MULTISCALE AND MULTIPHYSICS MODELLING OF DURABLE INFRASTRUCTURE MATERIALS

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MULTISCALE AND MULTIPHYSICS MODELLING OF DURABLE INFRASTRUCTURE MATERIALS

BY
SUMERU NAYAK

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN CIVIL AND ENVIRONMENTAL ENGINEERING

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BY

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ABSTRACT

Infrastructure is the backbone of America’s 18.57 trillion-dollar economy. The current condition of America’s deteriorating infrastructure network, however, is the cause of serious safety, quality of life, and economic concerns. According to the recent American Society of Civil Engineers’ (ASCE) 2017 Report Card, America’s Infrastructure received a score of D+. According to ASCE’S annual report, the US economy is expected to lose $4 trillion in GDP by 2025 and $14 trillion in GDP by 2040 if current concerns are not addressed and infrastructure continues to deteriorate at current rates. Clearly, there is a need for bold and forward thinking solutions that adopt modern technologies, materials and design methodologies in these critical infrastructures. Improvement of the health of our infrastructure depends not only on closing the investment gap in the building and repair of these systems and networks, but also on development of innovative design-driven technologies to build the next-generation of durable infrastructure for our future. The central objective of this thesis stems from the afore-mentioned concerns and realities; to develop innovative durable infrastructure materials. Thus, this thesis explores development of innovative cementitious systems and polymer composites for durable infrastructure. Virtual design and numerical modelling of the innovative materials as applied to structures form a salient feature of this thesis that can enable designers and engineers alike with tools to facilitate optimized design. While concrete is notorious for its poor fracture performance, its exposure to freeze-thaw cycles and deicing salts in the temperate areas leading to loss of design life is a key concern. A part of this thesis addresses this by incorporating waste metallic particulates to improve fracture performance and phase change materials to improve freeze-thaw resistance. The phase change materials
incorporated in cementitious systems are found to reduce the number of freeze-thaw cycles in a concrete structure thus significantly reducing the freeze-thaw induced cyclic damage and associated chloride ingress. Alternative binders such as alkali-activated blast furnace slag that can reduce cement consumption have been also been studied. Incorporation of metallic particulate reinforcement in such alternative binder enhances fracture performance of the composite by crack bridging and deflection. To enhance the life of existing infrastructure, the other part of this thesis aims to develop piezoresistive composites that can enable strain and damage sensing. Such smart composites are achieved by nano-engineered interfaces or waste iron powder in cementitious systems and the incorporation of CNTs in polymer composites. Multi-physical simulations that can capture the sensing capabilities of such heterogenous systems have been developed in an electro-mechanical framework. Owing to the heterogenous nature of such materials, accurate predictions entail capturing of detailed microstructural features which are facilitated by multiscale simulations. Damage sensing as enabled by electromechanical experiments leading to tomographic observations have also been carried out to validate the efficiency of inclusions in the smart composites. The application of nanoengineered films in aggregates in concrete and polymer weaves enables reversible strain sensing thus fostering a real-time health monitoring. The simulations involving the separation of inclusion-matrix interface and ensuing matrix damage when coupled with electromechanical responses of the constituents in a multiscale framework serve to elucidate the strain and damage sensing behavior of the composites. In a similar multiscale framework, the baseline conductivity serves as a-priori information in iron powder incorporated cementitious systems thereby enabling determination of spatial conductivity distribution inside the sample for spatial damage
sensing by Electrical Resistance Tomography. The key findings of the studies involve the efficiency of iron powder volume fraction up to 40% demonstrating spatial damage sensing with suitable accuracy. For the self-sensing nanoengineered composites, the thin films brought about by percolating CNT networks similarly show reversible strain sensing ability thus elucidating the efficiency of such systems achieved by 0.01% volume fraction of CNTs in films as thin as 10 microns.
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The thesis presents the multiple chapters towards durable infrastructure materials in a manuscript format whereby the section, figure, table and equation numbering pertain to the specific manuscript in which it appears. The US infrastructure is in dire need of resurrection given that many of the roads and bridges are reaching the end of their lifespan and are dangerously overstretched, thus hampering the safety of commuters. Consequently, there is an urgent need for development of innovative durable infrastructure materials for improved design life of structures. Concrete continues to be one of the most successful and widely adopted infrastructure materials throughout the history of industrial revolution. However, concrete is inherently weak in tension, and its fracture strength must be considered as one of the factors that controls its rate of deterioration. Localized stresses arise in concrete due to expansion, shrinkage or loss of cohesion of the aggregate and paste due to a variety of physical and chemical interactions. This leads to the initiation of micro-cracks and subsequently to the growth and propagation of both micro- and macro-cracks. The potential for deterioration can range from its introduction at the level of manufacture of the cement to incompatibility of the design. The factors for degradation or failure of structures with the exception of design errors, are related to either the cement paste microstructure, the macro-environment or the fracture strength of the concrete. Moreover, the fracture strength controls the extent of the rate of the deterioration of concrete. Thus, the permeability and the fracture strength of concrete can be singled out as the primary variables for assessing durability. More often than not, a synergistic degradation is brought about by the influence of these parameters in conjunction with several degradation processes that include electrochemical (corrosion of embedded reinforcement), physical
(freeze-thaw), diffusion (chloride attack and carbonation). Thus, the susceptibility of reinforced concrete structures to corrosion and their rate of deterioration can be approximated, provided that the macro-environment, the cement paste microstructure and the fracture strength of the concrete can be rationally defined. Freeze-thaw, chloride attack and reinforcement corrosion are the most prevalent causes of concrete deterioration [1]. The combination of either of the degrading phenomena coupled with concrete’s poor fracture performance leads to crack development and deterioration of the structure. Since concrete is the mostly widely used construction material in history, degradation of concrete structures affects the QOL thereby necessitating durable structures.

As mentioned earlier, freeze-thaw attack is one of the most significant causes of deterioration of concrete especially in areas with severe winters. This study attempts the use of PCMs in the New England area of United States to tackle the freeze-thaw damage. A literature survey on the use of PCMs shows its applicability towards indoor thermal comfort in buildings and enhancement of building energy efficiency[2–6]. Besides, PCMs have been shown to reduce early age hydration heat release and the early-age thermal cracking in large concrete structures and pavements[7–9]. Availability of these PCMs with a wide range of transition temperatures [10,11] opens up various innovative avenues towards beneficial utilization of these materials in infrastructure materials. Application of PCMs towards reduction in freeze-thaw cycles in concretes pavements has been proposed [11,12]. Deicing salts are commonly used to remove snow and ice from the pavement surface [11–16]. But, such process is labor-intensive and causes damage to the pavements [11,12,17,18]. Alternatively, incorporation of PCMs in concretes has been suggested [10,12,19] to solve this issue by the means of high latent heat of fusion of PCMs. A recent
experimental study [12] has shown significant reduction in snow formation when PCMs are incorporated in concrete. Chapters 1 and 2 describe the application of PCMs to superstructures and the subsequent gains in durability thus obtained.

Another cause of degradation pertaining to the inherent relatively weaker tensile properties of concrete has been tackled with use of metallic particulate reinforcements. While several modified and alternative cementitious materials such as supplementary cementitious materials [20,21], alkali activated binders [22–24], carbon-negative binders [25–27] etc. have been widely studied over the past few decades to improve sustainability credential of concrete, the issue of poor fracture response has been addressed incorporating steel fibers [28,29], glass fibers [30,31], carbon fibers [32,33], wollastonite [34,35], textile reinforcement [36,37] etc. This paper incorporates waste iron powder as cement-replacement. This waste iron powder is an industrial byproduct and it is generated in large quantities in electric-arc furnace (EAF) steel production facilities and shot-blasting operations of structural steel sections. Traditionally, this waste iron powder is landfilled since it is not economically feasible to recycle such waste materials. Several million tons of such waste product is being landfilled all over the world. Thus the waste iron powder is expected to address the concern related to poor sustainability credential of cementitious materials by replacing cement partially thereby reducing the carbon-footprint of concrete. On the other hand, the elongated iron particulates in iron powder, as observed in previous studies [27,38,39], are likely to contribute towards improved crack-bridging mechanism and enhanced fracture response of mortars which are explored in detail in this study. Chapters 3, 4 and 5 explain the metallic particulate reinforcement in AAS and cementitious binders to enhance fracture properties of such composites. From a numerical simulation
perspective, the classical theory of solid mechanics, because of its reliance on partial
differential equations, is inherently limited when applied to failure of materials [40–42].
The non-existence of the spatial derivatives at the crack tips introduces singularity, which
is alleviated with supplemental relations for stable numerical modeling. Finite element
based fracture simulations stipulate explicit damage initiation and propagation laws, as
demonstrated in Chapters 3 and 5. Chapter 4, however, applies Peridynamics based
approach for fracture study in metallic particulate reinforced mortars. The motivation of
the study stems from the need for reformulation of the fundamental equations of continuum
mechanics for universal application regardless of discontinuities arising from
deformations. Peridynamics uses integral equations and maintains the integrity of the
mathematical structure in the event of a discontinuity [43–45]. In this approach [46,47],
any failure is treated as a natural outcome of the deformation arising out of the equations
of motion and the constitutive model [41]. This eliminates the need for supplemental
kinetic relations which would otherwise be necessary in fracture mechanics to define crack
initiation and propagation [48,49]. The approach has been applied and contrasted with FE
simulations, as demonstrated in Chapter 4.

The other aspect of the current study is to extend the life of existing structures by
Structural Health monitoring (SHM). SHM can provide valuable information on the
reliability and safety of the structures besides helping to develop strategies to save the
structures before critical damage threatening the structural integrity [50,51]. Strain- and
damage-sensing are integral aspects of SHM. Most of the load-bearing structures are very
sensitive to damage and it can cause catastrophic failures leading to immense loss of life
and property [50,52]. Therefore, costly routine inspections have been used for maintenance
of these structures. Traditionally, various non-destructive testing (NDT) techniques such as ultrasound testing, radiographic tests (X-ray) etc. have been used, although they are impractical and expensive for large structures. Thus, there has been a need for a real-time mixed global/local damage-sensing approach. For real-scale industrial structures, use of smart composites is gaining popularity in recent times for strain-sensing in structures [53–55]. In particular, such smart composites achieve damage-sensing capability by utilizing piezoresistivity which is an electromechanical phenomenon that enables certain electrically conductive composites to respond electrically under the influence of strain [56–63]. Electrical resistance methods in these composites have been shown to be sensitive to minor and microscopic changes that include defects or damage [59,63–65]. Bulk electrical response obtained from electrical impedance spectroscopy (EIS) has been used for detection of cracks [66,67], fiber distributions [68,69], fiber orientations [70], and corrosion rate of reinforcing bars [71–74] in conductive cementitious composites. In order to achieve spatial distribution of features (say damage), tomography techniques enabled by electrical responses are achieved in smart composites by a technique called electrical resistance tomography (ERT). In ERT [75–78], several electrode pairs, attached to the surface of the sample, measure potential differences in response to an injected current and a spatial conductivity distribution map is obtained by solving an ill-posed problem [78–80]. In the current scope, nano-engineered cementitious systems have been demonstrated to be strain-sensing in Chapter 6 while ERT has been used to reconstruct damaged zones in iron powder based cementitious systems, as described in Chapter 7. The studies point to an integrated implementation of material tweaks and superior monitoring to achieve enhanced durability. Additionally, strain sensing has been demonstrated in smart polymer composites enabled
by CNT incorporation in textile weaves. Textile composites are widely used in aerospace, astronauts, marine, automotive and off-shore applications owing to their lightweight nature and exceptional mechanical performance [81,82]. Unlike traditional unidirectional laminated composites which are susceptible to inter-laminar damages, the woven fabrics offer enhanced through-thickness reinforcement thus significantly enhancing the damage tolerance. However, with the ever-expanding domain of applications of such fiber reinforced composites, a variety of unforeseen circumstances have appeared including material defects, manufacturing errors, environmental-induced degradation, excessive loading, fatigue amongst others that can cause significant damages in forms of delamination, matrix-cracking, inter-laminar fracture, debonding and their combinations which can lead to catastrophic structural failure [83,84]. The intricacy of such damage mechanisms in a heterogeneous structural material such as fiber-reinforced woven polymers pose a tremendous challenge in damage detection. The damages that initiate at micron scale between fibers and matrices or laminae are imperceptible to visual inspection and macroscale sensors like strain gauges, transducers and accelerometers. This paves the way for development of intrinsic sensors that can enable continuous monitoring while offering superior performance brought about via incorporation of nano-sensors like CNTs which are multifunctional in nature [85,86]. Toward that end, nano-engineered composites with CNT-incorporated thin films deposited on fiber weaves have been demonstrated in an experimental study [86] for strain sensing and damage detection. The mechanisms governing the strain sensitivity of such smart weave are the mechanically induced deformations that alter CNT positions or induce damage in matrix or interface thereby varying the overall current distribution in the microstructure. Strain sensing ability of such
smart textile composites has been established through experimental evaluation [86,87]. While the previous studies evaluated the performance of such composites experimentally, this study assimilates a finite element based framework that entails multiple hierarchical length scales toward obtaining macroscopic electro-mechanical response with a view to enable multiscale simulation-based design of such smart composites. This is achieved by an integration of the various length scales to form a holistic framework capable of capturing piezo-resistive characteristics in a sequential multiphysics framework that can even be extended with thermomechanical characteristics [88], environmental degradation [89] or piezoelectric effects [90]. Such an approach offers robustness in its ability to incorporate nanoscale modifications that can significantly alter thin film characteristics thereby altering the sensing efficiency of the smart weave composites, as described in Chapter 8.

