A Review of Multi-Scale Modelling of Concrete Deterioration: Fundamentals, Techniques and Perspectives

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Abstract:

The properties of concrete are degraded during service by coupled physical and chemical processes that operate at several length scales, and the prediction of its performance in engineering structures requires multi-physics, multi-scale modelling approaches. The aim of this paper is to provide a comprehensive overview of the current modelling techniques for analysis of concrete deterioration. The paper covers the fundamentals of modelling at several length scales, as well as the bridging/transition between scales, and the numerical methods based on continuum and discrete formulations appropriate to different scales. Considered are the key chemical and physical deterioration processes of carbonation, chloride ingress, freeze-thaw damage, and abrasion. The paper also reviews the validation and verification of multi-scale models and discusses future trends such as data science integration and sustainable concrete design. It is expected that the information presented here will be a valuable resource for researchers and practitioners in the field, highlighting advancements and stimulating future research in multi-scale modelling of concrete deterioration.

Keywords: Multi-scale modelling; concrete deterioration; finite element method; discrete element method; molecular dynamics

1. Introduction

Concrete deterioration refers to the progressive degradation of performance of concrete structures over time. It is a natural process influenced by a combination of factors such as environmental conditions, material properties, design choices and construction practices (Dasar et al. 2017; Yi et al. 2020). Understanding the mechanisms causing deterioration is crucial for effective maintenance and management of existing, as well as for improved design of future, concrete infrastructure.

Chemical deterioration of concrete occurs when aggressive substances penetrate the concrete matrix and react with its components. One common form is carbonation, where carbon dioxide from the atmosphere reacts with the calcium hydroxide in concrete to form calcium carbonate, leading to a decrease in alkalinity and potential corrosion of reinforcement (Ho & Lewis, 1087; Sulapa et al. 2003; Leemann & Moro, 2017). Chloride ingress, primarily through exposure to seawater or de-icing salts, can cause corrosion of embedded steel, resulting in cracking and spalling (Gunevisi et al. 2007; Zhu et al. 2016; Hajkova et al. 2018). Sulphate attack occurs when sulphates in groundwater or soil react with the components of concrete, leading to the formation of expansive products and subsequent cracking (Al-amoudi, 2002; Neville, 2004; Zao et al. 2020).

Physical deterioration of concrete involves mechanical forces and environmental factors. Freeze-thaw cycles expose concrete to repeated freezing and thawing, causing the expansion and contraction of water within the pores. This process can lead to internal pressure and damage, including surface scaling, cracking and loss of strength (Rosenqvist et al. 2015; Matalkah & Soroushian, 2018; Zao et al. 2022). Abrasion and erosion occur due to the repetitive action of heavy loads, vehicular traffic, or water flow, resulting in the wear and

degradation of the concrete surface (Scott & Safiuddin, 2015). Thermal stresses arise from temperature variations, causing differential expansion and contraction, which can lead to cracking and structural distress (Wisnom et al. 2006; Mackiewicz, 2014).

Multi-scale modelling has emerged as a powerful tool for studying and predicting concrete deterioration. It involves integrating different length scales, from the macroscopic behaviour of the structure to the microscopic interactions at the material level. Multi-scale models consider factors such as material properties, chemical reactions, and physical processes to simulate the behaviour and degradation of concrete accurately (Maekawa et al. 2008; Bosco et al. 2020: Pan & Ramaswamy, 2023). By capturing the complex interactions between various deterioration mechanisms, multi-scale modelling enables researchers to evaluate the long-term performance of concrete structures, predict service life and optimise maintenance strategies. The development of advanced multi-scale modelling techniques has expanded our understanding of concrete deterioration processes. Computational models based on finite element analysis, discrete element methods, molecular dynamics and hybrid approaches provide insights into the deterioration mechanisms, damage propagation and structural response (Nguyen et al. 2017; Lau et al. 2018). These models help researchers explore different scenarios, test the effectiveness of preventive measures, and optimise material choices and designs.

Furthermore, multi-scale modelling facilitates the optimisation of concrete material properties and design strategies to enhance durability (Geikaer et al. 2017; Zhang et al. 2021). It enables the assessment of various materials, reinforcement configurations and protective measures, leading to the identification of optimal solutions to mitigate specific deterioration mechanisms. In addition to its engineering applications, multi-scale modelling offers cost and time efficiency compared to traditional experimental testing. It allows researchers to virtually simulate diverse deterioration scenarios, evaluate different design alternatives and predict the effectiveness of repair or prevention strategies. Moreover, multi-scale modelling contributes to the optimisation of maintenance strategies by providing insights into deterioration processes (Avril et al. 2005; Sun et al. 2020). It aids in identifying critical areas requiring attention and evaluating the effectiveness of maintenance scenarios such as surface treatments, cathodic protection, or crack repairs.

The motivation for this paper lies in the need to address the complex challenges associated with concrete durability. Traditional empirical approaches are limited in capturing the intricate multi-scale phenomena involved in concrete deterioration. By integrating various length scales, multi-scale modelling offers a powerful tool to understand and predict the behaviour of concrete structures. This review aims to consolidate recent advancements in multi-scale modelling techniques, provide a critical analysis of their applications in concrete deterioration studies and highlight their significance in advancing our understanding of concrete durability. By doing so, it aims to contribute to the development of more sustainable and resilient concrete infrastructure.

While this review provides valuable insights and analysis, it is important to acknowledge certain limitations. Firstly, due to the vastness of the topic, it may not cover all the possible multi-scale modelling techniques and applications in concrete deterioration. Secondly, the review relies on existing literature and therefore, the availability and quality of research articles may influence the comprehensiveness of the analysis. Additionally, the review may not delve into specific case studies or experimental validations of the multi-scale models discussed. As with any review paper, there is always a potential for bias in the selection and interpretation of the included studies. It is crucial for readers to consider these limitations and further explore the topic to gain a comprehensive understanding of multi-scale modelling of concrete deterioration. Lastly, the scope of the review is concrete as a material. The use of the approaches presented here in performance assessment of structural members is a topic requiring a separate review.

2. Fundamentals of Multi-scale Modelling

The fundamentals of multi-scale modelling in the context of concrete deterioration are essential to understand the complex behaviour of the material at different length scales. Multi-scale modelling involves bridging the gap between macroscopic and microscopic phenomena, enabling a more accurate representation of the material's response to deterioration mechanisms. It encompasses the concepts and principles of scale transitions, where information from smaller scales is integrated into larger scales and vice versa. This integration allows capturing the heterogeneity, interactions, and interdependencies among different length scales, which are crucial in accurately simulating the deterioration processes. By considering the fundamentals of multi-scale modelling, researchers can better understand the underlying mechanisms driving concrete deterioration and develop more effective strategies for mitigation and durability enhancement.

2.1 Concepts and Principles of Multi-scale Modelling

Multi-scale modelling is founded on the principles of capturing the interactions and behaviours of materials at multiple length scales. In the context of concrete deterioration, it involves understanding the fundamental concepts and principles that govern the material's behaviour and degradation mechanisms. At the core of multi-scale modelling is the concept of hierarchy. Concrete is composed of different components, such as cement paste, aggregates, and interfacial transition zones, each with its own unique characteristics and behaviours. These components interact with each other and contribute to the overall performance of the material. Multi-scale modelling aims to represent and simulate these components and their interactions accurately. The schematic of multiscale modelling of concrete is shown in Fig. 1. The first is a model of the cement meso-structure (top) consisting of different phases and pores. It is a structure between atomic scale and cement considered as a homogeneous continuum. The second is a model of the mortar meso-structure (middle) consisting of cement, fine aggregates, ITZs (and pores). This is a structure between the individual constituents listed and the mortar considered as a homogeneous continuum. The third is a model of the concrete meso-structure (bottom) consisting of mortar, coarse aggregates, ITZs (and pores). This is a structure between the individual constituents listed and the concrete considered as a homogeneous continuum (for engineering scale models).

To achieve this, multi-scale modelling relies on the concept of scale transitions. It involves defining relationships and interfaces between different length scales to ensure the flow of information and energy across scales. This requires identifying the relevant phenomena and mechanisms at each scale and understanding their interdependence. For example, at the nanoscale, modelling the hydration process and the formation of the cementitious matrix is crucial, while at the macroscale, the modelling of cracking and structural response becomes significant (Wang et al. 2017; Wang et al. 2019).

Another principle of multi-scale modelling is the coupling of different physical processes (Gong et al. 2017; Gallyamov et al. 2020). Concrete deterioration is often a result of the interplay between various degradation mechanisms, such as chemical reactions, physical stresses, and transport phenomena. Multi-scale modelling allows for the integration of these processes, enabling a comprehensive understanding of their combined effects on concrete deterioration. Moreover, multi-scale modelling considers the inherent heterogeneity and variability present in concrete (Achour et al. 2020; Yu et al. 2022; Tong et al. 2023). The material exhibits spatial variations in properties, such as aggregate distribution, pore structure and material composition. These variations impact the behaviour and degradation patterns of concrete. Multi-scale modelling accounts for this heterogeneity, either through stochastic approaches or by explicitly considering spatial variations, to capture the realistic response of the material.

By embracing the concepts and principles of multi-scale modelling, researchers can gain deeper insights into the mechanisms of concrete deterioration. It facilitates a more comprehensive understanding of the material's behaviour, prediction of its performance over time and exploration of mitigation strategies. Through the integration of different length scales, hierarchical structures and coupled processes, multi-scale modelling provides a powerful tool for studying and simulating concrete deterioration in a detailed and accurate manner.

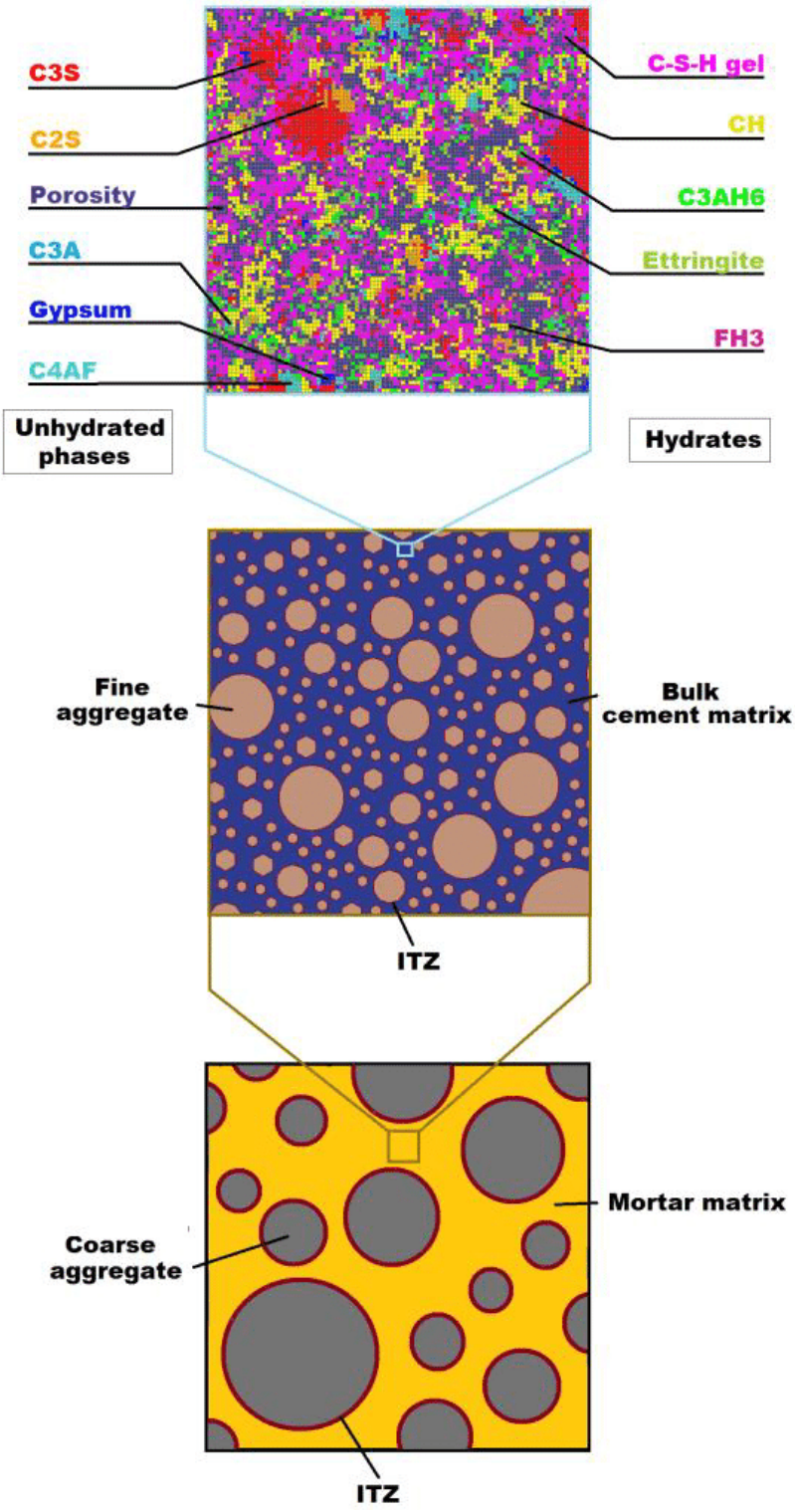

Fig. 1: A schematic of multiscale modelling of concrete

2.2 Importance of Scale Transitions in Concrete Deterioration Modelling

The importance of scale transitions in concrete deterioration modelling cannot be overstated. Concrete is a complex material with a hierarchical structure, consisting of various length scales, from the nanoscale to the macroscale (Wang et al. 2019; Zhang et al. 2023). Each scale contributes to the overall behaviour and performance of the material and capturing these interactions is crucial for accurate modelling and prediction of concrete deterioration. At the nanoscale, scale transitions are essential for understanding the fundamental processes that drive concrete deterioration (Sanchez & Sobolev, 2010). This includes the hydration of cement particles, the formation of hydration products and the chemical reactions that occur within the material. These nanoscale phenomena directly influence the mechanical and chemical properties of concrete and dictate its durability (Zadeh & Bobko, 2013).

Moving to the mesoscale, scale transitions become crucial for capturing the interactions between the cement matrix, aggregates, and interfacial transition zones (Gao et al. 2013; Baji et al. 2019; Wei et al. 2020). The mesoscale structure and composition play a significant role in concrete's mechanical strength, permeability, and resistance to deterioration mechanisms such as cracking, alkali-silica reaction, or chloride ingress. By considering scale transitions, models can effectively account for the influence of mesoscale features on the overall deterioration behaviour.

At the macroscale, scale transitions are vital for capturing the behaviour of concrete structures and the propagation of deterioration mechanisms. Concrete structures are subjected to various environmental and loading conditions, leading to localised damage, such as cracking, spalling, or corrosion. Scale transitions enable the modelling of these localised phenomena and the interaction between different regions of the structure, enhancing the accuracy of predictions and assessment of structural integrity (Camborde et al. 2000; Unger & Eckardt, 2011). Furthermore, scale transitions facilitate the integration of experimental data and computational models (McDowell & Dunne, 2010). Laboratory experiments often provide data at a specific length scale, while simulations allow for the investigation of concrete behaviour at multiple scales. By incorporating scale transitions, models can bridge the gap between experimental observations and numerical simulations, allowing for the validation, calibration and refinement of the models based on experimental data. The different scales and models used in the suggested multiscale analysis are depicted in Fig. 2 (Sherzer et al. 2017).

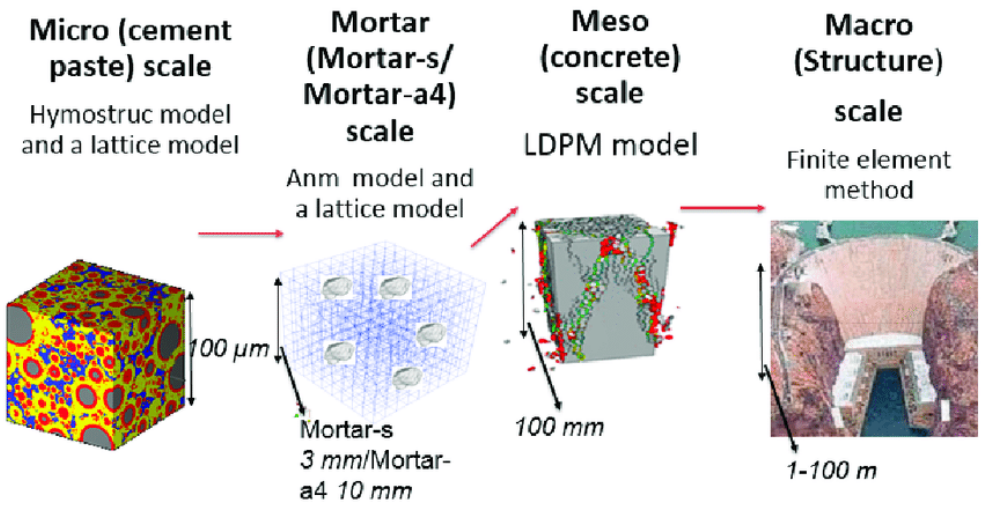

Fig. 2: The different scales and models used in the suggested multiscale analysis (Sherzer et al. 2017).

Incorporating scale transitions also enables the consideration of heterogeneity in concrete materials. Concrete exhibits spatial variations in properties, such as aggregate distribution, pore structure and material composition (Bouguerra et al. 1998; Zou et al. 2021). These variations can significantly impact the initiation and progression of deterioration mechanisms. By accounting for scale transitions, models can capture the heterogeneity and spatial distribution of properties, leading to more realistic predictions of deterioration patterns and localised damage.

