Boltzmann Method (LBM) or finite-volume implementations of the Darcy-Stokes equations. This integration would allow the explicit resolution of fracture-flow interactions and the identification of preferential transport pathways through evolving crack networks. Such hybrid models would provide physically grounded predictions of permeability evolution, self-healing phenomena, and

the ingress of aggressive species, including chlorides, sulfates, and CO_2 . These capabilities are essential for a quantitative assessment of durability under variable environmental exposures.

The extension of PD modeling to low-carbon and recycled aggregate concretes (RAC) represents another strategic research avenue. In these materials, alternative binders, recycled aggregates, and modified ITZ characteristics fundamentally alter fracture and transport processes. The combination of high-resolution X-ray μCT -based mesostructural characterization and PD simulation would enable detailed quantification of microstructural effects on durability and mechanical integrity. Such studies would support the formulation of new design strategies for low-carbon cementitious systems that balance environmental impact, mechanical robustness, and long-term resilience.

Finally, the incorporation of chemical–mechanical coupling within the PD framework constitutes an essential step toward a unified multiscale understanding of concrete degradation. Reaction–diffusion mechanisms such as carbonation, chloride ingress, and sulfate attack can be integrated with fracture evolution to capture the synergistic interaction between mechanical damage, mass transport, and chemical transformation. The resulting chemically informed PD models would provide a physically consistent basis for predicting deterioration kinetics, assessing service life, and optimizing material formulations for enhanced durability and sustainability.

2.2 Dynamic Behavior of Concrete Materials and Structures

Beyond environmental durability, the peridynamic method offers a robust and versatile platform for investigating the dynamic response of concrete materials and structures subjected to extreme mechanical loads. Its intrinsic ability to represent discontinuities without additional damage criteria, coupled with its compatibility with rate-dependent constitutive laws, makes it particularly well suited for simulating impact, blast, and penetration events.

Future research should therefore focus on extending the PD framework to model projectile penetration and high-velocity impact in concrete and ultra-high-performance concrete (UHPC). Such simulations would provide detailed insights into the mechanisms of energy dissipation, crack branching, spalling, and fragmentation under high strain rates. By capturing the entire sequence of impact-induced damage—from microcrack initiation to large-scale material fragmentation—the PD approach can bridge the gap between mesoscale material behavior and structural-level performance. These studies would offer valuable guidance for designing protective and resilient infrastructures.

The coupling of PD simulations with experimental penetration and spalling tests will be critical for model calibration and validation. Incorporating strain-rate-dependent constitutive models and dynamic fracture criteria into the PD framework would further enhance predictive accuracy. Additionally, combining PD with advanced measurement techniques, such as high-speed imaging and digital image correlation, could provide a comprehensive understanding of dynamic fracture processes and facilitate the development of energy-based damage indices for impact-resistant materials.

Improving computational scalability is also essential for enabling realistic simulations at engineering scales. Future work should pursue high-performance implementations through GPU acceleration, adaptive domain decomposition, and variable-horizon discretization. Such advances would permit large-scale three-dimensional simulations with complex aggregate morphologies and realistic boundary conditions, thereby bridging the mesoscale and structural domains. This capability would make PD a practical predictive tool for the assessment and optimization of concrete structures exposed to extreme loading environments.

In summary, the methodologies and insights developed in this thesis provide a robust foundation for advancing both the durability and dynamic performance of cementitious materials through peridynamic modeling. By extending PD to encompass coupled environmental and chemical processes, sustainable material formulations, and high-rate dynamic behavior, future research can contribute to a unified, multiphysics, and multiscale understanding of concrete. This integrated approach will support the rational design of next-generation materials and infrastructures that are simultaneously durable, sustainable, and resilient throughout their service life.

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