In summary, Chapters 1 and 2 explain the frost resistance of PCM incorporated concrete and demonstrate their applications in pavement and bridge respectively. Chapter 2 extends the study in a multiphysical domain by predicting chloride ion diffusivity in frost damaged concrete.

Chapters 3, 4 and 5 demonstrate the enhanced fracture performance brought about by inclusion of metallic waste powder incorporation in cementitious composites that serves as particulate reinforcement. While Chapters 3 and 4 demonstrate the fracture response of traditional mortars, Chapter 5 involves an alternative cementitious binders. Chapter 3 adopts FE based technique requiring explicit damage laws while Chapter 4 adopts peridynamics that can handle discontinuities (crack propagation) autonomously. A contrast of the techniques is brought about in Chapter 4.
Chapters 6, 7 and 8 demonstrate strain and damage sensing in piezoresistive composites. While Chapters 6 and 7 involve smart cementitious systems, Chapter 8 demonstrates strain sensing ability of a polymer composite systems. Strain sensing is enabled by nano-engineered films deposited on aggregates (Chapter 6) for cementitious systems and fiber weaves (Chapter 8) in textile composites. Chapter 7 demonstrates spatial damage sensing in waste iron powder incorporated cementitious systems using electrical resistance tomography (ERT).
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Chapter 1

Influence of Phase Change Materials (PCMs) on the Freeze-thaw response of Concrete Pavements

Published in Construction and Building Materials (2019), Elsevier
Abstract: The use of phase change materials in infrastructure has gained significant attention in the recent years owing to their robust thermal performance. This study implements a numerical simulation framework using finite element analysis to evaluate the influence of Phase Change Materials (PCMs) on the thermal response of concrete pavements in geographical regions with significant winter weather conditions. The analysis is carried out at different length scales. The latent-heat associated with different PCMs is efficiently incorporated into the simulation framework. Besides, the numerical simulation framework employs continuum damage mechanics to evaluate the freeze-thaw induced damage in concretes. The simulations show significant reductions in the freeze-thaw induced damage when PCMs are incorporated in concrete. The numerical simulation framework, developed here, provides efficient means of optimizing the material design of such durable PCM-incorporated concretes for pavements by tailoring the composition and material microstructure to maximize performance.
1. INTRODUCTION

Use of Phase change materials (PCMs) in cementitious composites for enhanced energy efficiency is an active research area [10,12,91,92]. PCMs have been shown to be advantageous in structural concretes due to their ability to store and release heat [2,12,91,93]. A large number of studies have focused on the use of PCMs towards indoor thermal comfort in buildings and enhancement of building energy efficiency [2,4,5,94]. Besides, PCMs have been shown to reduce early age hydration heat release and the early-age thermal cracking in large concrete structures and pavements [7–9]. In addition to the above-mentioned applications, availability of these PCMs with a wide range of transition temperatures [10,11] opens up various innovative avenues towards beneficial utilization of these materials in infrastructure materials. For example, application of PCMs towards reduction in freeze-thaw cycles in concrete pavements has been proposed earlier [11,12]. Deicing salts are commonly used to remove snow and ice from the pavement surfaces [11–16]. But, such process is labor-intensive and causes damage to the pavements [11,12,17,18]. Alternatively, incorporation of PCMs in concretes has been suggested [10,12,19] to solve this issue by the means of high latent heat of fusion of PCMs. A recent experimental study [12] has shown significant reduction in snow formation when PCMs are incorporated in concrete. Another recent study confirmed improved frost resistance of the concrete containing PCMs [19]. Numerical studies involving freeze-thaw performance of cementitious materials are also implemented using one dimensional finite difference technique [7,11,19].

This paper focuses on microstructure-guided numerical simulation using finite element analysis to evaluate the influence of microencapsulated paraffinic PCMs with transition temperature around 5°C on the freeze-thaw response of macro-scale concrete pavements. The numerical simulation framework, presented in this study, performs numerical homogenization using finite element analysis at multiple length scales. The effective properties, obtained using multi-scale numerical homogenization, are employed in a macro-scale FE model of concrete pavement to obtain pavement temperatures under the effects of the ambient temperature and solar radiation whilst considering conduction, convection and radiation modes of heat transfer with the subgrade and the atmosphere. The pavement temperatures, thus obtained, are used to quantify frost damage at multiple length scales using continuum damage mechanics [95–98] that can capture the progressive freeze-thaw induced damage. Thus, this study integrates the material microstructure and thermo-mechanical properties of the constituent phases to predict the freeze-thaw response of macro-scale concrete pavement. The numerical simulation framework, presented in this study, provides efficient design strategies to tailor the composition and microstructure towards development of concretes.
with improved frost-damage performance without compromising its strength. Hence, the methodology developed herein would be extremely useful for pavements in areas with severe winter weather conditions.

2. NUMERICAL SIMULATION TO ELUCIDATE THE INFLUENCE OF PCM ON THERMAL RESPONSE OF CONCRETE PAVEMENTS

In this paper, a thermal analysis is carried out at multiple length scales with a view to evaluate the influence of PCMs in concrete pavements. Here two different material mixtures are considered. While the control concrete contains 70% aggregates (40% coarse aggregate and 30% fine aggregate) by volume, the PCM-incorporated concrete contains 64% aggregates (40% coarse aggregate and 24% fine aggregate) and 6% microencapsulated paraffinic PCMs (as 20% volumetric sand-replacement) by volume. Such dosage of PCM has been shown to provide equivalent mechanical performance as compared to conventional mortars [99]. In this study the dosage of PCMs is fixed at 20% by volume sand substitute since incorporation of higher volume fraction of PCMs has been shown to result in decrease in compressive and flexural strength in a previous study [99]. PCM considered here has phase transition temperature of 5.1°C. It consists of a paraffin core encapsulated by melamine formaldehyde shell as detailed in [99].

The forthcoming sub-sections describe numerical homogenization for effective property-prediction and application of effective properties towards thermal response evaluation of a macro-scale pavement section with a view to highlight the influence of PCMs in concrete.

2.1 Multiscale Numerical Homogenization for Prediction of Effective Thermal Properties:

Here, a microstructure guided numerical simulation framework is employed at multiple length scales to compute the effective properties of both the concretes. At every length scale, a representative volume element (RVE) is generated with the inclusion phases. Intrinsic thermal and mechanical properties are then assigned to the component phases in the RVE. Periodic boundary conditions [100,101] are applied. The RVE is meshed and FE analyses are carried out. A post processing module generates volume averaged responses that are computed to yield effective properties. The basic framework for the procedure is illustrated in Figure 1.
The following sub-sections present the multiscale numerical homogenization procedure to obtain the effective properties of both the concretes.

### 2.1.1 Generation of Microstructure and Boundary Conditions:

3D representative volume elements (RVEs) are generated using the Lubachhevsky-Stillinger algorithm [102–105]. A hard particle contact model is employed, while ensuring there is no particle overlap. The formulations regarding the generation of the RVEs are adequately described in [100,101,106]. The meshed microstructure is implemented in a Python script and the analysis is performed in ABAQUS™ solver.

Periodic boundary conditions (PBC) [107–110] are applied on the RVE. Periodicity provides higher computational efficiency in smaller analysis domain and thus facilitates faster convergence [101]. Periodic boundary conditions (PBC) ensure continuity of temperature and heat flux at the boarder of neighboring unit cells. PBCs have been applied successfully towards prediction of effective properties of heterogeneous composites [100] and are detailed adequately in [107–110]. Figure 2 presents the microstructures generated for multi-scale homogenization.
A three step homogenization procedure is followed for the case of control concrete. The first step homogenizes air voids with hardened cement paste (Figure 2 (a-1)) whereas the second step homogenizes sand into the homogenized matrix obtained from first step (Figure 2 (a-2)). The final step incorporates coarse aggregates into the homogenized matrix obtained from second step (Figure 2 (a-3)) and thus, effective property of concrete is computed.

While a three-step homogenization is employed for control concrete, an additional step involving homogenization of PCMs is adopted for PCM-modified concrete. The first step of homogenization remains the same as control concrete case. In the second step, microencapsulated PCMs are incorporated into the homogenized matrix obtained from the first step as shown in Figure 2 (b-2). The third and fourth steps homogenizes sand (Figure 2 (b-3)) and coarse aggregate (Figure 2 (b-4)), respectively, into the homogenized matrix obtained from the previous step. These homogenizations are performed here at multiple steps in order to reduce the computational cost while maintaining computational efficiency [111]. The relative edge lengths of RVEs with respect to inclusion sizes are computed (Shown in Figure 2) based on sensitivity study. Similar relative
sizes of RVEs with respect to inclusion sizes were obtained elsewhere [100,101]. The size distribution of inclusions (air voids, PCMs, sand and coarse aggregates) are adopted from [96,99,100]. The absolute volume fractions of component phases are shown in Table 1. The volume fractions of the individual components of control concrete are denoted as $V_f^a$ whereas those for PCM-modified concrete are denoted as $V_f^b$. The thermal analyses of the cases involving PCM are carried out at a temperature below the transition temperature implying that the microencapsulated PCMs are in the solid state.

Table 1 - 1 A table showing the volume fractions of the components of control concrete ($V_f^a$) and PCM-incorporated concrete ($V_f^b$)

<table>
<thead>
<tr>
<th>Component</th>
<th>$V_f^a$ (Control Concrete)</th>
<th>$V_f^b$ (PCM-Concrete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCP</td>
<td>24%</td>
<td>24%</td>
</tr>
<tr>
<td>Void</td>
<td>6%</td>
<td>6%</td>
</tr>
<tr>
<td>PCM</td>
<td>NA</td>
<td>6%</td>
</tr>
<tr>
<td>Sand</td>
<td>30%</td>
<td>24%</td>
</tr>
<tr>
<td>CA</td>
<td>40%</td>
<td>40%</td>
</tr>
</tbody>
</table>

2.1.2 Effective Property Computation

Once the RVE is generated using the Python script, it is meshed and subjected to FE analysis under externally applied unit temperature gradient along the X-direction. The FE analyses are carried out in ABAQUS™ solver. A MATLAB© script operates on the result files containing the volume of the elements and the responses to obtain the effective properties as explained before. The intrinsic thermal properties of the constituent phases of both the concretes are shown in the Table 2.