Overall, the importance of scale transitions in concrete deterioration modelling lies in their ability to integrate different length scales, capture the multiscale nature of deterioration mechanisms, bridge the gap between experiments and simulations, account for heterogeneity and enhance the accuracy of predictions. By incorporating scale transitions effectively, models can provide valuable insights into concrete deterioration processes, aid in the development of effective mitigation strategies and contribute to the sustainable design and maintenance of concrete structures.

3. Multi-scale Modelling Techniques

Multi-scale modelling techniques involve the study and simulation of complex systems at different levels of detail and resolution. By capturing interactions and phenomena across various scales, these techniques enable a more comprehensive understanding of the system's behaviour. They are particularly valuable in fields such as materials science, biology, and engineering. Multi-scale modelling integrates different models and computational methods, ranging from atomistic simulations to continuum models, to bridge the gap between microscopic and macroscopic scales. This approach allows researchers to explore emergent properties, predict system behaviour and design optimised materials or processes. Ultimately, multi-scale modelling techniques empower scientists and engineers to tackle complex problems and make informed decisions in diverse domains.

3.1 Continuum-based Multi-scale Modelling Approaches

Continuum-based multi-scale modelling approaches provide a framework for simulating complex systems by incorporating different length and time scales. The Finite Element Method (FEM) is a widely used technique that discretises the system into finite elements, allowing for the analysis of mechanical behaviour and stress distribution. Lattice Element Method (LEM) extends FEM by considering the lattice structure of materials, enabling the modelling of materials with microstructural features. The Multi-scale Finite Element Method (MsFEM) combines FEM with sub-scale models, capturing the effects of heterogeneities and local behaviour. These approaches facilitate the simulation of large-scale systems by efficiently incorporating information from smaller scales, making them valuable tools in fields such as structural engineering, materials science, and geomechanics.

3.1.1 Finite Element Method (FEM)

The Finite Element Method (FEM) is a powerful numerical technique used to solve a wide range of complex engineering and scientific problems. It provides a systematic approach to approximately solve boundary value problems, i.e., problems formulated by partial differential equations that govern the behaviour of physical systems in prescribed domains, supplemented by boundary conditions that describe the interactions of these domains with the rest of the world. At its core, FEM involves discretising a continuous domain into smaller finite elements (Reddy, 2019). These elements are typically triangles or quadrilaterals in two dimensions and tetrahedra or hexahedra in three dimensions. The corners of these elements are defined by nodes, which serve as the vertices of the elements.

The first step in the FEM process is to establish a set of governing equations that describe the behaviour of the system. These equations are derived from the fundamental physical principles of conservation of mass/energy and linear/angular momentum, supplemented by empirical laws relating gradients of fields and fluxes referred to as the constitutive relations (Huebner et al. 2001). For example, in structural analysis, the equations represent conservation of momenta (equilibrium) via constitutive relations between gradient of displacement field (strains) and momentum flux (stress). In thermal analysis, the equations represent conservation of heat energy via constitutive relations between gradient of temperature field and heat flux. Next, the domain is divided into finite elements and the governing equations are approximated within each element. This involves representing the unknown quantities, such as displacements or temperatures, using interpolation functions defined over the element. The coefficients of these interpolation functions, known as nodal values, are then determined by solving the resulting algebraic equations.

To assemble the system of equations for the entire domain, the element equations are combined based on the connectivity of the nodes. This results in a global system of equations that needs to be solved to obtain the nodal values. This is typically done using numerical techniques such as matrix algebra and optimisation algorithms. Once the system of equations is solved, the FEM can provide detailed information about the system's behaviour. It can determine quantities such as stress distribution, deformation, temperature gradients, fluid flow rates and electromagnetic fields (Ma et al. 2014). These results help engineers and scientists understand and analyse the system's response to different inputs, such as forces, displacements, or boundary conditions. The details of a FEM modelling are shown in Fig. 3.

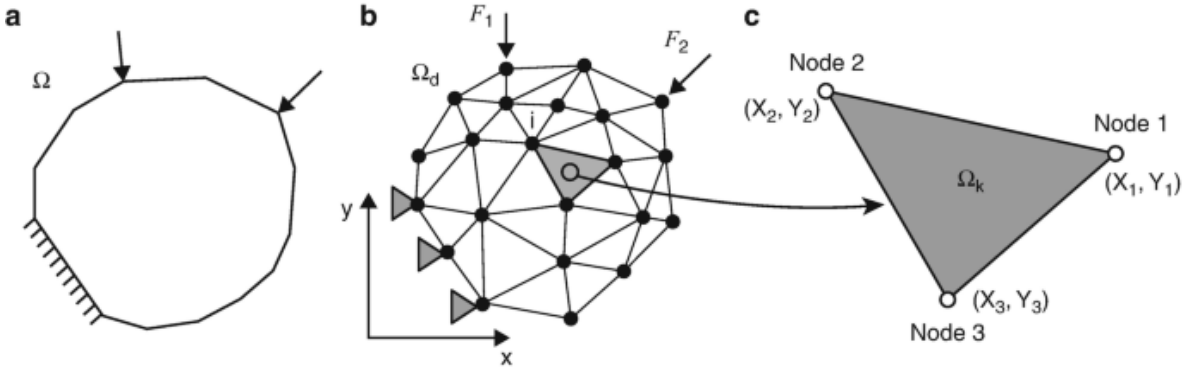

Fig. 3: Details of a FEM modelling (Tekkaya & Soyarslan, 2014)

One of the key advantages of FEM is its ability to handle complex geometries and material properties. Irregular shapes and varying material properties can be easily accommodated by appropriately dividing the domain into smaller elements. FEM also offers a flexible framework for incorporating different types of boundary conditions and constraints, making it suitable for modelling real-world scenarios accurately. Additionally, FEM allows for efficient computational solutions by exploiting the inherent structure of the system of equations. Sparse matrix techniques and iterative solvers are commonly employed to solve large-scale problems. Furthermore, adaptive mesh refinement techniques can be utilised to enhance the accuracy and efficiency of the solution.

The Finite Element Method finds extensive applications in various fields of engineering and science. It is widely used in structural analysis to analyse the behaviour of bridges, buildings, and mechanical components under different loading conditions. FEM is also employed in heat transfer problems to study temperature distributions and thermal gradients. In fluid dynamics, it is used to simulate fluid flow patterns, pressure distributions and turbulence. FEM is also utilised in electromagnetics to analyse electric and magnetic fields and their interactions with materials.

3.1.2 Multi-scale Finite Element Method (MsFEM)

The Multi-scale Finite Element Method (MsFEM) is a computational technique that combines the advantages of the Finite Element Method (FEM) with sub-scale models to accurately simulate and analyse complex systems across multiple length scales. MsFEM is particularly useful when dealing with heterogeneous materials or structures with varying microstructural features (Ibrahimbegović & Markovič, 2003; Saucedo-Mora & Marrow, 2015). In MsFEM, the domain of interest is divided into two or more scales: a macroscopic scale and one or more sub-scale domains. The macroscopic scale captures the overall behaviour of the system, while the sub-scale domains represent local regions with distinct material properties or microstructures. These sub-scale domains can be considered as representative volume elements (RVEs) or inclusion regions. Jun et al. (2020) discussed the MsFEM and its extension based on polyhedral coarse grid elements for modelling heterogeneous materials and structures (Fig. 4) In this study, the authors presented an enhanced version of MsFEM that incorporated polyhedral elements in the coarse grid to capture the geometric complexity of heterogeneous materials. The proposed approach enabled a more accurate representation of material interfaces and heterogeneities, resulting in improved predictions of the mechanical response of such materials and structures. The paper provided valuable insights into the application of MsFEM for modelling heterogeneous systems, opening avenues for advanced simulations in various engineering disciplines.

The MsFEM is applied at the macroscopic scale to model the global behaviour of the system. The macroscopic MsFEM provides an approximation of the solution and describes the overall deformation and stress distribution. However, at this scale, the MsFEM may not accurately capture localised effects or microstructural details. To overcome this limitation, sub-scale models are introduced within the sub-scale domains. These models, which can be analytical, numerical, or even experimental, capture the behaviour of the local regions more accurately. They account for the microstructural details, such as material heterogeneity, interfaces, or localised deformation mechanisms. The sub-scale models are then integrated with the macroscopic MsFEM through a process called the coupling scheme. The coupling scheme exchanges information between the macroscopic and sub-scale domains, ensuring compatibility and consistency between the two scales. This integration enables the transfer of localised information from the sub-scale models to the macroscopic scale, improving the accuracy of the overall simulation.

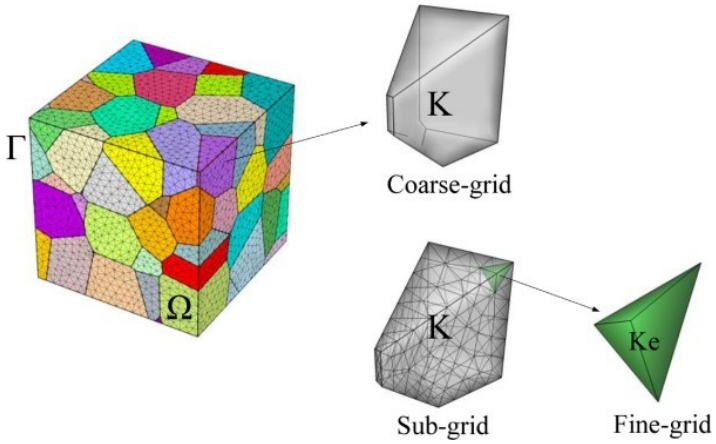

Fig. 4: Details of Extended multiscale finite element method based on polyhedral coarse grid elements (Jun et al. 2020)

The MsFEM offers several advantages. It allows for the accurate representation of materials with complex microstructures and heterogeneous properties. It also captures localised effects, such as stress concentrations or strain localization, which are critical in many applications. By

incorporating sub-scale models, MsFEM provides a more comprehensive understanding of the system's behaviour and can predict phenomena that are not captured by conventional macroscopic models.

MsFEM finds applications in various fields, including materials science, geomechanics and structural analysis. It is used to study the mechanical behaviour of composite materials, heterogeneous media, or materials with inherent length-scale effects. MsFEM is also applied in the analysis of fractures, damage propagation, or the behaviour of materials with complex interfaces or inclusions.

3.2 Particle-based Multi-scale Modelling Approaches

Particle-based multi-scale modelling approaches are computational techniques that simulate complex systems by representing them as collections of individual particles. These methods capture the behaviour of systems at different scales, bridging the gap between microscopic and macroscopic phenomena. Two widely used approaches are the Discrete Element Method (DEM) and Smoothed Particle Hydrodynamics (SPH). DEM models the interactions between particles, making it suitable for granular materials and particulate systems. SPH, on the other hand, represents fluids as a collection of particles and is ideal for simulating fluid flows and interactions. These particle-based methods provide valuable insights into the dynamics, behaviour and interactions of particles or fluids, enabling the analysis of multi-scale systems in diverse fields such as engineering, physics and materials science.

3.2.1 Discrete Element Method (DEM)

The Discrete Element Method (DEM) is a computational technique used to simulate the behaviour of granular materials, powders and other particulate systems. It represents the system as a collection of individual particles that interact through contact forces, allowing for the study of particle-scale phenomena. In DEM, each particle is characterised by its position, velocity, mass and other properties (Ghaboussi & Barbosa, 1990; Radjai & Richefeu, 2009). The behaviour of the particles is governed by contact laws, which describe the forces and moments that arise when particles come into contact. These laws consider factors such as particle shape, friction and cohesion.

Through numerical integration, DEM calculates the motion of each particle over time, taking into account the forces and torques exerted by neighbouring particles. The simulation captures various phenomena, including particle-particle collisions, compaction, flow and segregation. DEM finds applications in diverse fields such as civil engineering, geotechnical engineering, mining, pharmaceuticals and food processing. It is used to analyse the behaviour of soils, granular structures, powders and bulk materials in processes like mixing, crushing and conveying (Ghaboussi & Barbosa, 1990; Tavarez & Plesha, 2007; Radjai & Richefeu, 2009; Coetzee, 2016; Coetzee, 2020). DEM simulations provide valuable insights into particle behaviour, structural stability and material flow, aiding in the design, optimisation and troubleshooting of industrial processes. Bertrand et al. (2008) focused on the application of the Discrete Element Method (DEM) for numerical modelling of a double-twisted hexagonal mesh. In this study, the authors utilised DEM to investigate the mechanical response and deformation characteristics of the double-twisted hexagonal mesh under various loading conditions. The paper provided valuable insights into the capabilities of DEM for modelling complex geometries and understanding the mechanical behaviour of geotechnical structures. It highlighted the potential of DEM as a powerful tool for analysing the stability and performance of such systems. The details of a DEM model are shown in Fig. 5.

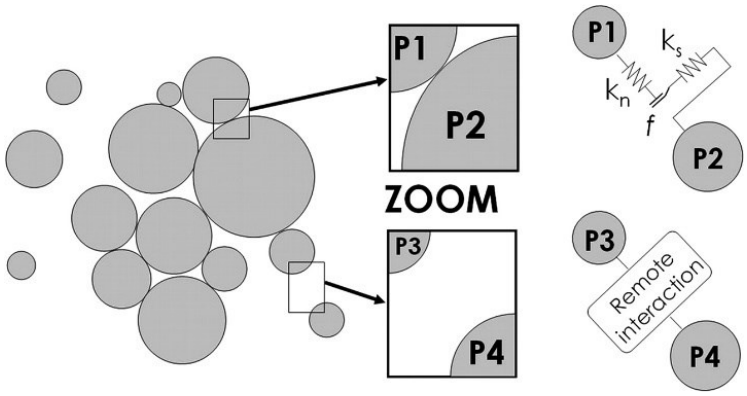

Fig. 5: details of a DEM model (Bertrand et al. 2008)

The advantages of DEM lie in its ability to capture the complex interactions and motions of individual particles. It allows for the study of systems with diverse particle shapes, sizes and material properties. DEM can account for particle-level phenomena, such as rotations, sliding and interparticle forces, providing detailed information about stress distribution, packing density and flow patterns. However, DEM also has challenges, including computational requirements for large-scale simulations and the need to calibrate contact parameters accurately. Researchers continue to develop enhancements to address these challenges, such as parallel computing algorithms and improved contact models.

3.2.2 Lattice Element Method (LEM)

The Lattice Element Method (LEM) is a continuum-based multi-scale modelling approach that extends the FEM by considering the lattice structure of materials. LEM is particularly useful for simulating materials with microstructural features, such as granular materials, foams, or cellular solids (Schlangen & Van Mier, 1992; Birck et al 2016; de Medeiros et al. 2022). In LEM, the material is represented as an interconnected network of lattice elements. Each lattice element corresponds to a small representative volume within the material, often referred to as a lattice cell. The lattice elements are connected at nodes, forming a lattice structure that captures the material's microstructural characteristics. The behaviour of each lattice element is described using constitutive equations that govern its deformation and interaction with neighbouring elements. These equations can be derived based on the material properties and microstructural features under consideration (Liu et al. 2020). For example, in granular materials, the constitutive equations may account for contact forces and frictional behaviour between particles.

Nikolić et al. (2018) explored the LEM and its peculiarities in structural modelling. The authors discussed various aspects of LEM, such as lattice configurations, element formulations and integration schemes. They highlight the advantages and limitations of LEM, including its ability to capture localised phenomena and its computational efficiency compared to continuum-based methods. The paper provides valuable insights into the application of LEM and serves as a reference for researchers and engineers interested in employing this method for structural analysis and design. The details of LEM model are depicted in Fig. 6.

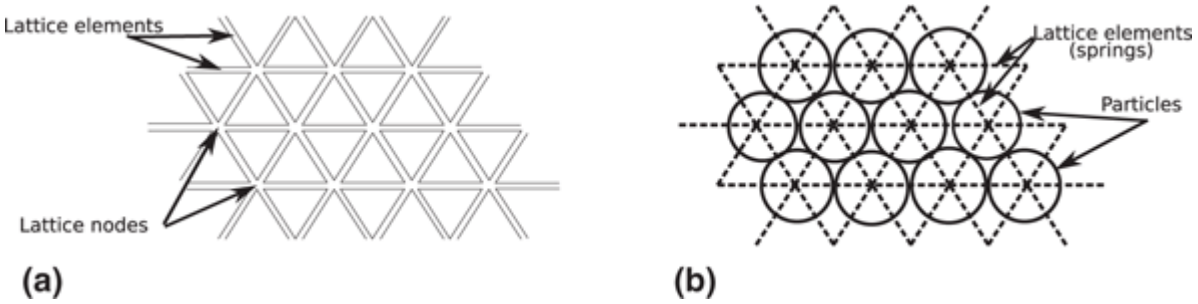

Fig. 6: Details of LEM model (Nikolic et al. 2018)

To simulate the response of the material, the lattice elements are subjected to external forces or displacements. The resulting deformation and stress distribution within the lattice structure can be obtained by solving the system of equations governing the behaviour of each lattice element. This solution provides insights into the material's overall response, including properties such as deformation patterns, stress concentration and failure mechanisms.

LEM offers several advantages over traditional continuum models. By explicitly considering the microstructure, LEM can capture localised effects, such as stress concentrations or strain localization, that are critical in materials with complex internal structures. It also enables the investigation of phenomena such as buckling, collapse, or compaction at the microscale. Furthermore, LEM provides a bridge between microscopic and macroscopic scales, allowing for the study of how microstructural properties influence the overall behaviour of the material. It can be used to investigate the impact of varying microstructural parameters, such as particle size or arrangement, on the material's mechanical response.

The LEM finds applications in various fields, including geomechanics, materials science and biomechanics. In geomechanics, LEM can simulate the behaviour of granular soils, rock masses, or underground structures subjected to loading or excavation (Sattari et al. 2017). In materials science, LEM helps understand the mechanical properties of foams, cellular solids, or composite materials with complex microstructures (Ravari et al. 2014). In biomechanics, LEM can be used to study the behaviour of biological tissues or implants with intricate architectures (Cerrolaza et al. 2017).