Table 1 - 2. Thermal conductivity ($\lambda$) [100], specific heat capacity (C) [93] and latent heat L [11,12] at 5.1°C for hardened cement paste (HCP), Sand, coarse aggregate (CA) and PCM

<table>
<thead>
<tr>
<th>Phases</th>
<th>$\lambda$ (W/m K)</th>
<th>C (J/ kg K)</th>
<th>L (kJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCP</td>
<td>0.75</td>
<td>750</td>
<td>NA</td>
</tr>
<tr>
<td>Sand</td>
<td>2.8</td>
<td>1150</td>
<td>NA</td>
</tr>
<tr>
<td>PCM</td>
<td>0.15</td>
<td>2600</td>
<td>150</td>
</tr>
<tr>
<td>CA</td>
<td>2.3</td>
<td>790</td>
<td>NA</td>
</tr>
</tbody>
</table>

A thermal analysis is carried out on the RVE containing C3D8R elements under a unit thermal gradient across opposite faces of the RVE along the X-direction. The thermal analysis results for different homogenization steps are shown in Figure 3 (a-1), (a-2) and (a-3) for the control concrete and in Figure 3 (b-1), (b-2), (b-3) and (b-4) for the PCM incorporated concrete.
Figure 1-3 Heat flux for (a) control concrete corresponding to different homogenization steps (RVEs shown in Figure 2): (a-1) Step I: air voids in HCP: Homogenized thermal conductivity ($\lambda$): 0.73 W/m K; (a-2) Step II: sand in homogenized matrix from step-I: Homogenized $\lambda$: 0.56 W/m K; (a-3) Step III: coarse aggregate in homogenized matrix from step-II: Homogenized $\lambda$: 1.76 W/m K and for PCM incorporated concrete corresponding to: (b-1) Step I: air voids in HCP: Homogenized $\lambda$: 0.6 W/m K; (b-2) Step II: PCM in homogenized matrix from step-I: Homogenized $\lambda$: 0.53 W/m K; (b-3) Step III: sand in homogenized matrix from step-II: Homogenized $\lambda$: 1.43 W/m K; (b-4) Step IV: coarse aggregate in homogenized matrix from step-III: Homogenized $\lambda$: 1.78 W/m K. All the heat flux values correspond to externally applied unit temperature gradient ($1^\circ$C/mm) in X-direction.

A post processing module (MATLAB® subroutine) computes the volume average of the heat flux. The volume-averaged heat flux is used to obtain the effective thermal conductivity using Equation 1 [100].

$$\lambda_{eff} = \overline{q}^e \left( \frac{L}{T_{x=L} - T_{x=0}} \right)$$  [1-1]
where $\lambda_{\text{eff}}$ is the effective thermal conductivity, $\bar{q}^e$ is the homogenized (volume averaged of all elements) heat flux in RVE, $L$ is the edge length of RVE. The temperatures on the two opposite faces of the unit cell along the X-direction are denoted by $T_{x=0}$ and $T_{x=L}$. Thus, $(T_{x=L} - T_{x=0})$ is the imposed temperature difference. The aforementioned 3D numerical homogenization technique for effective thermal conductivities has been successfully validated in a previous study [100] against experimental thermal conductivities obtained using a guarded hot plate apparatus in accordance with ASTM C177-13 [112]. The effective thermal conductivities of a multi-inclusion porous systems is often predicted on the basis of a microstructure guided study [100,113] which have shown substantial agreement with experimental results.

In order to obtain the effective volumetric heat capacity, the reaction heat flux is obtained at the nodes under applied unit temperature gradient along X-direction. The ratio of the volume-averaged reaction heat flux to the temperature difference yields the effective volumetric heat capacity $(\rho C_p)_{\text{eff},s}$ [114]. For the case of PCM incorporated concrete, a similar procedure is followed to obtain $(\rho C_p)_{\text{eff},s}$ that has PCM in the solid state. However, at the transition temperature of the PCMs, the latent heat released by the PCM during phase transformation is appended to the volumetric heat capacity as shown in Equation 2 [93].

$$
(\rho C_p)_{\text{eff},t} = (\rho C_p)_{\text{eff},s} + \left((\phi_c \rho_c h_{sf})/\Delta T_{pc}\right)
$$

where $(\rho C_p)_{\text{eff},t}$ is the effective volumetric heat capacity at transition temperature, $(\rho C_p)_{\text{eff},s}$ is the effective volumetric heat capacity for solid phase PCM, $\phi_c$ is volume fraction of PCM, $\rho_c$ is density of PCM, $h_{sf}$ is latent heat of fusion of PCMs and $\Delta T_{pc}$ is the phase change temperature window. It is to be noted that all the calculations involved herein consider PCMs in solid state only, for the sake of simplicity. Similar approach has been successfully implemented in [11,93].

The effective properties obtained using the above-mentioned framework for both control and PCM-modified concretes are presented in Table 3. The values obtained for control concrete are in line with experimental values reported in literature [11,93]. For the cases of PCM inclusions, the values match closely with the ones reported in [93,100]. The effective thermal properties, thus obtained, are used in macro-scale simulation of pavement in the forthcoming section to elucidate the influence of microstructural modifications imparted by PCMs on the macro-scale structures.

Table 1 - 3. The effective properties obtained after homogenization

<table>
<thead>
<tr>
<th>Materials</th>
<th>$\lambda$ (W/m K)</th>
<th>$(\rho C_p)_{\text{eff},s}$ (J/kg K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concrete</td>
<td>1.4</td>
<td>880</td>
</tr>
</tbody>
</table>
2.2 Simulation of Thermal Response of Macro-scale Concrete Pavements:

In this section macro-scale FE analysis is performed to elucidate the influence of PCMs on the thermal performance of concrete pavement. Consequently, the temperature profiles of the pavement are obtained under the local weather conditions in Providence, Rhode Island, United States. Forthcoming sub-sections present the model geometry, boundary conditions, analysis procedure and the thermal responses obtained from the numerical simulation as follows:

2.2.1 Model Geometry and Boundary Conditions:

A three-dimensional pavement section is modeled in FE commercial software ABAQUS™ as shown in Figure 4. The pavement section, considered here, is 13.3 m long and 9.15 m wide. The thickness of the top layer, made of concrete, is 406 mm which is lying over a subgrade of 12.20 m thickness. Such a configuration ensures that the subgrade is semi-infinite since the boundary effects are mitigated on the top pavement section when such a depth is considered [115].

Figure 1-4. 3D geometry of pavement section showing the ambient interactions and thermal boundary conditions

The boundary conditions of the macro-scale pavement model are determined by the ambient conditions. The daily weather data for Providence, Rhode Island, United States are obtained from

10
the National Oceanic and Atmospheric Administration (NOAA) [116]. It includes hourly global horizontal irradiance (GHI) data and hourly atmospheric temperature data. GHI encompasses the short wave radiations diffused in the atmosphere and the solar radiation incident on a surface normal to the rays thus resulting in the total amount of short wave radiation received per unit area of a horizontal surface on the ground. The ambient interactions and the temperature boundary conditions are shown in Figure 4. The daily maximum GHI ($q_s$) values are adjusted for absorption by concrete with its absorptivity ($\beta_s$) being 0.59 [117] and are applied as surface heat flux thermal load valid only during the day in the model. The hourly ambient temperature ($T_0$) is used to define the heat transfer interactions. Convection is defined by the product of surface convection coefficient ($h_0$) and the difference of the pavement surface temperature ($T(0, t)$) and ambient temperature ($T_0$) [118]. The value of $h_0$ is a function of wind velocity which can be assumed to be 26 W/m$^2$K for the air-concrete interface at low wind speeds [119] and is applied as a surface film coefficient in the model that defines the convective interaction between the pavement surface and the atmosphere. The Stefan-Boltzmann radiation constant ($\sigma$) and the surface emissivity of concrete ($\varepsilon$) with values 5.6697 x 10$^{-8}$ W/m$^2$K$^4$ and 0.92 respectively, when multiplied with the difference of the fourth powers of ambient temperature ($T_0$) and pavement surface temperature $T(0, t)$ ( $\varepsilon\sigma(T_0^4 - T(0, t)^4)$ ) give the radiative heat transfer. This is modelled by defining a surface radiation interaction between the pavement surface and the atmosphere with an ambient temperature of $T_0$. The temperature at the base of the pavement (here below the subgrade) ($T_g$) is a function of the ambient temperature $T_0$ and the relationship is shown as follows [120]:

$$T_g(t) = 0.83 \times T_0(t) + 3.7$$ \hspace{1cm} [1-3]

Temperature boundary conditions are applied to the base of the pavement model. Another boundary condition stems from the heat flux continuity equation at the interface between the top concrete layer and bottom subgrade layer. This interaction is defined in the model with a surface-to-surface contact, thereby ensuring a conductive heat flow at the interface. While the conductivity of concrete is obtained from numerical homogenization (Table 3), conductivity of subgrade is adopted as 1.75 W/(m.K) [121]. For the case of PCM incorporated concrete, the significant jump in internal energy during phase change is accounted for by defining the latent heat as a thermal property of the material. A nonlinear transient heat analysis step in the model ensures that the latent heat in conjunction with the density of the material successfully attenuates the heat capacity in the phase change temperature window as mentioned earlier. Thus, as the pavement in the model cools down in absence of solar radiation and plunging ambient temperature, the PCMs having a volume fraction of 6% ($V_f$), release 150 kJ/kg ($h_{sf}$) at 5.1°C ($T_{pc}$). Density of 300 kg/m$^3$ for PCMs is adopted here
This study incorporates a phase transformation temperature window ($\Delta T_{pc}$) of 1°C which is in line with values reported elsewhere [93]. At the transition temperature of the PCMs, the latent heat released by the PCM during phase transformation is added to the volumetric heat capacity (Equation 2), obtained using numerical homogenization as explained before.

2.2.2 Finite Element Simulation of Macro-scale Response:

A MATLAB© script extracts the data from the weather data files and feeds it into the ABAQUS™ model. The conductive, radiative and convective heat transfer processes are considered in the python script for ABAQUS™ solver. A transient heat transfer FE analysis is carried out in ABAQUS™ solver. A mesh convergence study was performed. The top concrete layer containing 280 linear hexahedral DC3D8 elements and the bottom subgrade layer containing 630 linear hexahedral DC3D8 elements ensured converged solution. A post processing module extracts the temperature data of the pavement for both concrete and PCM-modified concrete cases which are reported in Figure 5 for the months of December 2015, January 2016 and February 2016.
The ambient temperature is also depicted in Figure 5 for reference. As can be seen from the figure, the pavement surface temperature for both concrete systems is higher than the peak ambient temperature which can be attributed to the solar radiation that heats up the surface. Similar observations were noted elsewhere [7,11]. Figure 5 also clearly shows that temperature peak of control concrete is higher than the temperature peak of the PCM-incorporated concrete when the temperature is greater than the phase transition temperature of 5.1°C. The reduced temperature peak obtained in the PCM incorporated concrete substantiates the effective solar energy storage capacity of PCMs which would otherwise be wasted in raising the surface temperature as obtained in the control concrete. The effectiveness of the PCM incorporated concrete lies in its ability to store the energy during its phase change as a latent heat in the charging cycle (under incoming solar radiation) that can be released at lower temperatures in the discharging cycle towards effective defrosting. From Figures 5(a), (b) and (c), it is clear that the amplitude of temperature variations
(difference between maximum and minimum pavement temperature) reduces significantly when PCM is incorporated. The difference is more pronounced for lower ambient temperatures. This is attributed to the release of latent heat during phase-transformation (liquid to solid) of PCMs at transition temperature of 5.1°C. Thus, the temperature profiles shown here reflect the effectiveness of these PCMs in keeping the pavement surface warmer even under very low ambient temperatures, thereby establishing the fact that such PCMs are extremely effective in the New England area of the United States facilitating enhanced service life. Similar observations were found experimentally in [11]. In order to shed more light, Figure 6 shows the pavement temperature profiles for January 7, 2016. Figure 6 (a-1) and (b-1) correspond to maximum ambient temperature of 7.2°C and peak solar radiation of 384 W/m² for control concrete and PCM-incorporated concrete respectively.

PCM-incorporated concrete shows slightly lower temperatures under the same ambient temperature as expected. Figures 6 (a-2) and (b-2) show the pavement temperatures corresponding to minimum ambient temperature (−7.1°C).
ambient temperature of the day for control concrete and PCM-incorporated concrete respectively. While the control concrete pavement shows significantly lower pavement temperatures (minimum temperature \(-5.4\, ^\circ\mathrm{C}\)), the PCM-incorporated concrete shows relatively higher pavement temperatures (minimum temperature \(-1.3\, ^\circ\mathrm{C}\)). This is attributed to the heat released by PCMs during phase-transformation thus helping to keep the pavement warmer. Considering a water-freezing temperature of \(-6.1\, ^\circ\mathrm{C}\) in concrete [11,122], the control concrete pavement is expected to freeze at this minimum ambient temperature of on January 7, 2016 whereas the PCM-incorporated concrete does not freeze. Overall, considering a freezing and thawing temperature of \(-6.1\, ^\circ\mathrm{C}\) and 0\, ^\circ\mathrm{C}\) respectively in concrete [11,122], the control concrete experiences 25 freeze-thaw cycles, whereas the PCM-incorporated concrete experiences 13 number of freeze-thaw cycles during December 2015 – February 2016 (Surface temperatures reported in Figure 5) thereby reinforcing the idea that PCMs have the potential to enhance the service life of pavements. In order to shed more light into the effectiveness of the PCMs, simulation of frost-damage in both the concretes is elucidated in the forthcoming section.

3. INFLUENCE OF PCM ON THE FREEZE THAW RESPONSE OF CONCRETE AND MORTAR MICROSTRUCTURE

While the previous section employed microstructure-guided numerical simulation at different length scales to obtain the macro-scale thermal response of concrete pavement, this section applies the pavement surface temperatures, obtained in the previous section for February 2016, to the meso scale so as to elucidate the fundamental difference in freeze-thaw response imparted by PCMs in concretes. The forthcoming sub-sections show microstructure-guided numerical simulation for frost-damage response in concretes and mortars using continuum damage mechanics. The analysis involves generation of meshed 2D representative element areas (REAs) by Python scripts. The physical change in the phase transformation of water to ice during the freezing cycle leads to a volume increase of 9% in the micro-pores [123]. The damage in the cementitious matrix of the REA is implemented in ABAQUS™ with the help of a user defined subroutine UMAT that implements the damage laws. A post processing module computes the degraded Young’s modulus from the results obtained by ABAQUS™ solver. The analysis procedure and the results are presented as follows:

3.1 Microstructures and Material Properties:

The damage analysis is carried out at the mortar scale. Here, 2D REAs are chosen to reduce computational demand as a trade-off between computational efficiency and demand [124]. The REAs are generated using Lubachevsky–Stillinger algorithm [100,102–105]. The edge lengths of
REAs are chosen as five times the mean diameter of inclusions based on a sensitivity study. Similar RVE sizes relative to inclusion sizes are implemented successfully in [101,106]. Figure 7(a) shows the control mortar microstructure containing 40% hardened cement paste with 10% voids and 50% sand by volume. The REA for PCM-incorporated mortar is shown in Figure 7(b) which contains 20% PCM as sand-replacement. The PCM-modified mortar microstructure contains 40% hardened cement paste with 10% voids, 40% sand and 10% PCM (20% sand replacement) by volume. The size distribution of PCM and sand are adopted from [99].

![Microstructure Images](image)

Figure 7.7 The generated REAs for: (a) mortar matrix containing 50% sand and 40% hardened cement paste (HCP) with 10% void; (b) PCM-modified mortar containing 40% HCP, 10% void, 40% sand and 10% PCM by volume.

The analysis requires the material properties for the matrix and inclusion phases which are shown in Table 4. The poison’s ratio for all components except PCMs is taken as 0.2. A poison’s ratio of 0.4 is adopted for PCMs [99].

![Material Properties Table](table)

<table>
<thead>
<tr>
<th>Component</th>
<th>E (GPa)</th>
<th>α (µε/℃)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCP</td>
<td>22.4</td>
<td>15</td>
</tr>
<tr>
<td>Sand</td>
<td>70</td>
<td>5</td>
</tr>
<tr>
<td>PCM</td>
<td>4.45</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 4. Input material properties for numerical simulation of damage [96,99,111]

3.2 Numerical Simulation of Isotropic Damage in Concretes:

The damage analysis is implemented in python language program which is later used in ABAQUS™ solver to obtain results. A user-defined subroutine in ABAQUS™ applies the volume expansion (due to freezing) in the voids embedded in the cement paste matrix. The resulting mechanical response is captured by the framework that applies the damage law. The mechanical
properties are used from Table 4 while the size distribution is similar to what has been implemented earlier in the study. Finally, a post processing module computes the stress-strain response after every freeze-thaw cycle and yields the degraded material properties of the mortar which is scaled up to the concrete level and validated with experimental results reported in [123].

Periodic boundary conditions [107–110] are implemented in the REAs as described earlier. The framework assumes fully saturated voids. The analysis framework imports the surface temperatures of the pavement from the macro scale analysis (for the month of February 2016 as shown in Figure 5(c)) and applies volumetric expansion in the voids as soon as the freezing temperature of -6.1°C [11,125] is reached. The volumetric expansion is implemented using a user-defined subroutine in ABAQUS™ that incorporates volumetric thermal expansion of voids by means of artificial coefficient of thermal expansion of the void so as to obtain 9% volumetric expansion. The volume expansion is released when the average nodal temperature increases above 0°C (Thawing temperature [11,126]). Such freeze-thaw cycle induce damage around the voids which propagates with increasing number of freeze-thaw cycles.

The progressive damage in HCP matrix due to freeze-thaw cycles is implemented by user defined subroutine UMAT [127–129] in ABAQUS™. The progressive degradation of both the mortars due to frost-damage is modeled here by continuum damage mechanics while considering the heterogeneity in these materials [95–97]. Assuming isotropic stiffness degradation, the damage variable, $D$ is given as [95–98,130]:

$$\sigma = (1 - D) \mathbf{C} : \varepsilon$$  \[1-4\]

Where the effective stress tensor is denoted by $\sigma$, $\mathbf{C}$ denotes fourth order tensor of elasticity and $\varepsilon$ is the strain tensor. The value of damage, $D$ ranges from 0 (undamaged) to 1 (completely damaged). The damage rate denoted by $\dot{D}$ assumes only zero or positive values which can be explained by its proportionality with the damage energy release rate [96].

In order to characterize the damage in the cement paste matrix at the scale of the mortar (Figures 7(a) and (b)), an isotropic damage model is used that provides a damage evolution law as shown in Equation 5 [131].

$$\dot{D} = \xi \frac{\partial S(\varepsilon^{eq})}{\partial \varepsilon^{eq}}$$  \[1-5\]

Where $\xi$ is the Lagrange multiplier which when multiplied with the partial derivative of the constraint $S(\varepsilon^{eq})$ (as mentioned in Equation 6) with respect to the $\varepsilon^{eq}$ (elastic energy) gives the rate of scalar damage $\dot{D}$. The constraint $S(\varepsilon^{eq})$ is defined as follows:
\[
S(\varepsilon^{eq}) = 1 - \exp[-((\varepsilon^{eq} - a)/b)^c] - D
\]

\(S(\varepsilon^{eq})\) is constrained to be \(\leq 0\). The damage evolution law (Equation 5) is discretized by an implicit Euler scheme and it yields the instantaneous damage parameter \(D\). The fitting parameters \(a\), \(b\) and \(c\) (in Equation 6) for cement paste, adopted from [131], are 0.488, 0.1 and 3.0 respectively. For the PCM incorporated mortar, same damage parameter values are implemented since the matrix is HCP for both the cases.

3.3 Frost-damage Response:

Figure 8 shows progressive damage in mortars for both the cases. The figure shows progressive frost-damage in both the mortars for the month of February in the year 2016 in Providence, Rhode Island, United States. The model geometries for control and PCM-incorporated mortar are shown again in Figure 8(a-1) and (b-1) for the ease of reference. While Figures 8 (a-2) and (a-3) exhibit progressive damage on February 10 and February 28 respectively for the control mortar, Figures 8 (b-2) and (b-3) show the damage status on February 10 and February 28 respectively for the PCM-incorporated mortar. While the control concrete has experienced 10 freeze thaw cycles, the PCM incorporated concrete has experienced 5 such events over the month of February, 2016. As the damage progresses, on day 10, for the control mortar, the HCP matrix (Figure 8(a-2)) shows significant damage whereas the damage is negligible for the PCM incorporated HCP matrix in the PCM modified mortar (Figure 8(b-2)). This is attributed to the fact that PCMs act as heat storage and releases heat when the ambient temperature starts to drop decreasing the amplitude of diurnal temperature fluctuations in the pavement. As a result, the number of freeze-thaw cycle experienced by pavement reduces due to incorporation of PCM in the mortar which is reflected here in the form of significant reduction in damage when PCM is incorporated. This trend is continued till the end of the month (Day 28) as shown in Figure 8 (a-3) and (b-3).
Degraded Young’s modulus ($E_d$) values for both the mortars corresponding to days in the month of February 2016 are calculated from the damage values using equation 4 and are reported in Figure 9(a). The PCM-incorporated mortar experiences significant reduction in frost-degradation as compared to control mortar which is primarily attributed to the lower number of freeze-thaw cycles experienced by PCM-incorporated mortar due to thermal heat storage capacity of PCMs as explained earlier. Degraded Yong’s modulus values obtained for mortar are numerically homogenized with coarse aggregates (40% by volume) to obtain degraded Young’s modulus for concretes as shown in Figure 9(b). PCM incorporated concrete show a lesser degree of degradation than control concrete as expected. While the control concrete shows a 25.5% degradation, the PCM incorporated concrete shows a 15% for the same time period which fundamentally reinforces the efficacy of using PCMs towards improving freeze-thaw durability of cementitious materials.
Figure 0.9 Ratios of degraded Young’s modulus (\(E_d\)) to initial Young’s modulus (\(E_0\)) with number of days of February for (a) mortars and (b) concrete for control and PCM-incorporated concretes respectively highlighting Days 10 and 28 (see Figure 8).

In order to shed more light on the predictive capability of the numerical simulation framework, the frost-damage results from numerical analysis for control concrete are compared to experimental results reported in [123]. Here the ratios of degraded Young’s modulus (\(E_d\)) to initial Young’s modulus (\(E_0\)) are plotted for up to 10 number of freeze-thaw cycles. The predicted values correlate very well with the experimental values signifying robustness of the numerical simulation framework in predicting freeze-thaw response in cementitious materials. The numerical simulation framework thus integrates the material microstructure to the macro-scale structural performance and provides an efficient means to optimize these concretes for durable infrastructure.