3.2.3 Smoothed Particle Hydrodynamics (SPH)

Smoothed Particle Hydrodynamics (SPH) is a meshless computational method used to simulate fluid flows and fluid-structure interactions. It represents fluids as a collection of particles, where each particle carries certain physical properties such as mass, position, velocity and other relevant parameters. In SPH, the behaviour of fluid is modelled by solving the governing equations, such as the continuity equation and the Navier-Stokes equations, using interpolation techniques (Ferrand et al. 2013; Pan et al. 2014; Canelas et al. 2015). The key idea behind SPH is to approximate the fluid properties at any point by averaging the properties of neigh boring particles within a smoothing radius. To calculate the particle interactions, SPH employs smoothing kernels that define the weight or influence of neighbouring particles on a given particle (Sao & Lo, 2003; Solenthaler et al. 2007; Islam & Peng, 2019). These kernels effectively smooth out the particle information, allowing for the transfer of physical quantities such as density, pressure and velocity between particles.

Dai et al. (2016) focused on the application of Smoothed Particle Hydrodynamics (SPH) for modelling the post-failure behaviour of landslides triggered by the 2016 Kumamoto earthquake (Fig. 7). In this study, the authors utilised SPH to investigate the landslide dynamics, including the mobilization and spreading of debris. They discussed the

implementation of SPH in capturing the complex behaviour of landslides, such as flow acceleration, deposition and erosion. The paper provided valuable insights into the use of SPH for simulating geotechnical disasters, contributing to the understanding of landslide mechanisms and supporting risk assessment and mitigation efforts.

One of the advantages of SPH is its ability to handle complex fluid geometries and free surfaces without the need for mesh generation. It can accurately simulate fluid flows with large deformations, splashing and breaking waves. SPH is particularly useful in applications such as ocean modelling, dam break analysis and astrophysics, where traditional methods struggle due to extreme conditions or complex geometries (Springel, 2010; Kao & Chang, 2012; Lowe et al. 2019). However, SPH simulations can be computationally expensive, especially when dealing with large-scale problems or high-resolution simulations. Efforts are made to improve the efficiency of SPH through parallel computing techniques and adaptive refinement strategies. In recent years, SPH has been extended to simulate other physical phenomena, such as solid mechanics, multiphase flows and even biological systems. This versatility and adaptability make SPH a valuable tool in various fields of research and engineering.

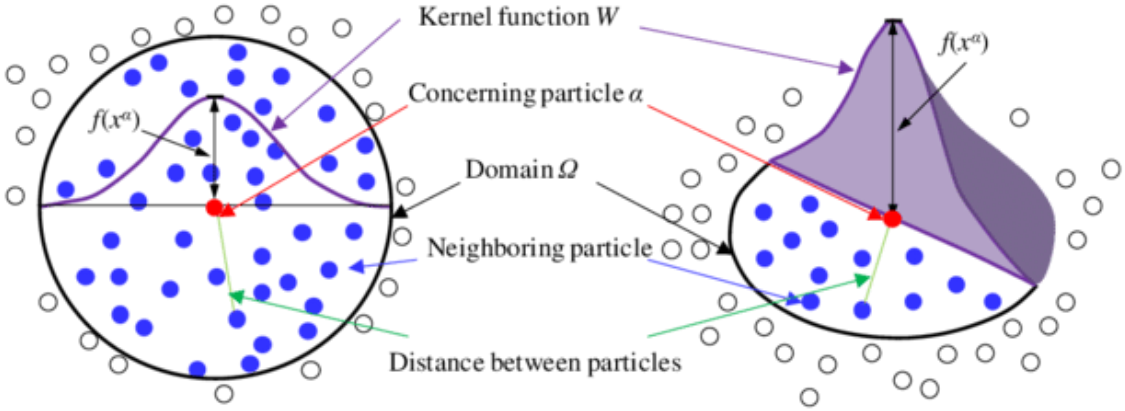

Fig. 7: Details of SPH-based numerical modelling (Dai et al. 2016)

3.2.4 Peridynamics Model (P)

Peridynamics is a mathematical framework that describes the behaviour of materials at a mesoscale level (Tong & Li, 2016). It is an alternative to classical continuum mechanics that focuses on modelling the interactions between individual material points rather than assuming a continuous distribution of matter. In the peridynamics model, a material is represented as a collection of points (sometimes called nodes) that interact with each other through pairwise forces. These forces are typically based on a non-local formulation, meaning that the interactions extend over a finite range rather than being limited to neighbouring points as in classical continuum mechanics. The governing equations of peridynamics are typically expressed in terms of integral equations, which describe the evolution of the displacement or deformation of the material points over time (Silling & Askaru, 2005; Buryachenko, 2020). The integral equations involve an integral over the entire material domain, capturing the interactions between all pairs of points. Figure 8 shoes the Illustration of concentration bonds (left) and Peridynamics flux between connected points (right) (Yan et al. 2020).

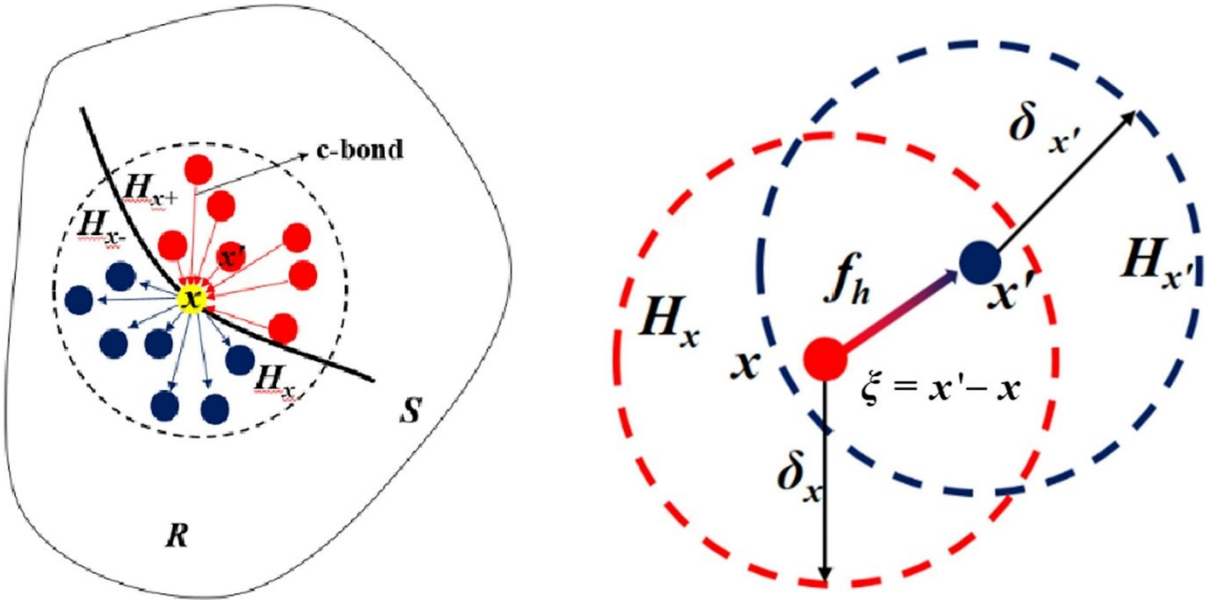

Fig. 8: Illustration of concentration bonds (left) and Peridynamics flux between connected points (right) (Yan et al. 2020)

One of the advantages of peridynamics is its ability to model discontinuities, such as cracks and fractures, naturally (Macek & Silling, 2007; Habibian et al. 2021). Since the interactions are not limited to neighbouring points, peridynamics can capture long-range effects and propagate failure over a larger area. This makes it particularly useful for simulating brittle materials or materials with complex failure mechanisms. Peridynamics has found applications in various fields, including solid mechanics, fracture mechanics, and materials science (Ni et al. 2018; Chen et al. 2021; Liu et al. 2023). It has been used to study fracture propagation, impact and blast effects, fatigue, and other failure phenomena. The numerical implementation of peridynamics involves discretizing the material domain into a mesh of points and solving the governing equations using computational methods such as finite differences or meshless methods. It is worth noting that peridynamics is still an active area of research, and its implementation and applications continue to evolve. Researchers are constantly exploring new developments and improvements to make peridynamics more accurate and efficient for a wider range of materials and problems.

3.3 Molecular Dynamics (MD) Simulations

Molecular Dynamics (MD) simulations are powerful computational techniques used to study the behaviour of atoms and molecules at the molecular level. MD simulations simulate the motion and interactions of particles by numerically integrating the equations of motion derived from classical mechanics or quantum mechanics. In MD simulations, the system is represented as a collection of atoms or molecules, each characterised by its position, velocity, and mass (Jain et al. 1993; Dupuy et al. 2005; Chowdhary et al. 2013). The forces between particles are described by interatomic or intermolecular potentials, which capture the interactions due to chemical bonding, electrostatic forces, van der Waals forces and other interactions. A schematic of the molecular dynamics process is shown in Fig. 9.

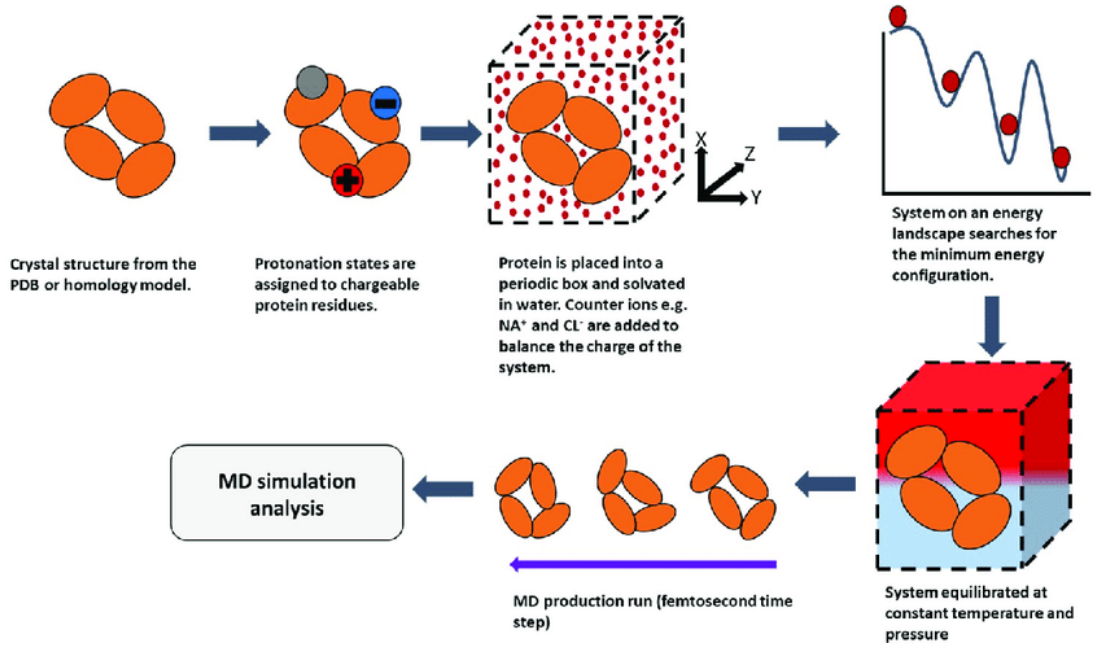

Fig. 9: A schematic of the molecular dynamics process (Pandya et al. 2018)

The simulation evolves the system over time, updating the positions and velocities of the particles based on the forces acting upon them. By repeatedly integrating the equations of motion, the simulation provides insights into the dynamics, thermodynamics, and structural properties of the system. MD simulations can be used to investigate a wide range of phenomena, such as the folding of proteins, chemical reactions, phase transitions and material properties (Duncan et al. 2011; Tang et al. 2016; Gissinger et al. 2017). They can reveal details about the energy landscape, reaction mechanisms, conformational changes and transport properties at the atomic or molecular level. MD simulations are particularly valuable when experimental measurements are challenging or expensive to obtain. They allow researchers to explore systems in silico, test hypotheses and provide atomistic-level understanding. Furthermore, MD simulations can be used to predict and design new materials, optimise drug candidates and guide the development of nanotechnologies.

However, MD simulations also have limitations. They rely on approximations and simplifications and the accuracy of the results depends on the quality of the force fields used. The computational cost can be high, especially for large systems or long simulation timescales. Additionally, MD simulations typically treat particles as classical entities, neglecting quantum effects, although methods such as ab initio molecular dynamics can incorporate quantum mechanics to some extent.

3.4 Hybrid Multi-scale Modelling Approaches

Hybrid multi-scale modelling approaches combine different modelling techniques to capture the behaviour of complex systems across multiple scales. These approaches aim to overcome the limitations of individual modelling methods by leveraging their respective strengths. In hybrid multi-scale modelling, different regions or components of the system are simulated using different techniques, which are then coupled together (Chen et al. 2013; Cilfone et al. 2015). For example, a continuum-based method like the Finite Element Method (FEM) may be used to model the macroscopic behaviour of a structure, while a particle-based method like the Discrete Element Method (DEM) can capture localised particle interactions in certain regions. The coupling between different modelling methods can be achieved through various techniques, such as overlapping or embedded domain methods, data exchange interfaces, or transition zones. These coupling schemes ensure compatibility and information transfer

between different scales, allowing for a seamless integration of different modelling approaches.

Hybrid multi-scale modelling offers several advantages. It allows for the efficient simulation of complex systems by utilising the most appropriate modelling technique for each region or scale. It can capture both macroscopic behaviour and microstructural effects, providing a comprehensive understanding of the system. Hybrid approaches also enable the investigation of phenomena that arise due to the interaction between different scales, such as the influence of microstructural features on the overall system response. These approaches find applications in various fields, including materials science, biomechanics, and geotechnical engineering. For example, in materials science, hybrid multi-scale modelling can simulate the mechanical behaviour of composite materials with different constituent phases (El Said et al. 2016). In biomechanics, it can capture the interaction between tissues and implants with varying length scales (Nikmaneshi & Firoozabadi, 2022). In geotechnical engineering, hybrid approaches can model the behaviour of soil-structure interaction considering both macroscopic and microscopic effects.

Despite the advantages, hybrid multi-scale modelling also presents challenges. The coupling between different modelling techniques can be complex, requiring careful calibration and validation. Computational costs may increase due to the use of multiple methods and the need for data exchange between scales. Furthermore, the choice of modelling techniques and the determination of appropriate transition zones or interfaces require expertise and knowledge of the system under investigation.

4. Multi-scale Modelling of Chemical Deterioration

Multi-scale modelling plays a crucial role in understanding and predicting the chemical deterioration of concrete. By considering multiple length and time scales, it enables a comprehensive analysis of the complex processes involved in chemical degradation. In the context of concrete deterioration, multi-scale modelling allows for the simulation of various chemical degradation mechanisms such as carbonation, chloride ingress, sulphate attack and alkali-aggregate reaction. It captures the interactions between the chemical species, pore structure and microstructure of concrete, providing insights into the spatial and temporal evolution of deterioration. Multi-scale modelling facilitates the evaluation of factors influencing chemical deterioration, including environmental conditions, material properties and structural design. It aids in the development of effective mitigation strategies, allowing engineers and researchers to optimise concrete formulations, design durable structures and enhance the service life of concrete infrastructure.

4.1 Carbonation Modelling

Multi-scale carbonation modelling is a sophisticated and comprehensive approach that plays a crucial role in understanding and predicting the process of carbonation in concrete. Carbonation is a complex chemical reaction that occurs when carbon dioxide (CO_2) from the atmosphere infiltrates the concrete and reacts with calcium hydroxide ($Ca(OH)_2$) in the cement matrix. This reaction leads to the formation of calcium carbonate ($CaCO_3$) and results in the reduction of the concrete's alkalinity. Multi-scale carbonation modelling considers various length scales, ranging from the macroscopic to the microscopic level, to provide a comprehensive understanding of the carbonation process. At the macroscopic level, these models consider the overall behaviour of the concrete structure, considering factors such as CO_2 diffusion, carbonation depth and distribution (Bary & Sellier, 2004; Phung et al. 2016). Environmental parameters such as CO_2 concentration, temperature, humidity, and material properties including porosity, permeability and carbonation rate constants are incorporated into these models to accurately simulate the carbonation process.

At the microscopic level, multi-scale carbonation models delve into the pore structure of concrete and analyse the chemical reactions occurring at the pore scale. They consider factors such as pore size distribution, capillary action, and the transport of CO_2 within the pores (Kwon & Song, 2010; Alizadeh et al. 2014). By studying the microstructure and pore network of concrete, these models provide insights into the local carbonation kinetics, including the influence of moisture content, cement composition, curing conditions and the presence of supplementary cementitious materials. This information is crucial in understanding the mechanisms and rate of carbonation in different regions of the concrete structure.

Iwama and Maekawa (2022) explored the modelling of carbonation, de-carbonation and re-carbonation processes in concrete subjected to high-temperature heating. While this study expanded the scope to include the effect of high temperatures, it specifically addressed the carbonation process during heating and may not have covered all aspects of carbonation in ambient conditions. Figure 10 shows the outline of carbonation, de-carbonation, and re-carbonation models during and after heating. The multi-scale modelling of carbonation in concrete had garnered significant attention from researchers in recent years. Maekawa et al. (2003) presented a comprehensive review of multi-scale modelling in concrete, including the integration of material and structural mechanics. While the paper provided a valuable overview of the topic, it predated recent advancements in multi-scale modelling techniques and may not have fully captured the state-of-the-art in carbonation modelling.

Torres et al. (2019) focused on the modelling of carbonation-calcination cycles for the calcium looping process, which involved the capture of CO_2 from flue gases. While the study was relevant for carbonation modelling, it primarily addressed a specific application rather than the general carbonation of concrete. Therefore, the direct applicability of the findings to the carbonation of structural concrete may have been limited. Zhan et al. (2021) investigated the mechanical behaviour and microstructural alteration of calcium silicate hydrate (CSH) in carbonated alite paste. The study offered valuable insights into the impact of carbonation on the microstructure and mechanical properties of concrete. However, it primarily focused on a specific phase of concrete and did not provide a comprehensive multi-scale modelling framework for carbonation.

The integration of information from multiple scales in multi-scale carbonation modelling enhances the accuracy and reliability of predictions related to the carbonation process. By considering various length scales, these models provide a more realistic representation of the complex interactions between CO_2, concrete constituents, and environmental conditions. This allows researchers and engineers to evaluate the long-term performance of concrete structures, estimate the carbonation depth and rate over time and assess the effectiveness of preventive measures or repair strategies. Furthermore, multi-scale carbonation modelling enables the optimisation of concrete mixes for enhanced durability and sustainability. By understanding the factors influencing carbonation, such as the role of pore structure, material composition and environmental conditions, researchers can design concrete with improved resistance to carbonation-induced deterioration. This knowledge can aid in the development of sustainable and resilient concrete structures that can withstand the challenges of carbonation in various environments.

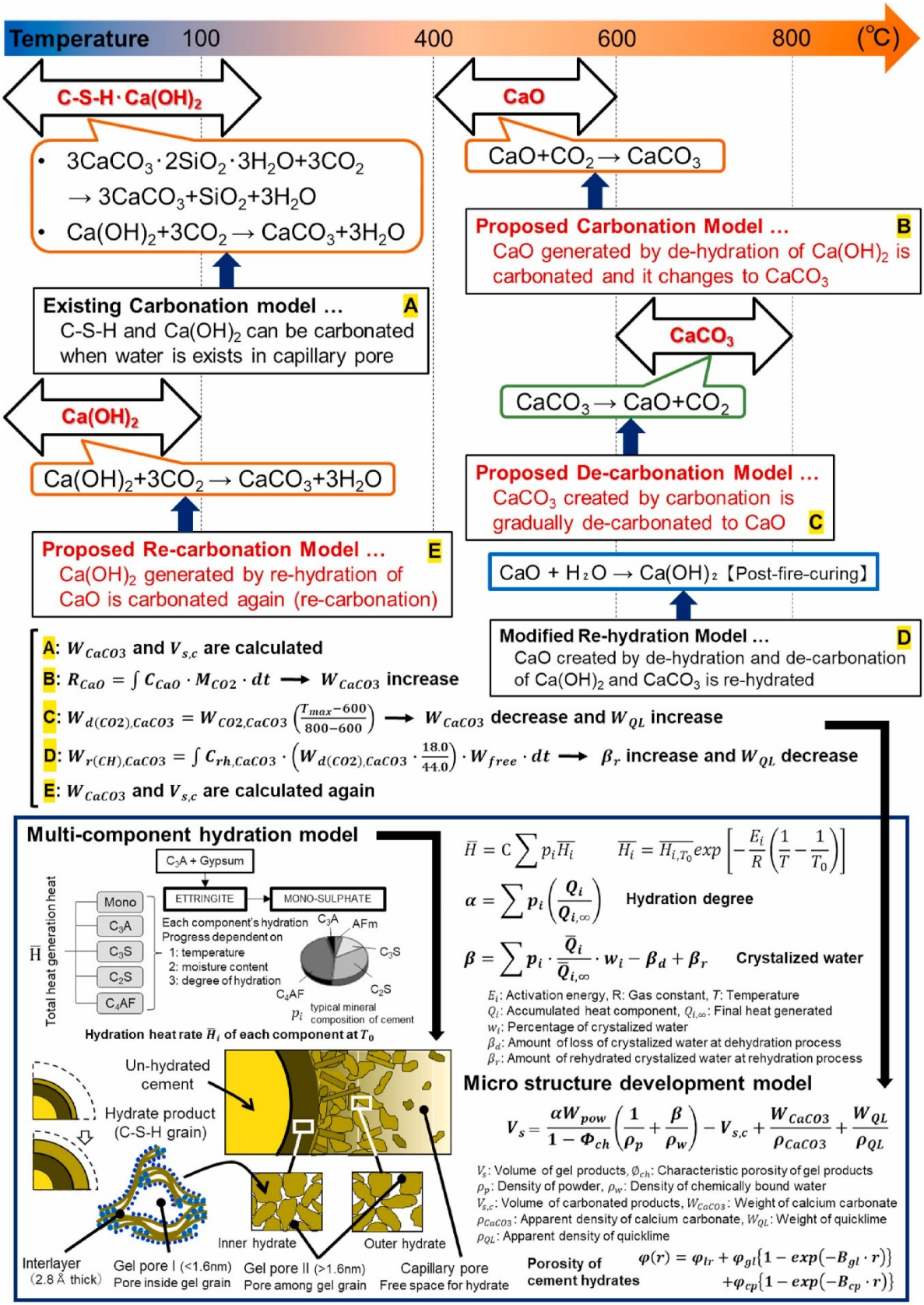

Fig. 10: Outline of carbonation, de-carbonation and re-carbonation models during and after heating (Iwama and Maekawa, 2022)

4.2 Chloride Ingress Modelling

Multi-scale chloride ingress modelling is a comprehensive approach used to study the transport and diffusion of chloride ions in concrete structures, which can lead to the corrosion of reinforcement steel and subsequent deterioration. This modelling technique integrates different length scales to provide a holistic understanding of chloride ingress and its impact on concrete durability. At the macroscopic level, models consider the overall behaviour of chloride ion transport in concrete, considering factors such as exposure conditions, concrete composition and diffusion coefficients. These models provide valuable information on chloride concentration profiles, penetration depth and the overall rate of chloride ingress into the concrete.

Moving to the mesoscopic level, multi-scale models examine the interaction between chloride ions and the cementitious microstructure, including the cement paste, aggregates, and pore network. These models consider factors such as pore size distribution, connectivity, and tortuosity, as well as the influence of admixtures or supplementary cementitious materials. They offer insights into the effects of microstructural characteristics on chloride diffusion and the transport pathways within the concrete. At the microscopic level, models focus on the molecular interactions between chloride ions and the cementitious materials. Molecular dynamics simulations and quantum chemical calculations are utilised to understand the fundamental mechanisms of chloride ingress at the atomic scale. These models consider the interactions between chloride ions, cement hydrates and other constituents, providing insights into the adsorption, diffusion, and binding of chloride ions at the nanoscale level.

The integration of multiple scales in chloride ingress modelling enables a more accurate representation of the complex phenomena involved in chloride transport and subsequent corrosion. It facilitates the prediction of chloride penetration depth, assessment of reinforcement corrosion risks and evaluation of preventive measures or mitigation strategies. By considering various scales, multi-scale chloride ingress modelling enhances our understanding of transport mechanisms, offers insights into factors influencing chloride ingress and supports the development of strategies to improve the durability of concrete structures. It aids in decision-making processes related to material selection, design optimisation and maintenance practices to mitigate the detrimental effects of chloride-induced corrosion.

In their study, Tong et al. (2023) proposed a predictive model for concrete, considering a 3-phase composition of aggregates, interfacial transition zones (ITZs) and mortar. The model assumed that only one side of the concrete was exposed to the ionic solution, while the remaining faces were non-flux (Fig. 11a). This unidirectional chloride transport from upstream to downstream allowed for the rational use of 2D randomness in the analysis of concrete durability. The Finite Element model developed in the study was depicted in Fig. 11b, with its corresponding mesh shown in Fig. 11c. To account for the influence of coarse aggregate shape on chloride diffusion, irregular shapes were assigned to the coarse aggregates in the model. Additionally, Figure 12 illustrated the process of parameter transfer across different scales and how the homogenisation methods facilitated the upscaling of heterogeneous characteristics from lower to upper scales within the proposed multi-scale predictive model.

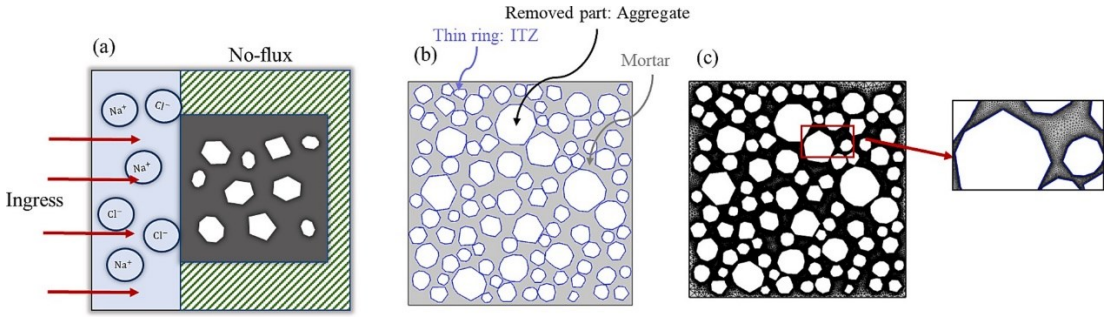

Fig. 11: The process of estimating the diffusivity of ions at concrete scale (a) Schematic diagram of chloride penetrating (b) Geometry of finite element model (c) Mesh generation of finite element model (Tong et al. 2023)

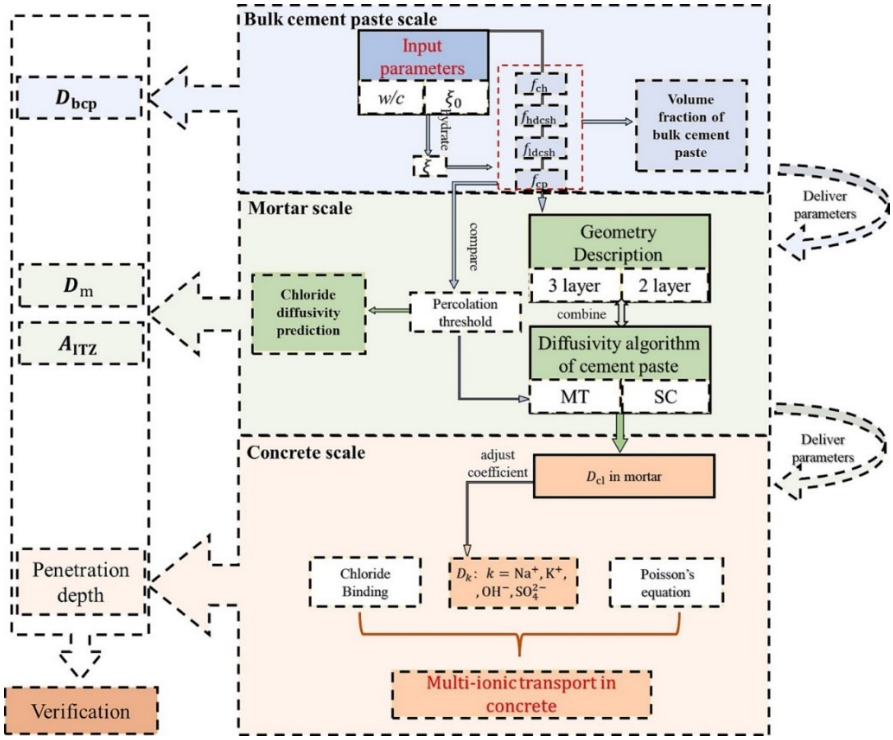

Fig. 12: The schematic diagram of coupling process for model validation (Input and output flowchart) (Tong et al. 2023)

In their study, Zhang et al. (2021) conducted a multi-scale modelling investigation on the ingress of chloride ions in concrete. The researchers employed a coupled multi-physics simulation approach to account for both saturated and unsaturated conditions in concrete. The study implemented a proposed model for simulating chloride transport in cementitious materials. The model utilised a discrete conduit network generated from the meso-scale geometry of the Lattice Discrete Particle Modelling (LDPM) approach. This involved constructing a discrete mesh that accounted for the geometric characteristics of concrete heterogeneity. Figure 13 illustrates the assumption of spherical coarse aggregates, which were randomly placed within the volume using a try-and-reject procedure. By applying Delaunay tetrahedralization, a system of polyhedral cells was created, representing the diffusion pathways and transport phenomena. The interconnected tetrahedrons (or triangles in 2D) formed a transport lattice network, with nodes coinciding with the tessellation points

and their connections defined the 1D transport conduits, as depicted in Fig. 13e. By integrating various physical phenomena, such as moisture flow, ionic diffusion and material properties, the multi-scale model provided a comprehensive understanding of chloride ingress behaviour in concrete. The study contributed to the advancement of predictive models for assessing the durability of concrete structures and facilitating the development of effective mitigation strategies against chloride-induced deterioration.

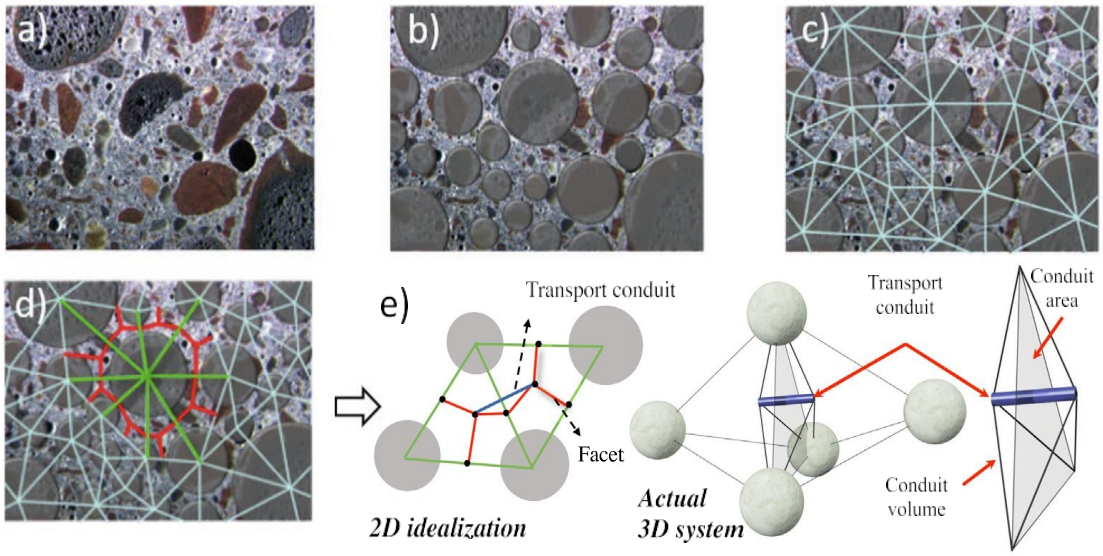

Fig. 13: Mesh generation: (a) Concrete material; (b) Supporting particles for grain generation; (c) Delaunay tetrahedralization (d) Tessellation (e) 2D idealization and 3D visualization of the conduit element connecting the centres of two tetrahedrons (Zhang et al. 2021)

The use of multi-scale modelling in studying chloride ingress in concrete has been explored in several research studies. Bentz (2000) investigated the influence of silica fume on the diffusivity of cement-based materials using multi-scale modelling. The study emphasized the importance of considering multiple scales in understanding concrete diffusivity, highlighting the role of silica fume as a microscale modifier. Dridi (2013) analysed the effective diffusivity of cement-based materials through multi-scale modelling. The research focused on understanding the diffusion process at different scales, contributing to the characterisation and prediction of chloride ingress in concrete. Du et al. (2014) proposed a meso-scale numerical method for simulating chloride diffusivity in concrete. The study highlighted the significance of considering the meso-structure of concrete in predicting the transport behaviour of chlorides. Jin et al. (2015) developed a multi-scale analytical theory to investigate the diffusivity of concrete subjected to mechanical stress. This work enhanced the understanding of how mechanical loading affects chloride transport in concrete, contributing to the assessment of durability under various conditions. Liu et al. (2016) presented a three-dimensional multi-scale method for simulating the ion transport behaviour in cement-based materials. The study focused on capturing the complex spatial distribution of ions within the material, enabling more accurate predictions of chloride ingress. Tong et al. (2023) conducted a multi-scale modelling and statistical analysis to examine the effect of heterogeneous characteristics on chloride transport properties in concrete. This research highlighted the importance of considering heterogeneity in predicting the ingress of chlorides and provided insights into statistical analysis methods. Guo et al. (2020) proposed multi-scale peri dynamic formulations for studying chloride diffusion in concrete. This approach provided a framework for capturing the multiscale behaviour of chloride ingress, enhancing the accuracy and efficiency of simulations.

The application of multi-scale modelling in studying chloride ingress in concrete has provided valuable insights into the complex transport phenomena at different scales. The published

literatures have contributed to the understanding of chloride diffusivity and its impact on concrete durability. However, a critical discussion reveals certain limitations and considerations that need to be addressed. One limitation is the assumption of idealized material properties and simplified boundary conditions in some of the studies. While multi-scale modelling allows for a more detailed representation of concrete's microstructure, the accuracy of the results heavily relies on the input parameters and assumptions made. Real concrete exhibits significant heterogeneity, which can affect the transport behaviour of chlorides. Therefore, it is crucial to consider the variability in material properties and boundary conditions to obtain more realistic predictions.

Another aspect to consider is the computational cost associated with multi-scale modelling. Incorporating multiple scales increases the complexity and computational requirements of the simulations. This can limit the size and scope of the models, restricting their applicability to real-world scenarios. Balancing the level of detail with computational efficiency is a challenge that needs to be addressed to ensure practical implementation. Furthermore, the validation and experimental verification of the multi-scale models are essential. While these studies present promising results, it is crucial to compare the model predictions with experimental data to assess their accuracy. Experimental data should include a wide range of concrete mixes, environmental conditions, and aging effects to ensure the models' robustness and reliability. Additionally, the integration of time-dependent and coupled effects in multi-scale modelling remains an area for further exploration. Chloride ingress is a dynamic process influenced by various factors such as moisture, temperature, and chemical reactions. Incorporating these time-dependent and coupled effects into the models can enhance the accuracy of long-term predictions and provide a more comprehensive understanding of chloride transport in concrete.