Figure 1.10 Predicted vs experimental ratios of degraded Young’s modulus (\(E_d\)) to initial Young’s modulus (\(E_0\)) for concrete.
4. CONCLUSIONS

This paper presents microstructure-guided numerical simulations at different length scales to evaluate the influence of PCMs on the freeze-thaw response of concrete pavements. Two different concretes were employed for evaluations. While the control concrete contains 70% aggregate by volume, the PCM-modified concrete contains 20% PCM as sand-replacement (6% absolute volume). A three-step numerical homogenization was performed for control concrete and an additional step involving PCMs was incorporated in PCM-modified concrete. The effective properties, thus obtained from the numerical homogenization, were employed in macro-scale concrete pavement model to obtain the pavement temperatures under the influence of ambient temperatures and solar radiation. The analysis was performed for ambient conditions at Providence, Rhode Island, United States during December 2015-February 2016. The PCM incorporated concrete pavements showed a significantly reduced amplitude of pavement temperature fluctuations as compared to that obtained for control concrete. This is attributed to the latent heat storage capability of the PCM which is released at its transition temperature. The results also indicate 50% reduction in the number of freeze-thaw cycles, experienced by pavement, when PCMs are incorporated. In order to shed more light into the influence of PCMs on the frost damage response of concretes, an isotropic damage model was employed to capture the progressive frost deterioration of the mortar and concrete. A superior frost damage-resistance of the PCM modified concrete was observed as compared to control concrete signifying effectiveness of the PCMs. For the month of February 2016, the control concrete experienced 25.5% loss of stiffness whereas the PCM-modified concrete showed about 15% loss of stiffness. This advocates the use of PCMs in concrete pavements with a view to enhance frost-damage resistance of concrete pavements. The microstructure guided numerical simulation framework, presented in this paper, provides an efficient means of designing concretes by tweaking the material at different length scales to maximize performance.
Chapter 2

Influence of Phase Change Materials (PCMs) on the chloride ion diffusivity of concrete

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Abstract: Use of phase change materials (PCMs) to tailor the thermal performance of concretes by efficient energy storage and transmission has gained traction in recent years. This study incorporates microencapsulated PCMs as sand-replacement in concrete bridge decks and performs numerical simulation involving multiple interactive length scales to elucidate the influence of PCM-incorporation in concretes subjected to combined freeze-thaw and chloride ingress-induced deterioration. The simulations show significant increase in durability against combined freeze-thaw and chloride ingress-induced deterioration in concretes when microencapsulated PCMs are incorporated. In addition, a reliability-based probabilistic analysis shows significant increase in life expectancy of bridge decks with PCM-incorporation. The numerical approach presented here provides efficient means to develop design strategies to tune dosage and transition temperature of PCMs to maximize durability of concrete structures in regions that experience significant winter weather conditions.
1. INTRODUCTION

Application of thermal energy storage capacity of microencapsulated paraffinic phase change materials (PCMs) towards enhanced energy efficiency of structures has been an active area of research in construction materials [10,12,91,92]. The ability of PCMs to store and release heat has been shown to introduce a thermal inertia in structural concretes thereby enhancing performance [2,12,91,93]. Previous studies have shown the effectiveness of PCMs towards improving energy efficiency of buildings and indoor thermal comfort [2,4–6]. PCMs have also been successfully used to arrest thermal cracking in concrete pavements during early ages of hydration. [7–9]. The modularity of PCMs in terms of availability of wide range of transition temperatures warrants various beneficial applications in infrastructure materials [10,11]. PCMs have been proposed for application in concrete pavements and bridges for improved performance under freeze-thaw cycles [11,12]. A common method of removing ice and snow from the surface of pavements and bridges is application of deicing salts [11–16]. Such process is not only labor intensive but also a major source of dissolved chlorides in concrete that can cause catastrophic damage to the underlying structures. A combined degradation of the concrete occurs by the freeze-thaw induced cracks and chloride diffusion through those cracks which can cause reinforcement-corrosion [11,12,17,18,132]. An efficient alternative method can be the incorporation of PCMs in concrete [10,12,19] which readily takes advantage of the high latent heat of PCMs that is released in freezing ambient conditions. A recent experimental study [12] corroborates the application of PCMs in concrete to reduce snow formation. The improved frost-resistance of such concretes has also been reported in another recent study [19]. Numerical studies involving one dimensional finite difference technique have also shown the effectiveness of PCMs in concrete subjected to freeze-thaw cycles [7,11,19].

While previous studies report on effectiveness of PCMs towards improved frost-resistance, this paper focuses on evaluation of the influence of PCMs on the performance and life-expectancy of concrete bridge decks subjected to combined freeze-thaw cycles and chloride-ingress using multiscale numerical simulations. The input properties of the materials used for macro-scale finite element analysis are obtained from multi-scale numerical homogenization. The effective properties, thus obtained, are used to obtain the surface temperature profile of a concrete bridge deck for a given period of time under ambient temperature and incident solar radiation. The simulation approach efficiently integrates the influence of latent heat of PCMs. The surface temperatures enable prediction of freeze thaw cycles. The volumetric expansion of the freezing pore solution causes stiffness-loss while the applied deicing salts (to remove snow) inundate the
surface with dissolved chlorides. To have a deeper insight into the material degradation and resulting accelerated chloride ingress, the heterogeneity of the concrete is encompassed in this study by a microstructure-guided analysis at the meso and micro scales. While continuum damage mechanics is used to quantify the progressive material degradation with freeze thaw cycles [95–98], Fick’s law of diffusion [133–135] is used to capture the resulting accelerated chloride diffusion behavior in the degraded concrete. Thereafter, a first-order reliability-based probabilistic analysis predicts the influence of PCMs on the life expectancy of bridge decks. This study achieves an integration between the material microstructure and the macro-scale bridge deck structure to predict lives of such structures subjected to combined freeze-thaw and chloride ingress-induced deterioration. The numerical approach thus provides a tool to designers and engineers alike to provide efficient design strategies which can be tailored to build durable structures in varying environments. Furthermore, this approach will facilitate the development of freeze-thaw resistant concretes with conventional strength that can find numerous applications not only in bridge decks but also in any exposed concrete surfaces subjected to chloride environments and harsh freezing ambient temperatures.

2. NUMERICAL SIMULATION OF FREEZE-THAW RESPONSE

In order to elucidate the influence of PCMs on the freeze-thaw response of concrete, a multi-scale analysis is carried out here using continuum micromechanics. The following sub-sections perform multi-scale numerical homogenization for effective properties of concrete which are used as input for macro scale analysis of thermal response of concrete bridge deck under ambient conditions in Providence, RI, United States. The macroscopic thermal responses for both the concrete decks are further used to obtain freeze-thaw induced damage response as detailed later in this section. A schematic diagram in Figure 1 shows the steps involved in the numerical framework. Firstly, a numerical homogenization approach predicts the effective properties of the cementitious systems which are used as an input to the thermal analysis of macro-scale bridge decks. The identified thermal response is used to characterize the freeze thaw induced damage in the microstructure. The damaged microstructure is thereafter subjected to chloride diffusion to predict the durability.
Figure 2 - 1 A schematic diagram showing the microstructure guided prediction of effective properties which are used for the thermal analysis of a macro-scale bridge deck followed by a detailed microstructural analysis of freeze thaw induced damage and ensuing chloride diffusion towards durability prediction

2.1 Prediction of effective properties

A numerical simulation approach involving microstructure-guided effective property prediction is implemented in this section at multiple length scales. The numerical homogenization approach is schematically illustrated in Figure 2. The approach involves: (1) representative unit cell generation implementing the known microstructural features of the material, (2) application of periodic boundary conditions (PBCs) [107–110] and (3) implementation of a post-processing module that yields effective properties as explained in the forthcoming sub-sections.

Figure 2 - 2 A schematic diagram showing the FE based numerical homogenization approach employed to obtain effective thermal responses
2.1.1 Representative Unit cell generation and Boundary Conditions:

The Lubachhevsky-Stillinger algorithm [102–105] is used here to generate the representative unit cell. In this algorithm, a hard contact model is employed that prohibits particle overlaps. The algorithm randomly distributes the desired inclusions inside a periodic bounding box with random initial velocities. Next, the radius of each particle grows as a function of time. The desired particle size distribution is obtained from the tailored growth rate. The forward Euler scheme is used to update the positions of the particles with a time step that is minimized with events of possible collisions between particles. Detailed formulations of the iterative process where particles change positions in the bounding box, collide and grow to achieve the desired volume fraction are mentioned elsewhere [136]. Periodic boundary conditions (PBC) [107–110] are applied to the generated unit cells. Such boundary conditions are computationally efficient and therefore suited for faster convergence in smaller analysis domains. [101]. For thermal analyses, the continuity of temperature/heat flux is ensured by PBC across the neighboring unit cells boundaries. PBCs are detailed adequately in [100] and successful application of PBCs in heterogeneous composites towards effective property prediction has been demonstrated in [106]. A Python script implements the microstructural formulations to generate a unit cell and mesh it. Thereafter, the script applies PBC to generate periodically bounded meshed microstructure that can be imported to ABAQUS™ solver for FE analysis.

The numerical homogenization procedure involves generation of periodically bounded unit cells at each length scale with intrinsic material properties assigned to each component phase. At each length scale, the unit cell is subjected to a FE analysis and the response to a unit temperature gradient leads to prediction of effective properties. This paper considers two different concrete mixtures: (i) control concrete containing 30% fine aggregates and 40% coarse aggregates; (ii) concrete containing 20% PCM as sand-replacement (24% fine aggregates, 6% PCMs and 40% coarse aggregates). The paraffinic PCMs are considered to undergo a phase transition at 5.1°C. For the control mixture, the effective properties are calculated from a three-step homogenization approach. In the first step voids are homogenized with hardened cement paste (HCP) matrix. The homogenized property is assigned as property of matrix in the mortar scale (step-II) where sand particles are embedded in the matrix. Finally, the coarse aggregates are numerically homogenized with the mortar matrix, obtained from step-II, to yield the effective properties of concrete. A similar homogenization procedure is followed for PCM-incorporated concrete where the PCMs are dispersed in the HCP matrix along with the voids in Step-I followed by similar homogenization steps (steps II and III) as explained earlier for control concrete. The median particle sizes ($d_{50}$) for
PCMs, voids, sand and coarse aggregates are 7\(\mu m\), 10\(\mu m\), 600\(\mu m\) and 13.75mm respectively[96,99,100,137]. Sizes of the RVEs adopted for the three length scales are 0.035 mm (Step-I), 12.75 mm (step-II) and 69.375 mm (step-III) respectively, obtained based on a sensitivity study. The numerical homogenization procedure is explained in detail in our previous publications [100,101].

### 2.1.2 Effective property computation

The RVEs obtained at each length scale are subjected to thermal FE analysis. The FE analysis proceeds with C3D8R elements under a unit temperature gradient. A MATLAB© script extracts the volume averaged responses to obtain effective properties. Effective thermal conductivity \(\lambda_{eff}\) is obtained from the volume averaged heat flux as per Equation 1 [100].

\[
\lambda_{eff} = \bar{q}^e\left(\frac{L}{T_L-T_0}\right)
\]

Where the volume-averaged heat flux for all the elements in the unit cell with edge length \(L\) is denoted by \(\bar{q}^e\); and the temperature difference imposed across opposite faces is denoted by \((T_L - T_0)\). The reaction heat flux is volume averaged for all elements in the unit cell and its ratio with the imposed temperature difference is obtained which yields the effective volumetric heat capacity \((\rho C_p)_{eff}\) [114]. However, the incorporated PCMs undergo a phase change at the transition temperature which necessitates the incorporation of the corresponding latent heat in calculation of effective volumetric heat capacity for PCM incorporated concretes. During phase-transition at the transition temperature, the released latent heat is added to the effective volumetric heat capacity \((\rho C_p)_{eff,s}\) as shown in Equation 2 [93] to obtain effective volumetric heat capacity \((\rho C_p)_{eff,t}\).