4.3 Sulphate Attack and Alkali-Aggregate Reaction Modelling

Multi-scale modelling of sulphate attack and alkali-aggregate reaction (AAR) in concrete involves a comprehensive analysis of the deterioration mechanisms at various length scales, spanning from macroscopic to microscopic levels. At the macroscopic level, models consider the overall behaviour of sulphate attack and AAR in concrete structures. Factors such as environmental conditions (e.g., temperature, humidity), concrete composition (e.g., cement type, aggregate properties) and the concentration of sulphates or alkalis in the surrounding environment are considered. These models provide insights into degradation patterns, expansion mechanisms and the overall performance of concrete structures subjected to these deterioration processes.

Transitioning to the mesoscopic level, multi-scale models explore the interaction between aggressive species (sulphates or alkalis) and the microstructure of concrete. They capture the influence of mineralogical composition, pore size distribution and connectivity on the transport of aggressive ions and subsequent expansion phenomena. These models consider the diffusion of aggressive ions into the concrete matrix, their interaction with cementitious phases and the formation of expansive reaction products. By incorporating the intricate interplay between microstructural features and chemical processes, these models enhance our understanding of deterioration mechanisms and aid in predicting the extent and location of damage.

At the microscopic level, multi-scale modelling focuses on molecular and atomic interactions between sulphates or alkalis and the cementitious materials. Molecular dynamics simulations and quantum chemical calculations are employed to investigate chemical reactions, diffusion processes and the potential formation of expansive reaction products at the atomic level. These models provide valuable insights into the atomic-level mechanisms driving sulphate attack and AAR, helping to elucidate fundamental processes involved. The integration of these multi-scale modelling approaches enables a comprehensive understanding of sulphate attack

and AAR in concrete. By considering multiple length scales, these models facilitate the prediction of degradation patterns, assessment of expansion risks and evaluation of preventive measures or mitigation strategies. They contribute to the development of more durable concrete formulations and the design of structures that are resilient to the effects of sulphate attack and AAR.

The use of multi-scale modelling in studying sulphate attack in concrete has been a topic of significant research. Feng et al. (2017) presented a multiscale microstructure model that considered the crystallization pressure during cement paste sulphate attack. This approach provided insights into the mechanisms and damage caused by sulphate attack at the microscale. Zuo et al. (2019) focused on the expansion response of hardened cement paste during the dormant period of external sulphate attack. Their multiscale numerical simulation shed light on the effects of sulphate attack on the mechanical behaviour of concrete and provided valuable information for assessing the durability of concrete structures.

Yin et al. (2020) proposed an integrated macro-microscopic model for concrete deterioration under external sulphate attack. This model aimed to capture the coupling between macroscopic mechanical properties and the microstructural changes induced by sulphate attack. Their research contributed to a better understanding of the overall degradation process and its implications for the structural performance of concrete. Socié et al. (2022) explored the simulation of both internal and external sulphate attacks using a reactive transport-poromechanical model. Their work highlighted the importance of considering the interactions between chemical reactions, transport phenomena and mechanical response to accurately simulate sulphate attack. This integrated approach provided a comprehensive framework for analysing the effects of sulphate attack on concrete durability.

The use of multi-scale modelling in the study of alkali-aggregate reaction (AAR) in concrete has gained significant attention. Cusatis et al. (2014) presented a multi-scale model for the degradation of concrete due to alkali-silica reaction. Their approach considered the interaction between the microstructural changes, material properties and macroscopic behaviour of concrete, providing insights into the mechanisms and progression of AAR-induced deterioration. Jen et al. (2019) focused on the evaluation of hybrid fibre restraint for controlling alkali-silica reaction expansion in concrete. Their multi-scale analysis provided a comprehensive understanding of the effectiveness of fibre reinforcement in mitigating AAR-induced damage. The study considered the interactions between the fibre reinforcement, aggregate properties and AAR expansion at different length scales.

Joo & Takahashi (2021) developed an AAR model that specifically accounted for the effect of aggregate size. By incorporating the influence of aggregate characteristics, their multi-scale model enhanced the accuracy of predicting AAR-induced expansion and damage in concrete structures. This work contributed to a better understanding of the role of aggregates in AAR and highlighted the importance of considering aggregate size in modelling approaches. Gallyamov et al. (2023) investigated the long-term behaviour of a dam affected by alkali-silica reaction using a multi-scale model. Their study examined the evolution of AAR-induced damage over time, considering the interplay between the macroscopic structural response and the microstructural changes at the mesoscale. This research provided insights into the long-term performance and stability of structures subjected to AAR. Multon & Sellier (2016) investigated the impact of alkali leaching on scale effects affecting expansion tests in AAR. The chemical approach used in this study is characterised by an alkali mass balance performed at two scales: the aggregate and the concrete scales (Fig. 14). Their multi-scale analysis considered both macroscopic and microscopic aspects, revealing the influence of alkali leaching on the expansion behaviour at different scales. This study highlighted the significance of incorporating scale effects in AAR modelling to accurately predict and understand the expansion phenomenon. By accounting for the intricate interactions between

various scales, multi-scale modelling contributes to the advancement of AAR research and aids in developing effective mitigation strategies.

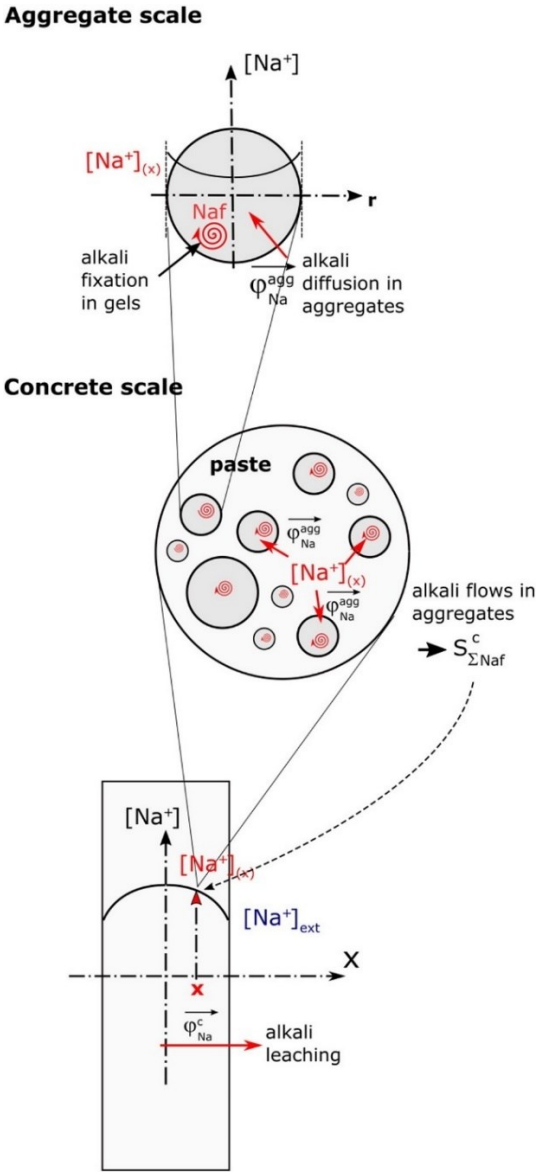

Fig. 14: Alkali mass balance at aggregate scale (with diffusion and fixation in ASR-gels), at concrete scale and at specimen scale (diffusion in the specimen) (Multon & Sellier, 2016)

Gallyamov et al. (2020) presented a multi-scale modelling approach that coupled mesoscopic damage evolution with macroscopic concrete behaviour to simulate AAR in concrete structures. By considering multiple scales, from the mesoscale to the macroscale, this approach captured the progressive damage evolution caused by AAR and its effects on the overall structural response. The study emphasized the importance of integrating different scales to accurately predict the long-term behaviour and durability of AAR-affected concrete structures. Such multi-scale modelling techniques enhance the understanding of AAR mechanisms and aid in the development of effective mitigation strategies. Figure 15 illustrates the configuration of the multi-scale setup employed in the validation test. The macro-scale specimen used in the numerical analysis has dimensions of 140x280 mm^2, while the size of the Representative Volume Element (RVE) remains consistent with the previously established

dimensions of 70x70 mm^2. In this approach, each macro-scale finite element is associated with a corresponding RVE, which captures the heterogeneous nature of concrete at the meso-scale. The number of RVEs corresponds to the number of finite elements in the macroscopic finite element mesh since each macroscopic element encompasses a single integration point. The coarser discretization of the macro-scale mesh is chosen to maintain a macro-element size equal to or larger than the RVE size, aligning with the concept of scale separation. Although a denser mesh could be employed for the macro-scale problem from a computational standpoint, a coarser discretization is favoured for consistency purposes.

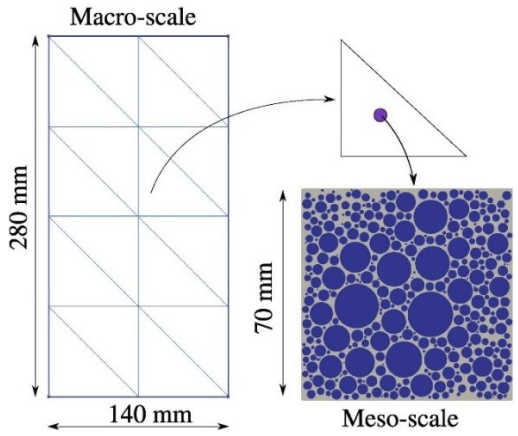

Fig. 15: Meshes used for the multi-scale simulation. Each of 16 macroscopic finite elements has a square concrete RVE at the meso-scale (Gallyamov et al. 2020)

4.4 Other Chemical Degradation Mechanisms

In addition to the well-known chemical degradation mechanisms such as carbonation, chloride ingress, sulphate attack and alkali-aggregate reaction (AAR), there are several other chemical degradation mechanisms that can significantly impact the long-term durability and performance of concrete structures. These mechanisms may occur individually or in combination, posing unique challenges for the understanding and prediction of concrete deterioration.

One of these mechanisms is acid attack, which occurs when concrete is exposed to acidic environments such as industrial waste, acid rain, or chemical spills. Acidic substances can react with the cementitious matrix, leading to the leaching of calcium hydroxide and the dissolution of cementitious phases. This process results in the loss of strength, degradation of the concrete's microstructure and increased permeability, ultimately compromising the structural integrity of the concrete.

Another important chemical degradation mechanism is the reaction between concrete and aggressive chemicals such as sulphates, nitrates, or chlorides present in the surrounding environment. These aggressive ions can penetrate the concrete pores and initiate chemical reactions with the cementitious phases. For example, sulphate ions can react with the calcium aluminate phases in the cement matrix, leading to the formation of expansive reaction products that induce internal stresses and cracking. Chloride ions can initiate corrosion of the embedded steel reinforcement, resulting in structural deterioration. The alkali-aggregate reaction (AAR) occurs when reactive minerals in aggregates react with alkalis from the cement paste, causing expansion and cracking of the concrete. Furthermore, concrete can be subjected to chemical degradation due to exposure to aggressive substances like organic compounds, acids, or alkalis. Organic compounds, such as petroleum products or solvents, can penetrate the concrete and interact with the cementitious phases, leading to the

degradation of the concrete's microstructure and reduced durability. Acids and alkalis can also attack the cement matrix, resulting in chemical reactions and weakening of the concrete.

To comprehensively understand and model these various chemical degradation mechanisms, multi-scale modelling approaches are employed. Multi-scale modelling considers the interaction of aggressive substances with the concrete at different length scales, from the macroscopic behaviour of the structure to the microscopic reactions occurring at the cementitious particle level. It considers factors such as environmental conditions, concrete composition, transport of aggressive ions, chemical reactions and the resulting changes in the concrete's microstructure. By simulating and analysing these mechanisms, multi-scale modelling provides valuable insights into the degradation processes, predicts the performance of concrete structures over time and aids in the development of effective strategies for mitigating chemical deterioration.

The accurate modelling of other chemical degradation mechanisms requires the integration of experimental data, fundamental understanding of chemical reactions and advanced computational techniques. It involves the consideration of factors such as the diffusion and transport of aggressive ions through the porous structure, the kinetics of chemical reactions, the role of pore solution chemistry and the influence of microstructural features on the performance of the concrete. Multi-scale modelling approaches provide a framework for capturing the complex interactions between aggressive substances and concrete, enabling researchers and engineers to gain a deeper understanding of the underlying processes and to make informed decisions regarding material selection, design, and maintenance practices.

5. Multi-scale Modelling of Physical Deterioration

Multi-scale modelling of physical deterioration in concrete encompasses a comprehensive analysis of the various mechanisms that lead to degradation at different length scales. At the macroscopic level, models consider the overall behaviour of physical deterioration processes such as freeze-thaw damage, abrasion, erosion, thermal stress, and mechanical fatigue. These models simulate the effects of environmental conditions, loading and material properties on the degradation patterns and performance of concrete structures. Moving to the microscopic level, multi-scale models delve into the microstructural characteristics of concrete and the interactions between different phases, aggregates, and the cementitious matrix. By capturing the intricate interplay between microstructure and physical processes, multi-scale modelling enhances our understanding of physical deterioration mechanisms and aids in predicting the extent and location of damage.

5.1 Freeze-Thaw Damage Modelling

Freeze-thaw damage is a phenomenon that occurs when water freezes and thaws within a material, leading to detrimental effects such as cracking, spalling and deterioration. It is a critical issue in various engineering applications, including infrastructure, transportation and building materials. To understand and predict the behaviour of materials under freeze-thaw conditions, multi-scale modelling approaches have gained significant importance.

Multi-scale modelling involves the integration of different length and time scales to capture the complex behaviour of materials. In the context of freeze-thaw damage, this approach considers the interactions between different levels of hierarchy, ranging from the molecular and microstructural scales to the macroscopic level. By incorporating the relevant physical and chemical processes at each scale, multi-scale models provide a comprehensive understanding of freeze-thaw damage mechanisms.

At the molecular scale, molecular dynamics simulations are employed to investigate the interactions between water molecules and the material's constituent atoms. These simulations

provide insights into the fundamental processes governing ice formation, crystal growth and the stresses induced by ice formation within the material's structure. Additionally, they help understand the effects of different material properties, such as porosity, on the behaviour of water at the molecular level. Moving to the microstructural scale, computational techniques such as finite element analysis (FEA) and lattice-based models are used. These models consider the heterogeneity of the material, including the presence of aggregates, pores, and interfaces. They account for the mechanical and thermal properties of the material, enabling the prediction of stresses, strains, and temperature distributions during freeze-thaw cycles. Additionally, these models can simulate the transport of water within the material, capturing the penetration and migration of water, which is crucial for freeze-thaw damage initiation.

As the analysis progresses to the macroscopic scale, continuum-based models become relevant. These models describe the behaviour of the material as a homogenized medium, considering the averaged properties of the microstructure. Continuum models, such as the phase field method or damage mechanics models, are employed to simulate the crack propagation and failure mechanisms due to freeze-thaw cycles. These models can predict the evolution of crack patterns, spalling and overall material degradation. The integration of these multi-scale models is achieved through the development of constitutive relationships and transfer algorithms that link the information between scales. This allows for a seamless transfer of information and the coupling of different physical phenomena, enabling the prediction of freeze-thaw damage behaviour from the molecular to the macroscopic scale.

The study conducted by Yao et al. (2023) investigated the use of multi-scale modelling in understanding the deterioration mechanism of recycled powder concrete under the combined effect of sulphate attack and freeze-thaw cycles. By employing a multi-scale approach, the researchers aimed to capture the intricate interactions between the macroscopic behaviour of the concrete and the microstructural changes occurring at the meso-scale. In Fig. 16a, the concrete matrix is divided into three distinct regions: the aggregate region, mortar region and recycled powder (RP) region. Interfaces are formed at the boundaries between these regions, namely the mortar-aggregate interface, RP-aggregate interface, and RP-mortar interface. Analysis of the MIP experimental results revealed that the RP region exhibited larger porosity, pore diameter, pore volume and critical pore size compared to the mortar region. Transition zones were observed at the mortar-aggregate interface and RP-aggregate interface, connecting the respective regions. The RP-mortar interface, formed by the RP acting as a hydration nucleation point, facilitated the exchange of substances between the RP and mortar regions through interconnected pore channels.

In Fig. 16b and Fig. 16c, the substance formation and transport processes at the mortar-aggregate interface and RP-aggregate interface were found to be similar. The sulphate solution showed a higher permeability towards the interface transition zone (ITZ). However, there were differences in capillary pore size and pressure between the mortar and RP regions. The smaller capillary pore size and higher capillary pressure in the mortar region led to the absorption of sulphate solution from the ITZ, mitigating deterioration at the mortar-aggregate interface. In contrast, the larger capillary pore size and lower capillary pressure in the RP region resulted in the enrichment of sulphate solution at the RP-aggregate interface rather than within the RP region. The findings highlighted the importance of considering the coupled effects of sulphate attack and freeze-thaw cycles on the performance of recycled powder concrete. This multi-scale modelling approach provided valuable insights into the underlying mechanisms of freeze-thaw damage, contributing to the development of more effective strategies for mitigating deterioration in concrete structures exposed to such environmental conditions.

Multi-scale modelling of freeze-thaw damage provides valuable insights for designing more durable materials and structures. It allows engineers and researchers to assess the performance of different materials, evaluate the effectiveness of preventive measures and

optimise material compositions. Moreover, it aids in the development of mitigation strategies and the design of novel materials that can withstand freeze-thaw cycles, reducing the economic and environmental impact of this type of damage.

The use of multi-scale modelling in understanding freeze-thaw damage in concrete has been investigated in several studies. Gong et al. (2018) employed multi-scale computational modelling to analyse concrete damage caused by mixed pore pressures, specifically focusing on the coupled effects of alkali-silica reaction and cyclic freeze/thaw. Xu et al. (2020) conducted a multi-scale damage characterisation of asphalt mix subjected to freeze-thaw cycles. Peng et al. (2022) developed a multi-scale computational model using the equivalent element method to simulate freeze-thaw damage in concrete. Li et al. (2022) investigated the durability degradation mechanism of aeolian sand concrete under freeze-thaw conditions through a multi-scale study. Gong et al. (2023) explored the multi-scale deterioration and microstructure of polypropylene fibre concrete under salt freezing.

These studies highlight the significance of multi-scale modelling in assessing the complex processes and interactions involved in freeze-thaw damage. By considering multiple length scales, from macroscopic to microscopic, these models provide a comprehensive understanding of the damage mechanisms and behaviour of concrete subjected to freeze-thaw cycles. The integration of various scales allows for the analysis of local effects, such as pore pressure and microstructural changes and their influence on the overall performance and durability of concrete.

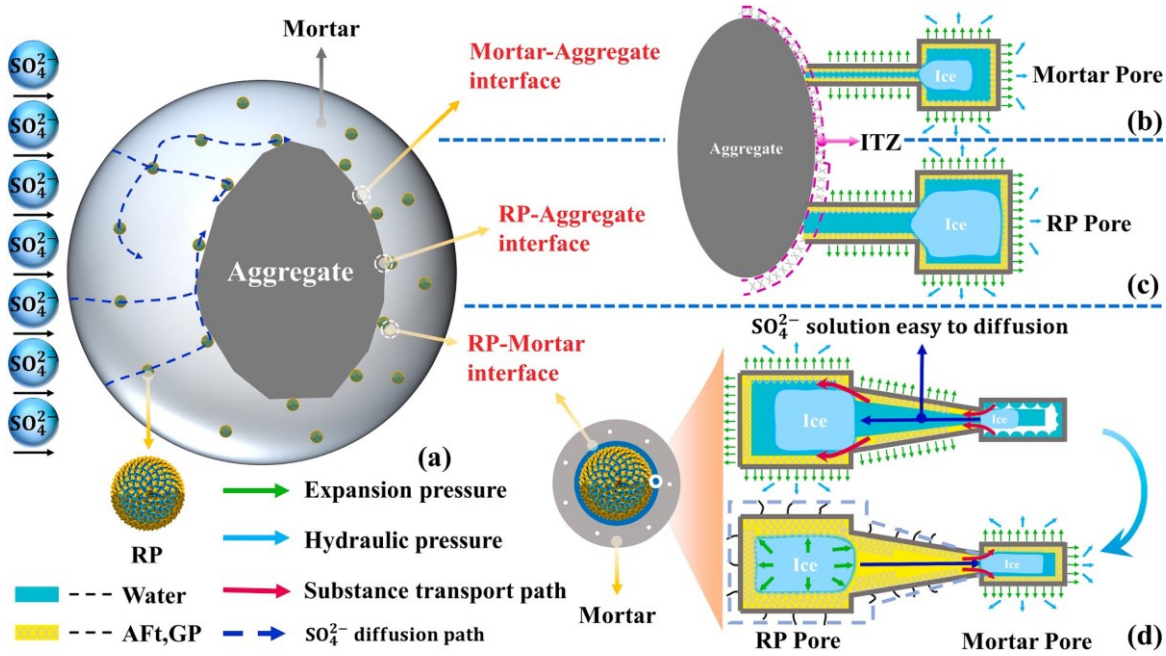

Fig. 16: RPC partition-interface under the coupled action of sulphate and freeze–thaw cycles (Yao et al. 2023)

The findings from these multi-scale modelling studies contribute to the advancement of knowledge in predicting and mitigating freeze-thaw damage in concrete. They offer valuable insights into the interplay between different factors, including material properties, environmental conditions, and structural behaviour. Furthermore, these models can aid in the development of effective strategies for enhancing the durability and performance of concrete structures exposed to freeze-thaw cycles. However, it is important to acknowledge that multi-scale modelling approaches still face challenges. The complexity of freeze-thaw damage phenomena requires the consideration of various parameters and their interactions, which can

make model calibration and validation more demanding. Additionally, incorporating accurate and reliable data at multiple scales remains a critical aspect of these models. Further advancements in experimental techniques, data acquisition and model validation will contribute to the refinement and wider applicability of multi-scale modelling approaches for freeze-thaw damage in concrete.

5.2 Abrasion and Erosion Modelling

Multi-scale modelling of abrasion and erosion involves a detailed analysis of material removal processes at different length scales. These processes occur when solid surfaces are subjected to mechanical wear or when fluid-borne particles impact and erode the material. Understanding and predicting the effects of abrasion and erosion are crucial for industries such as mining, manufacturing, and transportation. At the macroscopic scale, continuum-based methods like the Finite Element Method (FEM) or Finite Volume Method (FVM) are employed. These methods simulate the overall behaviour of the system and provide information on the global material loss, surface damage and wear rates. Macro-scale models consider the mechanical interactions between bodies, considering parameters such as contact forces, friction and surface properties.

However, to capture the local effects and intricate mechanisms of material removal, micro-scale models are necessary. These models focus on the interactions between individual particles or atoms and provide insights into the micro-scale wear mechanisms. The choice of micro-scale modelling technique depends on the specific problem and the desired level of detail. Discrete Element Method (DEM) is commonly used for particle-particle interactions, Molecular Dynamics (MD) for atomistic simulations and mesoscale methods like Lattice Boltzmann Method (LBM) for bridging the gap between micro and macro scales.

The coupling between different length scales is a critical aspect of multi-scale modelling. The information obtained from the micro-scale models, such as contact forces, particle velocities, or material removal rates, is incorporated into the macro-scale model. This ensures accurate representation of local wear phenomena and their impact on the overall system behaviour. Multi-scale modelling of abrasion and erosion provides a comprehensive understanding of the wear mechanisms and helps optimise equipment design and material selection. It allows for the evaluation of different operating conditions and the development of strategies to mitigate wear, prolong equipment lifespan, and reduce maintenance costs. However, multi-scale modelling of abrasion and erosion poses challenges. One of the main challenges is the calibration of material parameters, such as the wear coefficient or erosion rate, which depend on the specific material properties and wear mechanisms involved. Experimental data and empirical relationships are often used to validate and refine the model parameters. Additionally, multi-scale modelling can be computationally demanding, especially when simulating large systems or long-time durations. Efficient algorithms, parallel computing and model simplifications may be employed to manage the computational cost and increase simulation speed.

5.3 Thermal Stress Modelling

Multi-scale modelling of thermal stress involves the simulation and analysis of the effects of temperature gradients on the mechanical behaviour of materials. It aims to capture the interconnected behaviour of heat transfer and stress distribution at multiple length scales. At the macroscopic scale, continuum-based methods such as the Finite Element Method (FEM) or Finite Volume Method (FVM) are commonly employed. These methods solve the heat conduction equations coupled with the equations of linear elasticity or plasticity to predict the temperature distribution and resulting stress fields. Macro-scale models consider the material properties, boundary conditions and thermal loads to simulate the thermal stress behaviour of the entire structure or component. However, to accurately capture the local effects and

microstructural changes induced by thermal stress, micro-scale models are necessary. These models focus on the detailed representation of microstructural features, such as grain boundaries, inclusions, or phase interfaces. Techniques like crystal plasticity modelling, phase field methods, or discrete dislocation dynamics are used to simulate the microstructural response to thermal loading.

The integration between different length scales is a critical aspect of multi-scale modelling of thermal stress. Information obtained from the micro-scale models, such as local stress concentrations, phase transformations, or grain growth, is incorporated into the macro-scale model. This ensures the accurate representation of local thermal stress phenomena and their impact on the overall system behaviour. Multi-scale modelling of thermal stress provides insights into various phenomena, including thermal expansion mismatch, thermal fatigue, thermal shock and residual stress formation. It helps predict and understand failure mechanisms, deformation patterns and material response under varying thermal conditions. These models play a crucial role in designing thermal barrier coatings, predicting the lifetime of high-temperature components and optimising manufacturing processes.

Multi-scale modelling of thermal stress in concrete has emerged as a valuable tool for understanding and predicting the behaviour of concrete structures subjected to temperature variations. The stochastic multi-scale model proposed by Liu et al. (2013) for predicting the thermal expansion coefficient of early-age concrete is a notable contribution. By considering the heterogeneous nature of concrete at different scales, the model offers a more accurate estimation of thermal expansion, which is crucial for predicting early-age concrete behaviour and preventing potential issues associated with thermal stress.

Similarly, Monte et al. (2019) adopted a multi-scale experimental approach to evaluate concrete sensitivity to fire spalling. Their study highlights the importance of considering the multi-scale nature of thermal stress phenomena, as fire-induced spalling is a complex phenomenon influenced by various factors at different scales. By incorporating these considerations, the study provides insights that can aid in the development of fire-resistant concrete materials and structures. The thermo-mechanistic multi-scale model developed by Iwama et al. (2020) specifically focuses on structural concrete at high temperatures. This model considers the effects of temperature at the microstructural level, enabling more accurate predictions of thermal stress and deformation. By capturing the intricate interactions between temperature and microstructural changes, this model contributes to a better understanding of the behaviour of concrete under extreme thermal conditions. The introduction of a novel multi-scale model by Zhang et al. (2020) for predicting the thermal damage of hybrid fibre-reinforced concrete is another significant advancement. This model considers the interaction between different scales and accounts for the reinforcement effects, providing a comprehensive understanding of the performance of fibre-reinforced concrete under thermal loading. The insights gained from this model can guide the design of concrete structures that are more resistant to thermal damage.

Li et al. (2021) conducted a study on multi-scale fibre-reinforced cement-based materials under elevated temperatures, focusing on the effects of fibre distribution and orientation at different scales. By considering these factors, the study sheds light on the mechanical properties and behaviour of such materials, offering valuable insights for the design of fire-resistant concrete structures. This research emphasizes the importance of considering multi-scale effects when evaluating the performance of concrete under thermal loading conditions. Zhang et al. (2023) further contribute to the discussion by evaluating the uniaxial tensile properties of multi-scale fibre-reinforced rubberized concrete after exposure to elevated temperatures. Their study underscores the significance of considering multi-scale effects in assessing the performance of concrete materials under thermal loading conditions. By considering the behaviour of concrete at different length scales, the study provides a more comprehensive understanding of the material's response to elevated temperatures.

In their study Iwama et al. (2020), the authors focused on the multi-scale modelling of thermal stress in concrete (Fig. 17). The research aimed to understand the complex behaviour of concrete subjected to high temperatures by integrating thermal and mechanical aspects at different length scales. The study considered factors such as thermal gradients, material properties and the microstructure of concrete to accurately predict the development and distribution of thermal stresses. The findings from the multi-scale modelling approach provided valuable insights into the mechanisms of thermal stress generation in concrete and helped in assessing the structural response under high-temperature conditions.

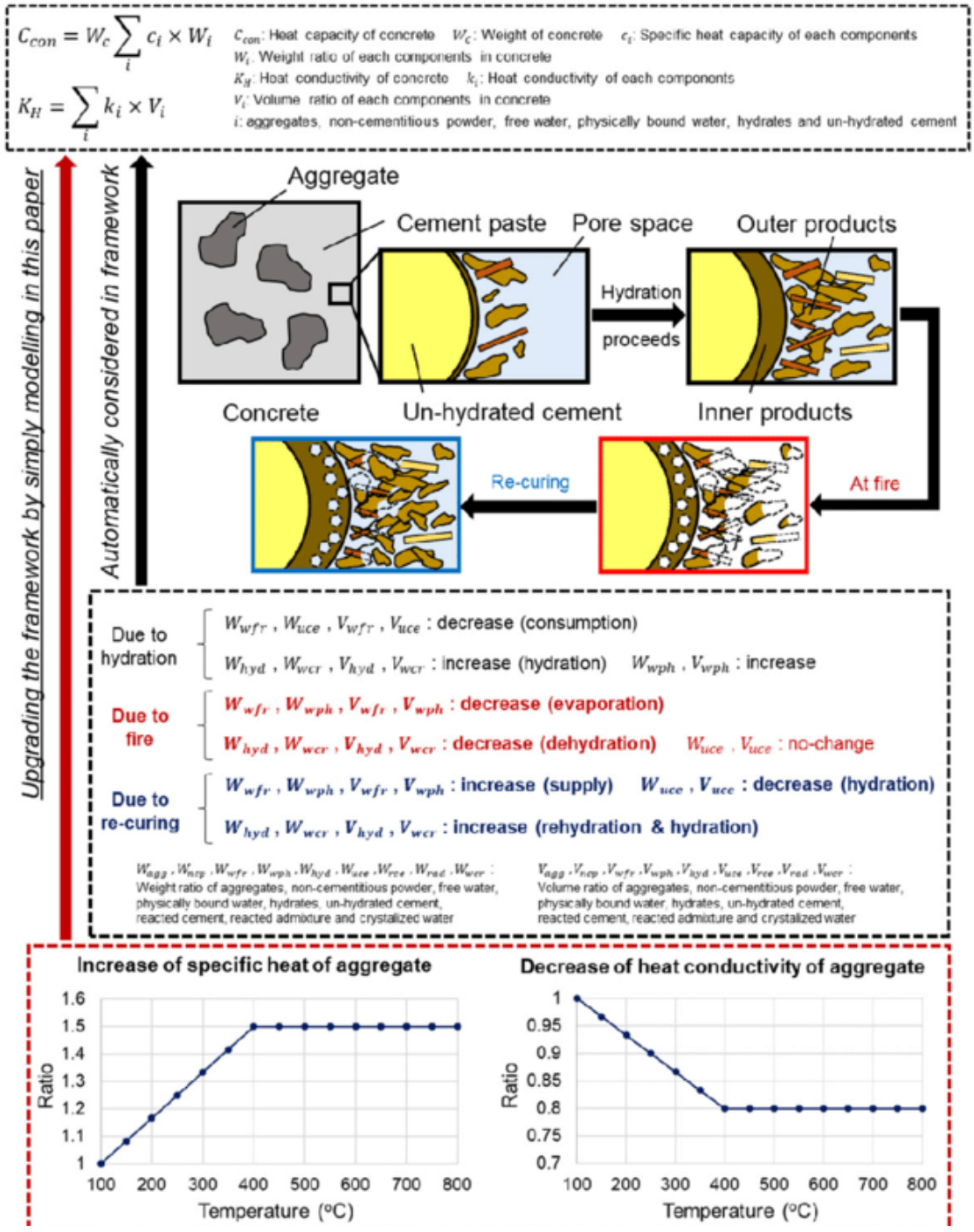

Fig. 17: Heat characteristics change of aggregates: heat capacity and heat conductivity.

5.4 Mechanical Fatigue Modelling

Mechanical fatigue modelling at the multi-scale level involves a detailed analysis of the progressive damage and failure mechanisms that occur in materials subjected to cyclic loading. Fatigue is a significant concern in engineering applications, as it can lead to catastrophic failures and reduced component lifespan. At the macroscopic scale, continuum-based models such as the Finite Element Method (FEM) or Finite Volume Method (FVM) are commonly used to simulate fatigue behaviour. These models consider the macroscopic stress and strain fields and utilise fatigue criteria, such as the stress-life (S-N) or strain-life (ε-N) approaches, to predict the fatigue life of the structure. Macro-scale models incorporate the material's mechanical properties, loading conditions and geometric features to provide insights into the overall behaviour and durability of the component.

However, to accurately capture the microstructural details and local effects that influence fatigue, micro-scale models are necessary. These models focus on the interaction between the material's microstructure and the applied loading conditions. Techniques such as crystal plasticity modelling, phase field methods, or cohesive zone modelling are employed to simulate the microstructural response and fatigue damage initiation and propagation. Micro-scale models consider the effects of grain boundaries, inclusions, precipitates and other microstructural features on the fatigue behaviour. The integration of different scales is crucial in multi-scale fatigue modelling to capture the interactions between microstructural phenomena and macroscopic behaviour. Information obtained from the micro-scale models, such as crack nucleation sites, crack growth rates, or damage accumulation, is incorporated into the macro-scale model. This enables a more accurate representation of local fatigue phenomena and their influence on the overall structural response.

Multi-scale modelling of mechanical fatigue provides insights into various fatigue mechanisms, including crack initiation, propagation and interaction with microstructural features. It helps predict the fatigue life, assess component durability and optimise design against fatigue failure. The models can also account for environmental factors, temperature effects and variable amplitude loading.

The use of multi-scale modelling in analysing mechanical fatigue in concrete has been explored in various research studies, providing valuable insights into the behaviour and performance of concrete structures under different loading conditions. Rossi and Parant (2008) investigated damage mechanisms in a multi-scale fibre-reinforced cement-based composite subjected to impact and fatigue loading conditions. Their study highlighted the capability of multi-scale modelling to analyse complex interactions between fibres, matrix and interfaces, contributing to a better understanding of damage evolution in the composite material. Ren and Li (2013) conducted a multi-scale fracture and damage analysis of steel fibre-reinforced concrete. Their study demonstrated that multi-scale modelling can effectively capture the crack initiation and propagation behaviour, offering insights into the fracture process and damage accumulation in the material. Tanaka et al. (2017) focused on the remaining fatigue life assessment of damaged reinforced concrete decks using a data assimilation approach with a multi-scale model. This study showcased the potential of integrating multi-scale modelling with site inspection data to accurately predict the remaining life of damaged structures, facilitating informed decision-making for maintenance and repair.