The PCMs are considered to be in the solid state for simplicity [11,93].

\[
(\rho C_p)_{eff,t} = (\rho C_p)_{eff,s} + \phi_c \frac{\rho_c h_{sf}}{\Delta T_{pc}}
\]

where \(\phi_c\) is the PCM volume fraction; \(\rho_c\) is the PCM density and \(h_{sf}\) is the latent heat of fusion and \(\Delta T_{pc}\) is the temperature window of phase transformation. The value of \(\Delta T_{pc}\) is assumed to be 1\(^{\circ}\)C [93]. For this study, the PCM has an absolute volume fraction of 6\% in concrete, latent heat of fusion 150kJ/kg and density of 300 kg/m\(^3\) [11,12,138,139]. Table 1 shows the intrinsic thermal conductivities (\(\lambda\)) [100] and specific heat capacities (C)[93] for each phase of both the concretes.
The effective thermal conductivities ($\lambda$) for both control and PCM-incorporated concretes, obtained from the aforementioned framework, are 1.4 W/m K and 1.78 W/m K for the control and PCM incorporated concretes respectively. The corresponding effective volumetric heat capacities ($\rho C_p_{eff,s}$) for the control and PCM incorporated concretes are 0.88 kJ/kg K and 0.928 kJ/kg K respectively. The obtained homogenized effective properties correlate well with the ones reported in the literature for control concrete [11, 93] and for PCM incorporated concrete [93, 100]. These effective properties are used in the forthcoming section to evaluate thermal response of a concrete bridge deck (macro-scale).

### 2.2 Upscaling to macro-scale freeze-thaw response

A macro-scale FE analysis is presented in this section to evaluate thermal responses of the control concrete as well as PCM-incorporated concrete. To illustrate the influence of PCM incorporation, the temperature profiles at the surface of the corresponding decks are obtained. The macroscale thermal analysis is performed under ambient weather conditions in Providence, Rhode Island, United States.

#### 2.2.1 Bridge Deck model

A commercial FE software ABAQUS™ is used to model the three dimensional bridge deck with a box girder section as shown in Figure 3. The length, breadth and thickness of the bridge deck are considered to be 17.09 m, 10 m and 240 mm respectively. Similar dimensions for box girder bridges are adopted in [140, 141]
Figure 3 also shows the thermal interactions of the structure with the ambience thereby forming the thermal boundary conditions. The weather data of Providence, Rhode Island is obtained from [116]. It includes hourly atmospheric temperature data and global horizontal irradiance (GHI) data. GHI embodies the short wave radiation received on unit horizontal ground surface which is composed of diffused short wave radiations and normal incident solar radiation. The absorptivity ($\beta_s$) of concrete is considered 0.59 [117] which is multiplied with the daily maximum GHI ($q_s$) to obtain the incident surface heat flux. This is applied as a thermal load applied to the heating step during the day in the simulation. The heat transfer interactions are determined by the hourly ambient temperature ($T_0$). The difference between the deck surface temperature and ambient temperature, $[T(0, t) - T_0]$ is multiplied with the surface convection coefficient ($h_0$) to yield the convective interaction [118,142]. The value of $h_0$ is considered to be 26 W/m$^2$ K for the interface of air and concrete for low wind speeds [143], which is incorporated in the model as a surface film coefficient. Convection occurs in the air inside the box and between the deck surface and the atmosphere. The radiative heat transfer is obtained by multiplying the Stefan-Boltzmann radiation constant ($\sigma$), the surface emissivity of concrete ($\varepsilon$) and the difference of the fourth powers of ambient temperature ($T_0$) and deck surface temperature $T(0, t)$ [142]. The values of $\sigma$ and $\varepsilon$ are considered to be $5.6697 \times 10^{-11}$ kW/m$^2$ K$^4$ and 0.92 respectively [142]. Surface radiation interaction is defined between the deck surface and the atmosphere (ambient temperature of $T_0$). The latent heat of the PCM incorporated concrete is defined as a material property that captures the change in internal
energy during phase change in the phase transformation temperature window ($\Delta T_{pc} = 1^\circ C$ [93]). The analysis is carried out with a non-linear transient heat analysis step. In the PCM incorporated concrete deck, the latent heat of 150 kJ/kg ($h_f$) is released by the PCMs at 5.1$^\circ C$ ($T_{pc}$); which when added to the volumetric heat capacity (see Equation 2) captures the complete change in internal energy.

2.2.2 Macroscale thermal response

The weather data is fed into the ABAQUS™ model by a MATLAB© script where the heat transfer interactions by conduction, radiation and convection are defined. Hexahedral DC3D8 elements are used to carry out the transient heat transfer analysis in ABAQUS™ solver. A mesh convergence study was performed and a mesh containing 1386 nodes and 880 elements yielded converged solution. A post processor subroutine operates on the output file and extracts the deck surface temperature data for January, 2018 in Providence, RI, as reported in Figure 4. As shown in Figure 4, the solar radiation causes the peak surface temperature to rise beyond the ambient temperature, as noted elsewhere [7,11]. However, the amplitude of temperature variation is significantly reduced for PCM incorporated concrete. The heat released at its transition temperature introduces a thermal inertia that results in higher deck temperatures compared to control concrete.

![Figure 4: Temperature profile at the top surface of the bridge decks under imposed ambient temperatures for January 2018 in Providence, RI](image)

The surface temperature profiles depict the effectiveness of PCMs in reducing the number of freeze thaw cycles since PCM-incorporated concrete decks demonstrate higher surface temperatures even under extreme low ambient temperatures. Table 2 shows the comparative statistical measures for
the distribution of minimum and maximum surface temperatures corresponding to ambient conditions for both control concrete and PCM incorporated concrete.

Table 0-2 Statistical measures of minimum and maximum surface temperatures (highest, lowest, mean and standard deviation) for PCM incorporated and control concretes

<table>
<thead>
<tr>
<th></th>
<th>Ambient</th>
<th>Control Concrete</th>
<th>PCM concrete</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Minimum (°C)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lowest</td>
<td>-19</td>
<td>-16.25</td>
<td>-14.75</td>
</tr>
<tr>
<td>Highest</td>
<td>0</td>
<td>-1.7</td>
<td>-3.2</td>
</tr>
<tr>
<td>Mean</td>
<td>-7.38</td>
<td>-6.61</td>
<td>-6.18</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>4.68</td>
<td>4.22</td>
<td>3.92</td>
</tr>
<tr>
<td><strong>Maximum (°C)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lowest</td>
<td>0.10</td>
<td>3.50</td>
<td>1.10</td>
</tr>
<tr>
<td>Highest</td>
<td>17.00</td>
<td>25.00</td>
<td>23.50</td>
</tr>
<tr>
<td>Mean</td>
<td>5.65</td>
<td>12.44</td>
<td>9.92</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>5.08</td>
<td>6.55</td>
<td>6.14</td>
</tr>
</tbody>
</table>

Consequently, considering a freezing temperature of -5.5°C and thawing temperature of 0°C for water filled pores in concrete [11,122], the number of freeze thaw cycles are computed to be 3 for PCM modified concrete and 10 for the control concrete during January 2018. The temperature profiles, thus obtained, are employed in the forthcoming section to quantify the beneficial impact of PCMs on the freeze-thaw-induced damage response in concrete which is further used later in this paper towards simulation of chloride ion diffusion in concrete, damaged due to freeze thaw cycles for a detailed insight.

2.3 Damage due to freeze-thaw cycles

The damage response analysis is performed involving two length scales as shown in Figure 5. First, a four-phase system is modelled with sand inclusions, interfacial transition zone (ITZ), voids and HCP matrix (see Figure 5 (a-1)) for control mortar. PCM-incorporated system contains an additional inclusion phase of PCMs as sand-replacement (see Figure 5 (b-1)). The thickness of ITZ is assumed to be 20μm [144–146]. The progressive damage in the matrix is implemented here using a user-defined subroutine in ABAQUS™. The effective degraded Young’s modulus of the mortars is computed by a post-processing subroutine, coded in MATLAB™ and used as matrix-property in the meso-scale (see Figures 5 (a-2) and (b-2)) where coarse aggregates are dispersed in the mortar.
matrix. Numerical homogenization for Young’s modulus is performed to obtain degraded Young’s modulus of the concretes as explained later in this paper.

Figure 2.5 The generated unit cells for: (a-1) mortar containing 10% voids, 40% hardened cement paste (HCP) and 50% sand with; (a-2) Control concrete containing 40% coarse aggregate (CA) and 60% mortar matrix; (b-1) PCM-incorporated mortar containing 10% voids, 10% PCM, 40% HCP and 40% sand by volume, (b-2) PCM-incorporated concrete containing 40% coarse aggregate and 60% PCM-modified mortar

2.3.1 Numerical Simulation of isotropic damage in matrix induced by freeze-thaw cycles

The volume expansion of the water filled voids in the cement paste matrix is implemented using a user defined subroutine for ABAQUS™ solver. The analysis approach adopted herein imports the bridge deck surface temperatures (Figure 4) and implements volumetric expansion in the pores for temperatures below -5.5°C [11,122]. An artificial coefficient of thermal expansion of the pores is implemented so as to obtain a 9% volumetric expansion in the pores due to freezing. Similar approach was successfully adopted in [142]. As the temperature rises above 0°C, the volumetric expansion is released.[147]. The ensuing mechanical damage is captured using continuum damage laws described later. The intrinsic Young’s modulus of HCP, sand, ITZ and coarse aggregates, adopted from literature [96,99,111,148] are 22.4 GPa, 70 GPa, 4.45 GPa and 74.5 GPa respectively. A Poisson’s ratio of 0.2 is assigned to all the component phases except PCMs. The Poisson’s ratio for PCMs is considered as 0.4 [99]. The median sizes of voids, PCM, sand and
aggregates are adopted as 10µm, 7µm, 600µm and 13.75 mm respectively [96,99,100,137]. The ITZ is considered 20 µm thick [144–146]. A post-processor subroutine computes the constitutive response of the degraded material and compiles the degraded Young’s modulus with varying freeze-thaw cycles.

This approach bridges the macro scale response of the concrete bridge deck to the micro and mesoscales by implementing volumetric expansion of water filled voids once the macro scale surface temperature drops below -5.5°C. In the analysis framework, the resultant hydraulic pressure in the pores due the strains causes an average stress that applies to the porous matrix, here the cement paste [149]. The stiffness degradation in the matrix results from a cyclic expansion during freezing and a contraction during thawing, with \( \frac{\Delta V}{V} \) being 0.09. The continuum damage implemented in the matrix is characterized by a damage variable \( D \) that has a value between 0 and 1 which signify undamaged and completely damaged states respectively. Assuming isotropic stiffness degradation, \( D \) is defined as per Equation 3 [95–98,130].

\[
\sigma = (1 - D)C : \varepsilon \tag{2-3}
\]

Where \( \sigma \) denotes the effective stress tensor, \( \varepsilon \) is the strain tensor and \( C \) denotes the elasticity tensor. The overall damage \( D \) is composed of its tensile (\( D_t \)) and compressive (\( D_c \)) parts (see Equation 4 [96,97])

\[
D = \alpha_t D_t + \alpha_c D_c \tag{2-4}
\]

A non-local equivalent strain \( \tilde{\varepsilon} \), defined in Equation 5 [95,96], is used to obtain \( D_t \) and \( D_c \).

\[
\tilde{\varepsilon} = \sqrt{\sum <\varepsilon_i^2>}_+ \tag{2-5}
\]

Where \( <\varepsilon_i^2>_+ \) is the positive part of the principal strain. The tensile and compressive components of damage (\( D_t \) and \( D_c \)) evolve as a function of \( \tilde{\varepsilon} \) as per the Equation 6 [95–98,130].

\[
D_{t,c}(\tilde{\varepsilon}) = 1 - \frac{\varepsilon_{Do} (1 - A_{t,c})}{\tilde{\varepsilon}} - \frac{A_{t,c}}{\exp [B_{t,c} (\tilde{\varepsilon} - \varepsilon_{Do})]} \tag{2-6}
\]

Where \( \varepsilon_{Do} \) is damage initiation threshold. Experimentally obtained uniaxial tensile and compressive curves can characterize the values of the parameters \( A_{t,c} \) and \( B_{t,c} \). The values of the parameters \( A_t \) and \( B_t \) for cement paste are 1 and 10^4 respectively while those of \( A_c \) and \( B_c \) are 1.2 and 1.5x10^3 respectively while \( \varepsilon_{Do} = 0.0001 \) [131].
2.3.2 Frost-damage response

The progressive damage in the paste matrix is shown in Figure 6 for the control and PCM incorporated cases for January 20th (See Figures 6 (a-2) & (b-2)) and January 31st (See Figures 6 (a-3) & (b-3)) respectively for the year 2018 in Providence, Rhode Island. Overall, the damage observed in control mortar is significantly higher than the PCM-incorporated mortar which demonstrates the durability benefit of PCM-incorporation. A significantly higher mechanical degradation, especially at the surface of a structure can be detrimental to its usability and mechanical integrity resulting from rebar corrosion in RC structures.

The degraded mechanical properties obtained in the micro-scale analysis is used as an input matrix property in the meso-scale to obtain a homogenized response of the concrete scale for both control and PCM-incorporated cases.

The normalized degraded modulus of elasticity (with respect to initial Young’s modulus) obtained for the control concrete are plotted along with experimental results obtained from [150] in Figure 7. The values show close correlation thereby validating the framework of frost-induced damage.

Figure 6 Frost-induced damage for: (a) control mortar: (a-1) initial geometry; (a-2) Day 20; (a-3) Day 31, (b) PCM-incorporated mortar: (b-1) initial geometry; (b-2) Day 20; (b-3) Day 31
2.4 Impact of PCM-incorporation on the freeze-thaw induced damage in concrete

The validated framework is used to quantify the damage response induced by freeze-thaw cycles for both the PCM-incorporated and control mortars as well as concretes. The relative degradation is captured by the ratio of degraded Young’s modulus ($E_d$) to the initial Young’s modulus ($E_0$). Figure 8(a) shows the relative performance of the PCM-incorporated mortar with respect to the control mortar for January 2018 in Providence, RI. A significant reduction in stiffness-degradation is observed for PCM-incorporated case implying superior freeze-thaw-durability of PCM-incorporated mortars due to its ability to stay relatively warm even in freezing ambient conditions. Figure 8(b) shows the performance of control and PCM-incorporated concretes. The freeze-thaw-durability efficiency of PCMs reduces in concrete when compared to mortars for the obvious dilution effect. However, a significant 18% reduction in the stiffness-degradation is still observed with PCM-incorporation in concrete highlighting the effectiveness of PCMs in improving freeze-thaw-durability of concrete. A major consequence of a degraded surface of a bridge deck is diffusion of water and dissolved ions in the concrete [151,152]. This can lead to corrosion of embedded steel reinforcement which is very pronounced in areas exposed to salts in the environment [153]. In order to study the beneficial impact of PCM-incorporation on the life of a bridge deck structure, it is necessary to obtain a comparative picture of the diffusion fronts of dissolved ions over a fixed duration. The forthcoming section describes a fluid diffusion model that computes a comparative assessment of the chloride resistance of both control and PCM-incorporated mortars subjected to freeze-thaw-induced damage.
3. NUMERICAL SIMULATION OF IONIC DIFFUSION IN FREEZE-THAW-DAMAGED CONCRETES

This section aims to depict the accelerated chloride diffusion in degraded concrete under freeze-thaw action. The transport behavior of chlorides is significantly affected by the void structure generated owing to freeze-thaw damage. Thus a coupled approach is adopted here that accounts for the influence of freeze-thaw-induced damage on the chloride ion diffusion at multiple length scales. Therefore, a better insight can be gained into the influence of PCMs on the life expectancy of structures from a detailed analysis of its microscale behavior. Figure 9 illustrates the coupled approach where the generated RVE is subjected to freeze-thaw-induced volume expansion and contraction resulting in mechanical damage. A remeshing module improves the mesh of the damaged/deformed structure and exports the damaged microstructure as a starting meshed geometry for the diffusion model. The damaged elements therein behave as cracks in the diffusion model which is subjected to a chloride concentration gradient. A post-processing module computes the volume averaged effective diffusion coefficient $D_e$ for each damage state.
3.1 Chloride ion diffusion in Concrete exposed to freeze-thaw cycle

Application of deicing salts (to melt snow and ice) on bridge decks and pavements results in presence of aqueous salt solution on the surface and it serves as a major source of dissolved chlorides which diffuse into the concrete structure thereby accelerating the damage. The chloride diffusivity of highly heterogeneous porous materials like cementitious composites strongly depends on the void-distribution in the microstructure and it is characterized by the diffusion coefficient which can be correlated with the properties of cement paste matrix and ITZ assuming impermeable aggregates [135]. Freeze-thaw cycle-induced damage causes an increased porosity in the microstructure that in turn accelerates chloride diffusion. Fick’s law expresses the flux of chlorides \( J \) as shown in Equation 7 [135].

\[
J = -D_k \nabla C
\]  

[2-7]

Where the Laplace differential operator \( \nabla \) operates on \( C \) (concentration of chlorides), and the diffusion coefficient of \( k^{th} \) phase (here: aggregate, ITZ and HCP) is denoted by \( D_k \). A necessary condition for mass conservation is given as [135]

\[
\frac{\partial C}{\partial t} = -\nabla J
\]  

[2-8]

Where \( t \) is the diffusion time. Equation 8 implies no accumulation of chlorides which has been reported to be the case with deicing salt application [132]. Combining the Equations 7 and 8, the following equation is obtained.

\[
\frac{\partial C}{\partial t} = D_k \nabla^2 C
\]  

[2-9]

Equation 9 relates the contribution of individual components in a heterogeneous material to chloride diffusion with time. Thus, the whole model establishes a quantitative relationship between
porosity and chloride diffusion by a nonlinear diffusion coefficient assigned to each phase of a random microstructure. Moreover, the coupled approach with frost-induced damage and chloride diffusion (see Figure 9) ensures an interactive framework of quantitative characterization of durability. The interaction is achieved by proportionally increasing the diffusion coefficient of the damaged elements in tandem with the progress of mechanical damage. The proportional increase of intrinsic diffusion coefficient of the damaged elements with the progressive damage $D$ is defined in Equation 10.

$$D_{det} = D_{cr} \cdot D$$

Where $D_{det}$ is the diffusion coefficient of the damaged element and $D_{cr}$ is the diffusion coefficient of a crack (implying damage state 1) and $D$ is the progressive damage variable. Such proportional intrinsic properties has been successfully assigned to degraded materials for electromechanical [136] and thermomechanical [154] analysis.

### 3.1.1 Model specifications and FE implementation

The deformed configuration (Figure 6) obtained from the mechanical FE analysis is re-meshed ensuring a good quality of elements (aspect ratio $\leq 3$). Thereafter, the re-meshed geometry is used for the diffusion FE analysis. The microstructure generated in Section 2.3 has circular aggregates which is sufficient for analysis since shape of aggregates has been shown to not impact diffusion [155,156]. The width of ITZ is 20 $\mu$m as mentioned earlier. A FE analysis of diffusion is carried out in ABAQUS™ solver using DCC2D4 elements. A differential concentration of 0.1 mol/m$^3$ is applied across the faces of the unit cell perpendicular to Y direction while the faces along X are impermeable. Application of deicing salts leads to a surface chloride concentration of around 3.5 kg/m$^3$ [132] which is 0.1 mol/m$^3$ as adopted in the paper. The initial condition of the model has a zero concentration gradient across the faces along x and y axis. The diffusion coefficient of HCP matrix $D_{cp}$ is taken to be $1.2 \times 10^{-12}$ m$^2$/s while that of aggregates is zero [157]. Since ITZ is porous, it has a higher diffusion coefficient than the matrix paste. In this study, the diffusion coefficient of ITZ is considered six times that of HCP that yields an apparent diffusion coefficient across the single element thick ITZ equaling thirty times that of HCP, as reported in [133].The diffusion model, adopted here, assumes isothermal conditions. With the progress of freeze-thaw-induced isotropic damage, the value of diffusion coefficient for completely damaged elements ($D = 1$) is assumed to reach a realistically possible high value implying that the chloride ions can readily diffuse through such elements. A sufficiently high value of $D_{cr} = 50,000$ times the $D_{cp}$ is adopted for the damaged matrix elements towards that end [133]. A post processing module computes the
volume averaged chloride surface concentration with time from ABAQUS™ solver to yield the apparent diffusion coefficient.

3.1.2 Accelerated chloride diffusion in frost-damaged microstructures

Figure 10 shows the chloride ingress with the progress of freeze-thaw induced damage for control mortar (Figure 10(a)) and PCM-incorporated mortar (Figure 10(b)). In both the cases, the chloride ingress progresses with time which is accelerated due to frost induced damage. While Figures 10(a-1) and 10(b-1) show the initial states for control and PCM-incorporated mortars respectively where there is no chloride ingress, the Figures 10(a-2) and 10(b-2) correspond to first 20 days of exposure in January 2018. Figures 10(a-3) and (b-3) correspond to 31 days of exposure for control and PCM modified concrete respectively. Overall, the extent of penetration and the rate of chloride diffusion is significantly reduced when PCMs are incorporated establishing the effectiveness of PCMs to improve the durability of mortars. The effective diffusion coefficient obtained at the mortar scale is used as a matrix input property in the concrete scale. A numerical homogenization yields the effective diffusion coefficient in the concrete scale where the impermeable coarse aggregates are dispersed in the mortar matrix. Implication of these results on the expected life of structures is explored in detail later in this paper.
Figure 2-10 Frost damage-induced chloride concentration distribution for: (a) control mortar: (a-1) initial geometry; (a-2) Day 20; (a-3) Day 31, (b) PCM-incorporated mortar: (b-1) initial geometry; (b-2) Day 20; (b-3) Day 31

The accelerated diffusion behavior obtained for the control concrete is expressed as a ratio of degraded diffusion coefficient ($D_e$) to the initial diffusion coefficient $D_0$ and is validated with experimental results [134] as shown in Figure 11. The values show close correlation thereby validating the framework of chloride diffusion in frost-damaged concrete.

Figure 2-11 Validation of accelerated diffusion analysis results with experimental results adopted from [134]
3.2 Influence of PCMs on chloride ion diffusivity of freeze-thaw-exposed concrete

The validated framework is used to quantify the chloride diffusion in the micro and meso-scales for both the PCM incorporated and control cases. Figures 12(a) and (b) show the relative performance in terms of the ratio of the accelerated apparent diffusion coefficient ($D_e$) to the initial diffusion coefficient ($D_0$) for control and PCM-incorporated cases at micro and meso-scales respectively for the same duration of January 2018 in Providence, RI. Due to the similarity in stiffness degradation up to Day 8, the accelerated diffusion ratio is similar for both the cases. However, for the rest of the duration, PCM incorporated materials show a vastly improved chloride resistance. Overall, for both mortar (Figure 12(a)) and concrete (Figure 12(b)), the PCM incorporated composite shows a significant decrease in diffusion coefficient and superior chloride resistance as compared to control cases pointing to improved durability against freeze-thaw cycles when PCMs are incorporated.

![Figure 12](image1.png)

Figure 12 - Relative ratios of accelerated apparent diffusion coefficient ($D_e$) to initial diffusion coefficient ($D_0$) during January 2018 for (a) mortars and (b) concretes

The forthcoming section uses the accelerated diffusion behavior to obtain a comparative probabilistic failure analysis of PCM incorporated and control RC decks with time.