Sun et al. (2019) applied multi-scale fatigue damage prognosis to long-span steel bridges under vehicle loading. Their study demonstrated the capability of multi-scale modelling to assess the fatigue damage and predict the remaining life of steel bridges, aiding in the development of proactive maintenance strategies. Kumar and Ray (2022) investigated multi-scale fracture characterisation in concrete under fatigue loading using critical energy dissipation. Their study showcased the ability of multi-scale modelling to analyse crack growth

behaviour, fatigue life and fracture toughness, providing a deeper understanding of concrete's fatigue response.

The use of multi-scale modelling in analysing thermal stress in concrete has shown promise in providing valuable insights into the behaviour and performance of concrete structures. The studies reviewed provide examples of how multi-scale modelling has been applied to investigate damage mechanisms, fracture behaviour, remaining fatigue life and fatigue damage prognosis in concrete under various loading conditions. One of the strengths of multi-scale modelling is its ability to capture the complex interactions between different length scales, such as fibres, matrix, interfaces, and cracks, which play a crucial role in the overall response of the material. By considering these interactions, multi-scale models can provide a more comprehensive understanding of the damage evolution process and accurately predict the remaining life of structures.

5.5 Other Physical Degradation Mechanisms

Multi-scale modelling plays a crucial role in understanding and predicting the behaviour of various physical degradation mechanisms beyond abrasion, erosion, thermal stress and mechanical fatigue. Here are some examples of other physical degradation mechanisms and how multi-scale modelling approaches can be applied to study them:

1. Corrosion: Multi-scale modelling can help analyse the complex electrochemical processes involved in corrosion (Lepech et al. 2015; Parvizi et al. 2021). It enables the simulation of microscopic phenomena, such as ion transport, surface reactions and corrosion product formation, as well as macroscopic effects, including material degradation and structural integrity. By integrating models at different scales, researchers can gain insights into the corrosion behaviour of materials, optimise corrosion prevention strategies and design corrosion-resistant alloys.

2. Wear: Multi-scale modelling facilitates the study of wear mechanisms, such as adhesive wear, abrasive wear and fatigue wear (Jiang & Zhang, 2012; Trommer et al. 2015; Wang et al. 2023). It enables the simulation of material interactions at different scales, ranging from atomic-level surface interactions to macroscopic contact and sliding between components. By incorporating material properties, surface roughness and environmental factors, multi-scale models can predict wear rates, identify critical wear locations, and guide the development of wear-resistant materials and lubrication strategies.

3. Impact and Shock: Multi-scale modelling can simulate the dynamic response of materials and structures subjected to impact and shock loading (Allix et al. 2001; Li et al. 2022). It involves capturing the behaviour of materials at different scales, from the propagation of stress waves at the microscale to the structural response at the macroscale. By integrating models of material behaviour, such as elasticity, plasticity, and fracture mechanics, with impact loading conditions, multi-scale simulations can provide insights into the energy absorption, deformation patterns and failure modes under impact and shock conditions.

4. Environmental Stress Cracking: Multi-scale modelling aids in understanding the mechanisms behind environmental stress cracking in polymers (Theodosiou & Saravanos, 2010; Meng et al. 2016). It combines models of polymer structure and chemistry with stress analysis to simulate the initiation and propagation of cracks in the presence of environmental agents. Multi-scale simulations can provide insights into the effects of material properties, environmental conditions, and stress states on crack formation, guiding the development of crack-resistant polymers and improved design practices.

5. Thermal Cycling: Multi-scale modelling is valuable for studying the effects of thermal cycling on materials and structures (Seiler et al. 2013; Xu et el. 2022). It involves capturing thermal

expansion, stress generation and fatigue damage mechanisms at different length scales. By integrating models of thermal behaviour, material properties and fatigue life, multi-scale simulations can predict the accumulation of thermal stresses, crack initiation and the overall durability of components subjected to thermal cycling conditions. This information can guide material selection, design optimisation and thermal management strategies.

6. Shrinkage: Multi-scale modelling of concrete shrinkage is a sophisticated approach that bridges the gap between the macroscopic behaviour of concrete structures and the intricate interactions at the microscale. It leverages computational techniques to simulate and predict how concrete undergoes shrinkage throughout its lifespan, considering factors like moisture content, temperature variations, and material properties. This modelling enables engineers and researchers to assess the potential cracking, deformation, and durability issues in concrete structures, offering invaluable insights for design and maintenance. By comprehensively understanding the complex processes of concrete shrinkage at various scales, this approach contributes to the development of more resilient and long-lasting infrastructure.

7. Creep: Multi-scale modelling of concrete creep is a powerful tool that allows us to investigate the time-dependent deformation of concrete structures. It integrates macroscopic behaviour with microscopic phenomena occurring at various scales, considering factors like material properties, stress history, and environmental conditions. By simulating how concrete gradually deforms under sustained load, this approach aids in predicting long-term structural performance, especially in structures like bridges and high-rise buildings. It provides essential insights for engineers to ensure safety, durability, and serviceability of concrete structures over their lifespan. Multi-scale modelling of creep advances our understanding of concrete behaviour, facilitating more efficient and sustainable construction practices.

Multi-scale modelling approaches provide a comprehensive understanding of the underlying physics and mechanics of various physical degradation mechanisms. They enable researchers and engineers to explore the behaviour of materials and structures across different scales, facilitating the development of more accurate models, improved materials and enhanced design strategies to mitigate degradation and enhance performance and durability.

6. Multi-scale Modelling of Coupled Degradation Mechanisms

Multi-scale modelling of coupled degradation mechanisms in concrete involves the integration of multiple length scales and degradation processes to understand the complex interactions that occur during concrete deterioration. It considers the interplay between chemical degradation mechanisms, such as carbonation, chloride ingress, sulphate attack, alkali-aggregate reaction, and physical degradation mechanisms, including freeze-thaw cycles, moisture transport and mechanical loading. By incorporating various length scales, from macroscopic to microscopic, these models provide insights into the degradation patterns, evolution of damage and overall performance of concrete structures. Multi-scale modelling of coupled degradation mechanisms enhances our understanding of the synergistic effects of different degradation processes and facilitates accurate prediction, assessment, and mitigation of concrete deterioration, contributing to the development of durable and sustainable infrastructure.

6.1 Chemical-Physical Coupling in Concrete Deterioration

Chemical-physical coupling in concrete deterioration refers to the intricate interaction between chemical and physical processes that contribute to the degradation of concrete over time. Concrete is a composite material that undergoes a range of chemical reactions and physical transformations when exposed to various environmental conditions and loads. The coupling

of these processes plays a significant role in the overall deterioration of concrete structures. The coupling between chemical and physical deterioration mechanisms arises from the interdependency and mutual influence of these processes. For instance, physical deterioration, such as cracking, can increase the permeability of concrete, allowing aggressive chemicals to penetrate deeper and accelerate chemical reactions (Wang et al. 1997; Yi et al. 2011). On the other hand, chemical reactions can lead to the formation of expansive reaction products that generate internal stresses and exacerbate the physical deterioration of the concrete structure (Gao et al. 2013; Ting et al. 2021; Wang et al. 2022).

Multi-scale modelling approaches have been developed to capture the complex nature of the chemical-physical coupling in concrete deterioration. These models integrate various length scales, from the macroscopic level of the entire structure to the microscopic level of individual components and interactions. At the macroscopic level, these models consider the overall behaviour of the concrete structure and simulate factors such as moisture transport, temperature gradients and stress distribution. At the microscopic level, the models delve into the microstructure of concrete, including the arrangement of aggregates, cement paste and pore network, to analyse chemical reactions, diffusion processes and mechanical behaviour.

By incorporating the coupling between chemical and physical deterioration processes, multi-scale modelling provides a comprehensive understanding of how different mechanisms interact and influence the overall performance of concrete structures. This knowledge is vital for predicting the service life of concrete infrastructure, designing more durable materials, and developing effective maintenance and repair strategies. Furthermore, multi-scale modelling allows for the exploration of various scenarios and the assessment of the effectiveness of preventive measures to mitigate the coupled degradation mechanisms. However, there are challenges in the accurate modelling of chemical-physical coupling in concrete deterioration. Obtaining reliable experimental data, quantifying material properties, understanding complex chemical reactions and capturing the dynamic nature of the processes pose significant difficulties. Additionally, the computational demands of multi-scale modelling require efficient algorithms and computational resources.

6.2 Multi-physics Modelling Approaches

Multi-physics modelling approaches have emerged as valuable tools for studying the intricate chemical-physical coupling in concrete deterioration. These approaches integrate multiple physical phenomena, such as heat transfer, moisture transport, chemical reactions and mechanical behaviour, to capture the complex interactions and mutual influences that occur during the degradation process (Pal & Ramaswamy, 2023; Wang et al. 2023). One of the key advantages of multi-physics modelling is its ability to simulate the coupled effects of chemical and physical processes on concrete deterioration. By considering the interdependency between these processes, these models provide a more comprehensive understanding of the deterioration mechanisms and enable accurate predictions of the performance and service life of concrete structures.

In the context of chemical-physical coupling in concrete deterioration, multi-physics modelling approaches can be applied to investigate several important degradation mechanisms. For example, the interaction between moisture transport, temperature variations and chemical reactions can be simulated to study the combined effects of freeze-thaw cycles and alkali-aggregate reactions (Gong et al. 2020). This enables a more accurate assessment of the resulting damage and deterioration in concrete structures. Similarly, multi-physics modelling can be used to study the interplay between moisture diffusion, chemical reactions, and mechanical loading to understand the combined effects of carbonation and mechanical stress on the degradation of concrete. By considering the changes in material properties, such as permeability, porosity and mechanical strength, these models provide insights into the

evolution of degradation and allow for the prediction of the structural integrity of concrete under various loading and environmental conditions.

Furthermore, multi-physics modelling approaches can also incorporate advanced techniques such as finite element analysis (FEA), computational fluid dynamics (CFD) and reactive transport modelling to simulate the complex interactions at different length and time scales. These models can account for the heterogeneity of concrete materials, the presence of different phases and the variability in environmental conditions, thereby providing a more realistic representation of the degradation processes. However, it is important to acknowledge the challenges associated with multi-physics modelling of chemical-physical coupling in concrete deterioration. These challenges include obtaining accurate and comprehensive experimental data for model calibration and validation, accurately characterizing the material properties and their variations, and handling the computational complexity and time requirements of the models.

The multi-scale modelling of coupled degradation mechanisms in concrete has gained significant attention in recent years, as it provides a comprehensive understanding of the complex deterioration processes that affect concrete structures. Lepech et al. (2015) presented a multi-physical and multi-scale modelling approach to couple corrosion and damage at the structural scale. The study highlighted the importance of considering the interaction between corrosion-induced deterioration and structural damage for accurate predictions. The work demonstrated the potential of multi-scale modelling in capturing the coupled effects and provided valuable insights into the behaviour of reinforced concrete structures.

Hu (2016) conducted a multi-scale numerical simulation analysis to investigate the influence of combined leaching and frost deteriorations on the mechanical properties of concrete. The study emphasized the need for incorporating multiple degradation mechanisms and their synergistic effects. By considering both the microstructural changes and the macroscopic mechanical response, the study shed light on the complex interactions and provided insights into the performance of concrete under combined deterioration processes. Gong et al. (2017) and Gong et al. (2018) explored the strong coupling between freeze-thaw cycles, alkali-silica reaction (ASR) and mixed pore pressures through multi-scale computational modelling. These studies highlighted the importance of considering the multi-scale poro-mechanical behaviour and the interplay between different degradation mechanisms. The research demonstrated the potential of multi-scale modelling in capturing the complex damage mechanisms and provided a foundation for assessing the durability of concrete structures.

Su et al. (2018) focused on the multi-scale performance simulation of hydraulic concrete subjected to leaching and frost. The study emphasized the importance of incorporating both the chemical and physical degradation processes in the modelling approach. By considering the multi-scale phenomena, the research provided insights into the evolution of material properties and the overall performance of hydraulic concrete under coupled deterioration mechanisms. Li et al. (2022) conducted a multi-scale study on the durability degradation mechanism of aeolian sand concrete under freeze-thaw conditions. The research highlighted the importance of considering the specific characteristics of different aggregates and the influence of environmental conditions in the modelling approach. The study provided insights into the degradation mechanisms and offered a foundation for assessing the performance of concrete structures in specific environmental contexts.

Overall, the studies discussed demonstrate the value of multi-scale modelling in understanding the coupled degradation mechanisms in concrete. They highlight the need for integrating various length scales, considering the interplay between different degradation processes, and incorporating relevant environmental and material factors. While these studies contribute significantly to the field, further research is needed to address challenges such as

data availability, model validation and computational efficiency. Continued advancements in multi-scale modelling techniques will enhance our understanding of coupled degradation mechanisms and contribute to the development of more durable and resilient concrete structures.

7. Validation and Verification of Multi-scale Models

Validation and verification are essential steps in assessing the accuracy and reliability of multi-scale models. Validation involves comparing model predictions with experimental or empirical data to ensure that the model captures the real-world behaviour accurately. It involves assessing various aspects, such as material properties, boundary conditions and system response. Verification, on the other hand, focuses on confirming the correctness of the model implementation and mathematical formulations. It involves comparing model predictions against analytical solutions or benchmark problems. By rigorously validating and verifying multi-scale models, researchers can gain confidence in their predictive capabilities, enabling the models to be used effectively in various engineering applications.

7.1 Experimental Validation Techniques

Experimental validation techniques are essential for assessing the accuracy and reliability of multi-scale models of concrete deterioration. These techniques involve conducting physical experiments that closely mimic real-world degradation conditions and comparing the experimental results with the predictions of the multi-scale models. By validating the models with experimental data, researchers can gain confidence in their predictive capabilities and identify areas for improvement.

One commonly used experimental validation technique is the comparison of macroscopic properties. This involves subjecting concrete specimens to specific degradation mechanisms, such as corrosion, carbonation, or freeze-thaw cycles and measuring macroscopic parameters like compressive strength, tensile strength, modulus of elasticity and dimensional changes. The experimental results are then compared with the model predictions for similar degradation conditions. If the model accurately captures the macroscopic behaviour of the concrete, it provides validation for the multi-scale approach.

Microstructural characterisation is another important validation technique. Advanced imaging and microscopy techniques, such as scanning electron microscopy (SEM), X-ray computed tomography (CT), or mercury intrusion porosimetry (MIP), are used to analyse the microstructure of degraded concrete specimens. The obtained microstructural information, such as pore size distribution, pore connectivity and damage patterns, can be compared with the model's predictions at the corresponding length scales (Garboczi & Bentz, 1996; Constantinides et al. 2006; Jadallh et al, 2016). This helps to assess the model's ability to capture the intricate degradation mechanisms and reproduce the observed microstructural changes.

In addition to laboratory-scale experiments, field validation techniques are employed to assess the performance of multi-scale models under real-world conditions. Monitoring and measuring the deterioration of actual concrete structures over time provide valuable data for comparison with the model predictions (Alexander & Beushausen, 2019). Field validation allows researchers to assess the model's ability to capture the complex interactions between various degradation mechanisms in real-world scenarios, accounting for factors such as environmental conditions, material heterogeneity and structural complexity. Furthermore, multi-scale models can be validated through tests conducted at different length scales. For instance, laboratory-scale experiments can focus on specific components of concrete, such as aggregates or cement paste and measure their behaviour under controlled degradation conditions. The obtained experimental data can then be compared with the model's

predictions at the corresponding length scales, ensuring that the model accurately captures the behaviour of individual components and their interaction.

7.2 Calibration and Verification of Model Parameters

Calibration and verification of model parameters are important steps in ensuring the accuracy and reliability of multi-scale models. Calibration refers to the process of adjusting the model parameters to achieve the best possible agreement between the model predictions and experimental or observed data. Verification, on the other hand, involves testing the calibrated model against additional independent data to assess its predictive capability.

The calibration process typically starts by selecting a set of initial model parameters based on prior knowledge or literature values. These parameters may include material properties, reaction kinetics, boundary conditions and other model inputs (Bernard et al. 2003; Otieno et al. 2011). The model is then simulated, and the results are compared with experimental data or observed behaviour. Statistical methods, optimisation algorithms, or sensitivity analyses are often employed to adjust the model parameters and minimise the discrepancy between the model predictions and the observed data.

During the calibration process, it is important to consider the uncertainties associated with the experimental data and model assumptions. Sensitivity analyses can help identify the most influential parameters and guide the calibration efforts (Esmaeili et al. 2014; Gu et al. 2019). Iterative adjustments and comparisons between model simulations and experimental data are carried out until a satisfactory level of agreement is achieved. Once the model is calibrated, it is necessary to verify its performance using independent data. Verification involves testing the model against different experimental conditions, varying input parameters, or data from other sources. This process helps assess the robustness and generalisation capability of the model. If the model consistently produces accurate predictions across a range of scenarios and experimental data sets, it provides confidence in its reliability and applicability.

It is worth noting that calibration and verification are iterative processes and multiple cycles of adjustment, simulation and comparison may be required to achieve an optimal level of agreement. Additionally, the calibration and verification processes should be documented rigorously, including details of the selected parameters, data sources, statistical analyses and any assumptions made.

In summary, calibration and verification of model parameters are critical for ensuring the accuracy and reliability of multi-scale models. The calibration process involves adjusting the model parameters to minimise the discrepancy between the model predictions and experimental data, while the verification process assesses the model's performance using independent data. By carefully calibrating and verifying model parameters, researchers can enhance the predictive capability and confidence in multi-scale models, enabling more accurate and insightful analyses of concrete deterioration and facilitating the development of effective mitigation strategies.

7.3 Comparison with Field Data

Comparing multi-scale models with field data is an essential step in evaluating the accuracy and reliability of these models in real-world applications (Sarker et al. 2019; Suwanmaneechot et al. 2020). Field data provides valuable insights into the actual behaviour and performance of concrete structures under various degradation mechanisms, such as corrosion, freeze-thaw, alkali-aggregate reaction, and others. To compare multi-scale models with field data, researchers typically collect relevant field measurements and observations, such as the extent of deterioration, material properties, structural response, and environmental conditions. These data serve as benchmarks for assessing the performance of the models.

The comparison involves examining the agreement between the model predictions and the field data. This can be done by evaluating various performance indicators, such as the carbonation depth, corrosion rate, crack propagation and structural integrity. Statistical analyses, such as root-mean-square error or correlation coefficients, may be used to quantitatively assess the level of agreement. Discrepancies between the model predictions and field data can arise due to various factors. These include uncertainties in the model parameters, limitations in the model assumptions or simplifications, variations in the actual field conditions and measurement errors (Shodja et al. 2010; Benitez et al. 2019). It is important to identify and understand these discrepancies to improve the accuracy of the models and address any shortcomings.

In cases where the model predictions do not align well with the field data, researchers may refine the model parameters, update the input data, or consider additional factors that were not accounted for in the initial model. This iterative process helps enhance the model's predictive capability and improve its agreement with the field observations. Moreover, qualitative comparisons between the model predictions and field data can also provide valuable insights. These may involve visual comparisons of crack patterns, degradation profiles, or other observable phenomena. Such qualitative assessments can help identify similarities or discrepancies between the model outputs and the real-world behaviour, leading to further model refinements. Comparing multi-scale models with field data is a crucial step in validating the models and gaining confidence in their applicability. It helps researchers and engineers understand the strengths and limitations of the models and supports informed decision-making regarding maintenance, repair, and design of concrete structures. By refining and improving the models based on the field data, researchers can develop more accurate and reliable tools for assessing the performance and durability of concrete infrastructure.

8. Challenges and Limitations in Multi-scale Modelling

Multi-scale modelling in concrete deterioration faces several challenges and limitations that researchers must address to improve the accuracy and applicability of these models. One challenge is the complexity and variability of the degradation mechanisms, which can involve multiple physical and chemical processes operating at different length and time scales. Capturing the interactions and coupling between these mechanisms requires detailed understanding and accurate representation in the models. Additionally, obtaining reliable and comprehensive experimental data for model calibration and validation poses a challenge due to the practical limitations of conducting large-scale tests. Furthermore, computational limitations and the need for computational resources and time pose constraints on the scale and complexity of the models. Balancing the trade-off between model accuracy and computational efficiency is crucial. Addressing these challenges will enhance the effectiveness and reliability of multi-scale modelling in predicting concrete deterioration and informing engineering decisions.

8.1 Computational Challenges and High-Performance Computing

The computational challenges in multi-scale modelling of concrete deterioration are driven by the need to accurately capture the complexity of the problem while efficiently utilising computational resources. As the number of scales and complexity of the model increase, so does the computational cost. Simulating multiple length and time scales simultaneously requires substantial computational power, which is provided by high-performance computing (HPC) platforms. Efficient algorithms play a crucial role in multi-scale modelling (Li et al. 2004; Provatas et al. 2007). These algorithms must effectively couple and synchronize the different scales, manage the exchange of information between them and ensure stable and accurate simulations. Developing innovative numerical techniques and advanced algorithms that can handle the multi-scale nature of the problem is a significant challenge.

The large volume of data generated in multi-scale simulations poses additional challenges. Storing, processing, and analysing the massive amount of simulation data require efficient data management strategies. Post-processing techniques are needed to extract meaningful information and insights from the results. To address these challenges, researchers rely on HPC techniques such as parallel computing, distributed computing, and domain decomposition methods. These techniques enable the efficient utilisation of computational resources, reducing simulation time and allowing for the exploration of larger and more complex systems.

However, accessing, and utilising HPC resources can be challenging. Limited availability of HPC resources, high costs associated with their usage and the need for specialized expertise in utilising these resources effectively can act as barriers for researchers and institutions. Collaborating with HPC centres, gaining access to shared resources, and providing training in HPC techniques are crucial steps in overcoming these challenges and promoting the widespread use of HPC in multi-scale modelling.

8.2 Uncertainty Quantification and Sensitivity Analysis

Uncertainty quantification (UQ) and sensitivity analysis (SA) play a crucial role in multi-scale modelling to account for the inherent uncertainties and variability in the system and to assess the impact of input parameters on the model predictions (Gu et al. 2019; Zheng et al. 2019; He et al. 2022). In multi-scale modelling, there are various sources of uncertainties, such as material properties, boundary conditions and model parameters. Uncertainty quantification aims to quantify and characterise these uncertainties to provide a comprehensive understanding of the reliability and robustness of the model predictions. This involves the propagation of uncertainties through the different scales of the model, considering the interactions and dependencies between them. Monte Carlo simulations, Latin Hypercube Sampling and Bayesian inference are commonly used techniques in UQ to capture the uncertainty distribution and estimate the probability distributions of the model outputs.

Sensitivity analysis is another important component of multi-scale modelling, as it helps identify the input parameters that have the most significant influence on the model outputs. It provides insights into the relative importance of different parameters and assists in prioritising efforts for parameter estimation and model calibration. Various methods, such as variance-based methods (e.g., Sobol' indices), local methods (e.g., derivative-based methods) and global methods (e.g., Morris method), can be employed for sensitivity analysis in multi-scale models.

Uncertainty quantification and sensitivity analysis are closely related and often conducted together to gain a comprehensive understanding of the model's behaviour and the impact of input uncertainties. By quantifying uncertainties and assessing parameter sensitivities, researchers can improve the reliability and accuracy of multi-scale models, enhance decision-making processes and guide model calibration and validation efforts. These techniques also provide valuable insights into the sources of uncertainties and guide future experimental and computational investigations to reduce uncertainties and improve the model's predictive capabilities. However, it is important to note that uncertainty quantification and sensitivity analysis in multi-scale modelling present their own challenges. The computational cost associated with performing UQ and SA can be significant, particularly in large-scale and complex multi-scale models. Approximations and surrogate models are often used to reduce computational burden without sacrificing accuracy. Furthermore, the availability and quality of experimental data for calibration and validation purposes can also pose challenges in the context of multi-scale modelling.

8.3 Data Requirements and Availability

Data requirements and availability play a critical role in multi-scale modelling as they provide the necessary input parameters, boundary conditions and experimental validation data to develop and validate the models. The quality and quantity of data greatly influence the accuracy and reliability of the model predictions. In multi-scale modelling of concrete deterioration, various types of data are needed at different scales. At the macroscopic scale, data related to the overall structural properties, such as dimensions, geometry, material composition and loading conditions, are required. This includes information about the concrete mix design, reinforcement details, environmental conditions and applied loads. These data can be obtained from engineering drawings, construction specifications and relevant design codes.

At the mesoscopic scale, data related to the microstructure of concrete are necessary. This includes information about the size, shape and distribution of aggregates, as well as the characteristics of cementitious materials, such as the composition, hydration kinetics and pore structure. Techniques such as X-ray computed tomography (CT), scanning electron microscopy (SEM) and mercury intrusion porosimetry (MIP) are used to gather such data. At the microscopic scale, data on the atomic and molecular interactions between concrete constituents are required. This includes properties of individual cementitious phases, such as the mineralogy, crystal structure and chemical reactivity. These data can be obtained through techniques like X-ray diffraction (XRD), nuclear magnetic resonance (NMR) and Fourier-transform infrared spectroscopy (FTIR).

While data availability varies depending on the specific research area and the level of detail required, there are challenges in obtaining comprehensive and accurate data for multi-scale modelling. Some limitations include:

1. Data Accessibility: Accessing certain types of data, such as proprietary information or experimental results from previous studies, can be restricted or require collaborations with industry partners or research institutions.

2. Data Completeness: Comprehensive data that cover all relevant aspects of the multi-scale modelling process may not always be available. In such cases, assumptions or simplifications may be made to fill in data gaps.

3. Data Quality: The quality and reliability of available data can vary and inconsistencies or errors may exist. Data validation and quality control measures are necessary to ensure the accuracy and consistency of the input data.

4. Data Scalability: As multi-scale models require data at different scales, there can be challenges in obtaining consistent and compatible data across the various scales. Upscaling or downscaling techniques may be required to reconcile data at different resolutions.

To address these challenges, collaborations between researchers, industry professionals and data providers are crucial. Sharing and archiving experimental data, establishing standardised testing protocols and promoting open data initiatives can enhance data availability and facilitate the development and validation of multi-scale models. Furthermore, advancements in data collection techniques, such as non-destructive testing methods and advanced imaging technologies, are continually improving the acquisition of high-quality data for multi-scale modelling applications.

9. Future Directions and Emerging Trends

In the field of multi-scale modelling of concrete deterioration, several future directions and emerging trends are shaping the research landscape. One key direction is the integration of advanced sensing technologies and real-time monitoring systems with multi-scale models to enable accurate and continuous assessment of concrete performance. This allows for early detection of deterioration mechanisms and timely intervention strategies. Additionally, the development of machine learning and artificial intelligence algorithms is expected to enhance the predictive capabilities of multi-scale models by enabling data-driven analysis and optimisation. Furthermore, there is a growing emphasis on sustainability and life-cycle analysis, leading to the incorporation of environmental factors and long-term durability considerations into multi-scale models. Finally, the utilisation of cloud computing and distributed computing platforms will facilitate the accessibility and scalability of multi-scale modelling tools, enabling broader adoption and collaboration among researchers and practitioners.

9.1 Advancements in Multi-scale Modelling Techniques

Advancements in multi-scale modelling techniques have revolutionized the field of concrete deterioration research, enabling more accurate and comprehensive analysis of complex degradation mechanisms. Several key advancements are driving the progress in this area.
Firstly, the development of advanced computational algorithms and numerical methods has significantly improved the efficiency and accuracy of multi-scale models. Techniques such as adaptive mesh refinement, domain decomposition and parallel computing have enhanced the ability to handle large-scale and computationally demanding simulations.

Secondly, the integration of experimental data and sensor measurements into multi-scale models has led to a more realistic representation of material behaviour and degradation processes. Data assimilation techniques, such as Bayesian inference and Kalman filtering, allow for the integration of real-time monitoring data to update and refine the model predictions.

Thirdly, the incorporation of coupled multi-physics phenomena in the models has expanded their scope and applicability. By considering the interactions between different degradation mechanisms, such as corrosion, alkali-silica reaction and freeze-thaw damage, multi-scale models can provide more comprehensive insights into the overall deterioration process. Furthermore, advancements in material characterisation techniques, such as high-resolution imaging, spectroscopy, and molecular dynamics simulations, have enabled a more detailed understanding of the microstructure and chemical processes occurring within concrete. This information can be incorporated into multi-scale models to improve their accuracy and predictive capabilities.

Lastly, the utilisation of high-performance computing resources and cloud computing platforms has facilitated the scalability and accessibility of multi-scale modelling tools. Researchers can now simulate larger and more complex systems and collaborate on a global scale, leading to accelerated advancements in the field.

9.2 Integration of Data Science and Machine Learning

The integration of data science and machine learning techniques has emerged as a promising approach in the field of multi-scale modelling. By leveraging large datasets and advanced analytical tools, this integration enables enhanced understanding, prediction and decision-making in the context of concrete deterioration.

Data science techniques play a crucial role in the pre-processing and analysis of diverse data sources, including experimental data, sensor measurements and historical records. They help in cleaning, aggregating and normalising data to ensure its quality and consistency. Additionally, data science techniques enable exploratory data analysis, pattern recognition and feature extraction, revealing hidden patterns and relationships within the data.

Machine learning algorithms, on the other hand, offer the ability to build predictive models and uncover complex nonlinear relationships between variables. They can learn from historical data to make predictions and identify patterns or anomalies in the deterioration process. By training models on data from multiple scales and degradation mechanisms, machine learning can capture the intricate interactions and dependencies, leading to more accurate and robust predictions.

The integration of data science and machine learning in multi-scale modelling provides several benefits. Firstly, it allows for the development of data-driven models that can effectively capture the complexities of concrete deterioration. These models can improve prediction accuracy, identify critical factors influencing degradation and support proactive decision-making for maintenance and repair strategies.

Secondly, data science and machine learning techniques facilitate the integration of real-time monitoring data into multi-scale models. By continuously updating the models with sensor measurements and feedback, they enable real-time assessment of structural health and deterioration, supporting condition-based maintenance approaches. Furthermore, the integration of data science and machine learning opens avenues for advanced analytics, such as uncertainty quantification, sensitivity analysis and optimisation. These techniques help assess the reliability and robustness of multi-scale models, identify influential parameters and optimise strategies for concrete durability. However, challenges exist in integrating data science and machine learning into multi-scale modelling. These include the availability and quality of data, the need for domain expertise to interpret and validate the results and the ethical considerations surrounding data privacy and security.

9.3 Standardisation and Interoperability of Multi-scale Models

Standardisation and interoperability of multi-scale models are essential for advancing the field of concrete deterioration modelling. These concepts refer to the development and adoption of common standards and frameworks that enable seamless integration, collaboration, and exchange of information among different multi-scale modelling approaches and tools. Standardisation ensures consistency in model representation, data formats and computational procedures, allowing researchers and practitioners to easily share and compare models. It promotes transparency, reproducibility and reliability in model development and validation, as well as facilitates the exchange of models and data across different platforms and software.

Interoperability focuses on the compatibility and connectivity of multi-scale models with other systems, such as data management platforms, simulation tools and decision support systems. It enables the seamless integration of models into larger frameworks and facilitates the exchange of data and information between different modelling components. Achieving standardisation and interoperability in multi-scale modelling poses several challenges. One key challenge is the diversity of modelling approaches and tools, each with its own specific requirements and capabilities. Developing common standards and frameworks that accommodate different modelling paradigms and scales is a complex task. Furthermore, data standardisation is crucial for effective interoperability. It involves the development of common data formats, metadata descriptions and ontologies that enable the exchange and integration of data from different sources. Data harmonization and normalization techniques may be required to ensure consistency and compatibility among datasets.

Collaborative efforts among researchers, practitioners and standardisation organisations are essential for advancing standardisation and interoperability in multi-scale modelling. These efforts involve the development of guidelines, protocols, and best practices, as well as the establishment of open repositories and data sharing platforms. Collaboration can also lead to the development of standardized benchmark problems and validation datasets, which facilitate model comparison and validation.

9.4 Multi-scale Modelling for Sustainable Concrete Design

Multi-scale modelling plays a crucial role in sustainable concrete design by providing insights into the performance, durability, and environmental impact of concrete structures. By considering the interactions between different length scales, multi-scale models enable a comprehensive understanding of the complex processes involved in concrete degradation and help optimise concrete design for enhanced sustainability.

One aspect of sustainable concrete design is the reduction of environmental impacts. Multi-scale models can assess the environmental performance of concrete by simulating the life cycle of a structure and analysing its carbon footprint, energy consumption and pollutant emissions. These models allow for the evaluation of alternative materials, mix designs and construction practices to minimise environmental impacts. Another important consideration in sustainable concrete design is the durability of structures. Multi-scale models can simulate various degradation mechanisms, such as corrosion, alkali-aggregate reaction, and freeze-thaw cycles, at different length scales. This enables the prediction of long-term performance, identification of vulnerable areas and evaluation of potential mitigation strategies. By optimizing the material composition, design parameters and maintenance practices, multi-scale modelling helps extend the service life of concrete structures and reduce the need for frequent repairs or replacements.

Furthermore, multi-scale models can aid in the development of novel and sustainable concrete materials. By investigating the interactions between different materials at the micro and nano scales, these models contribute to the design of high-performance concretes with improved strength, durability, and environmental properties. They can also guide the incorporation of alternative binders, supplementary cementitious materials, and recycled aggregates to reduce the use of virgin materials and promote circular economy principles. In addition to performance and durability considerations, multi-scale modelling can support sustainable concrete design by optimizing structural efficiency. By analysing the mechanical behaviour of concrete at different scales, these models help optimise the use of materials, reduce overdesign, and enhance structural performance while minimising material waste. However, the application of multi-scale modelling for sustainable concrete design faces challenges. These include the complexity and computational demands of multi-scale simulations, the need for accurate material properties and parameters and the integration of diverse modelling approaches and tools. Overcoming these challenges requires ongoing research, collaboration and advancements in computational methods, material characterisation techniques and data availability.

10. Concluding Remarks

The use of multi-scale modelling in the study of concrete deterioration has proven to be a valuable approach in enhancing our understanding of the complex processes involved. It provides insights into the degradation mechanisms at different length scales, from macroscopic to microscopic levels and allows for a more accurate prediction of concrete performance and durability. Through multi-scale modelling, researchers can simulate and analyse the interaction between various degradation mechanisms, such as corrosion, alkali-aggregate reaction, freeze-thaw cycles, and fatigue loading. This enables a comprehensive

assessment of the combined effects of multiple factors on concrete degradation, leading to more informed decision-making in the design, maintenance, and repair of concrete structures.

However, it is important to recognise the challenges and limitations associated with multi-scale modelling. These include the need for accurate and reliable experimental data for model calibration and validation, computational complexities, data storage and management issues and the requirement for specialized expertise and high-performance computing resources. To overcome these challenges, further advancements are needed in terms of model refinement, algorithm development and data availability. Collaboration between researchers, industry professionals and stakeholders is crucial in standardizing models, promoting data sharing and fostering interdisciplinary research.

Overall, multi-scale modelling holds great potential in advancing the field of concrete deterioration and plays a vital role in the development of sustainable and resilient infrastructure. By improving our understanding of degradation mechanisms, optimizing material formulations, and designing more durable concrete structures, multi-scale modelling contributes to the longevity, safety and sustainability of our built environment.

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