3.3 Probabilistic modeling of lifetime distribution

This section presents a probabilistic comparative analysis of the freeze-thaw and chloride diffusion-induced deterioration in RC bridge decks due to the vastly different chloride diffusive behavior shown by PCM-incorporated concrete and control concrete. In RC structures such as a bridge deck, chloride ingress is often the cause of reinforcement corrosion which otherwise stays passive embedded in the alkaline concrete. Once the chloride concentration exceeds a threshold value at the surface of the reinforcement, it destroys the protective passive layer causing catastrophic
degradation of the embedded reinforcement and thus its strength. Chloride ingress is accelerated due to material degradation that forms cracks on the surface. These provide an easy pathway for chloride diffusion across the concrete cover especially in frost deteriorated bridge decks. When deicing salts are applied on the surface of concrete decks, the chloride content $C(x, t)$ at a depth $x$ and time $t$ is can be defined as shown in Equation 11 [132].

$$C(x, t) = C_0[1 - \text{erf}(\frac{x}{\sqrt{2Dt}})]$$ \[2-11\]

Where $C_0$ is the surface chloride content, $D$ is the apparent chloride diffusion coefficient and erf is the error function. This model is based on the observation that no chlorides accumulate with time [158]. The critical chloride concentration at the surface of the reinforcement is assumed to be 1 kg/m$^3$ and the concrete cover to be 50 mm [132]. The statistical parameter $C_0$ follows a lognormal distribution with a mean of 3.5 kg/m$^3$ and coefficient of variation 0.5 [132]. The apparent diffusion coefficient is characterized with time as shown in Equation 12 [159].

$$D = D_0t^\alpha$$ \[2-12\]

Where $D_0$ is taken to be $2\times10^{-12}$ m$^2$/s [132] and the time coefficient $\alpha$ is determined from the variation of diffusion coefficient with time mentioned in Section 3.2 (Figure 12). The limit state function is bounded by the critical chloride concentration $C_{cr}$ as shown in Equation 13.

$$g(x, t) = C_{cr} - C(x, t)$$ \[2-13\]

The probability for chloride concentration at reinforcement to be less than the critical chloride reinforcement is computed following first order reliability method. This procedure involves definition of an appropriate limit state equation (here Equation 13 is used as limit state equation). A safety index $\beta$ governs the termination of the iterative procedure at a predetermined tolerance level (which is 0.001 [160] in this case). The iterative procedure proceeds with the computation of the random variable at every step as per Equation 14 [160].

$$x_i^* = \mu_{X_i}^N - \alpha_{X_i}^N\beta\sigma_{X_i}^N$$ \[2-14\]

Where $x_i^*$ is the design point (for $i=1,2,\ldots,n$) for the non-normal variable; $\mu_{X_i}^N$ and $\sigma_{X_i}^N$ are the mean and standard deviation for the equivalent standard normal variable $X_i$; $\alpha_{X_i}^N$ is the direction cosine at design point $x_i^*$ as shown in Equation 15.
\[
\alpha_{X_i} = \frac{\left(\frac{\partial g}{\partial X_i}\sigma_{X_i}^{N}\right)}{\sqrt{\sum_{i=1}^{N}\left(\frac{\partial g}{\partial X_i}\sigma_{X_i}^{N}\right)^2}}
\]  

[2-15]

The probability of failure \(P_f\) is obtained from \(\beta\) as per Equation 16.

\[
P_f = \varphi(-\beta)
\]  

[2-16]

Where \(\varphi\) is the normal cumulative distribution function defined for any variable \(p\) in Equation 17 [160].

\[
\varphi(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{p} e^{-t^2/2} dt
\]  

[2-17]

The probabilistic model is implemented in a MATLAB© script that incorporates a parametric variation of \(\alpha\) which has a value of 0.41 for control concrete and 0.23 for PCM incorporated concrete as obtained from regression analysis by fitting the relationships shown in Figure 12(b) to Equation 12. The parameter \(\alpha\) essentially captures the accelerated diffusion due to progressive freeze-thaw damage in control and PCM incorporated concrete. Figure 13 reports the cumulative probability of failure for both control and PCM incorporated concrete bridge deck cases. As observed in Figure 13, the probability of failure due to chloride ingress in frost-damaged RC deck is significantly lower in case of PCM incorporated concrete than control concrete and the efficiency increases progressively with increase in time. This comparative analysis depicts a conservative scenario where the same amounts of deicing salts are used for both cases. In a practical scenario, the lifetime of the PCM incorporated RC structure will be significantly enhanced owing to a reduced frequency of deicing salt demand. The numerical approach followed in this study explains a holistic gain in durability of the structure resulting from the improved freeze-thaw resistance of PCM incorporated cementitious materials. The reduced number of freeze-thaw cycles helps to maintain the integrity of the structure which in turn enhances its chloride resistance over its life span.
CONCLUSIONS

This paper presents a detailed evaluation of the effectiveness of microencapsulated PCM-incorporation in concrete bridge decks subjected to combined freeze-thaw and chloride ingress-induced deterioration. The evaluation is performed using a multiscale-numerical approach. A macro-scale bridge deck model predicts the surface temperature profiles for the month of January 2018 in Providence, RI based on solar radiation and ambient temperature. The model inputs effective material properties obtained by FE-based numerical homogenization of the inherent material properties of each component phases of the heterogeneous cementitious material at micro and meso scales establishing an efficient micro-macro relationship. A comparative analysis is drawn up between the control concrete and PCM-incorporated concrete with PCM replacing 20% of sand by volume. Consequently, the latent heat released by the PCMs reduces the number of freeze-thaw cycles as depicted by the surface temperature profile from the macroscale deck model. For the month of January 2018 in Providence, the PCM incorporated concrete shows a 70% reduction in the number of freeze thaw cycles which establishes the potential of its application. To obtain a holistic picture of the benefits of improved freeze-thaw resistance of PCM modified concrete, a microstructure guided approach is implemented to characterize the frost-induced deterioration and resulting chloride ingress in both the mortars as well as concretes. A mortar-scale model captures the damage induced due to freeze-thaw cycles in the cement paste matrix using a progressive continuum damage model initiated by the volume expansion of the freezing pore solution. Hereafter, a mass diffusion model quantifies the diffusivity of chlorides in the degraded matrix using Fick’s law of diffusion. The combined approach allows a detailed insight into the mutually dependent phenomena of freeze-thaw damage and chloride ingress. The reduced stiffness

Figure 2.13 Cumulative probability distribution of failure due to chloride ingress in frost damaged RC deck

4. CONCLUSIONS

This paper presents a detailed evaluation of the effectiveness of microencapsulated PCM-incorporation in concrete bridge decks subjected to combined freeze-thaw and chloride ingress-induced deterioration. The evaluation is performed using a multiscale-numerical approach. A macro-scale bridge deck model predicts the surface temperature profiles for the month of January 2018 in Providence, RI based on solar radiation and ambient temperature. The model inputs effective material properties obtained by FE-based numerical homogenization of the inherent material properties of each component phases of the heterogeneous cementitious material at micro and meso scales establishing an efficient micro-macro relationship. A comparative analysis is drawn up between the control concrete and PCM-incorporated concrete with PCM replacing 20% of sand by volume. Consequently, the latent heat released by the PCMs reduces the number of freeze-thaw cycles as depicted by the surface temperature profile from the macroscale deck model. For the month of January 2018 in Providence, the PCM incorporated concrete shows a 70% reduction in the number of freeze thaw cycles which establishes the potential of its application. To obtain a holistic picture of the benefits of improved freeze-thaw resistance of PCM modified concrete, a microstructure guided approach is implemented to characterize the frost-induced deterioration and resulting chloride ingress in both the mortars as well as concretes. A mortar-scale model captures the damage induced due to freeze-thaw cycles in the cement paste matrix using a progressive continuum damage model initiated by the volume expansion of the freezing pore solution. Hereafter, a mass diffusion model quantifies the diffusivity of chlorides in the degraded matrix using Fick’s law of diffusion. The combined approach allows a detailed insight into the mutually dependent phenomena of freeze-thaw damage and chloride ingress. The reduced stiffness
and accelerated diffusivity thus obtained in the mortar scale are scaled up to obtain the behavior of corresponding concretes. Finally, a comparison is depicted between the PCM-modified concrete and the control concrete in terms of the life of a RC deck subjected to freeze-thaw-induced damage and chloride ingress. Owing to the vastly reduced chloride ingress in the concrete cover of RC decks made from PCM-incorporated concrete, a significant improvement in its survival probability is observed for PCM-incorporated concrete deck as compared to control one. Thus the beneficial impact of PCM incorporation in concretes in terms of the frost-resistance advocates its use in concrete bridge decks. Moreover, the framework presented in the paper enables modification of material properties at different length scales for optimized performance of such durable concretes.
Chapter 3

Enhancement of fracture response of cementitious materials using metallic particulate reinforcement

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Fracture response of metallic particulate-reinforced cementitious composites: Insights from experiments and multiscale numerical simulations

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Finite element method

ABSTRACT

This paper presents an experimental and numerical investigation into the fracture response of mortars containing up to 30\% waste iron powder by volume as OPC-replacement. The iron powder-modified mortars demonstrate significantly improved strength and fracture properties as compared to the control mortars due to presence of elongated iron particulates in the powder. With a view to develop a predictive tool towards materials design of such particulate-reinforced systems, fracture responses of iron powder-modified mortars are simulated using a multiscale numerical approach. The approach implements multi-scale numerical homogenization involving cohesive zone-based damage at the matrix-inclusion interface and isotropic damage in the matrix to obtain composite constitutive response and fracture energy. Consequently, these results serve as input to macro-scale XFEM-based three-point bend simulations of notched mortar beams. The simulated macroscopic fracture behavior exhibit excellent match with the experimental results. Thus, the numerical approach links the material microstructure to macroscopic fracture parameters facilitating microstructure-guided material design.
1. INTRODUCTION

Concrete, being one of the most versatile building materials, is widely used all over the world. One of the major causes of concern related to manufacturing of cement is its poor sustainability credentials [161,162]. Manufacturing process of cement is considered to be a major contributor to global CO$_2$-emissions [163,164]. On the other hand, another concern regarding the use of cementitious materials has been their inherent brittleness and poor fracture resistance [165,166]. The central idea of this paper stems from addressing the above-mentioned concerns towards obtaining a material that reduces CO$_2$-emissions as well as provides improved resistance to crack growth and developing a numerical tool to design such materials comprehensively.

Several modified and alternative cementitious materials such as supplementary cementitious materials [20,21], alkali-activated binders [22–24], and carbon-negative binders [25–27] have been widely studied over the past few decades to improve sustainability credentials of concrete. On the other hand, several particulate reinforced composites have shown improved toughness [167,168]. Applications of carbon based nano-particles in polymer matrices [169–172], oxides or nitrides in metal matrix composites [173,174], metallic particles in ceramics [175,176] and nano-clay in polymers [177,178] have served as particulate reinforcements with beneficial fracture properties. The fracture behavior of brittle matrices has shown significant improvements when rigid inclusions are incorporated [179,180]. The issue of poor fracture response of quasi-brittle cementitious composites has been addressed incorporating steel fibers [28,29], glass fibers [30,31], carbon fibers [32,33], wollastonite [34,35], and textile reinforcement [36,37] in the cementitious matrix. Use of metallic waste particle-incorporation in heavy concrete has also been experimentally evaluated [181–183]. This paper incorporates waste iron powder as cement-replacement to address the concern related to poor sustainability credentials of cementitious materials by replacing cement partially thereby reducing the carbon-footprint of concrete. This waste iron powder is an industrial byproduct and it is generated in large quantities in electric-arc furnace (EAF) steel production facilities and shot-blasting operations of structural steel sections. Traditionally, this waste iron powder is landfilled since it is not economically feasible to recycle such waste materials. Several million tons of such waste product is being landfilled all over the world. Hence, use of such waste material in concrete as large volume cement-replacement would provide significant environmental benefit. In addition to the potential sustainability benefit, the elongated iron particulates in iron powder [27,38,39] are likely to contribute towards improved crack-bridging mechanism and enhanced fracture response of mortars which are explored in detail in this study using three-point-bend test on notched mortar beams coupled with digital image correlation (DIC) [27,184–186].
Another important aspect of this study is to develop a predictive tool towards the material design of such inclusion-modified cementitious systems. Accurate prediction of constitutive relationship and fracture response in these systems necessitates a reliable technique that is capable of handling more than just the volume fraction of component phases. The effective properties of cementitious materials have been predicted using various analytical homogenization techniques [187–189]. Presence of closed form solutions and ease of analysis make these techniques very popular. However, these techniques are incapable to predict the post-peak response in many cases and are proved to be insufficient when dealing with phases with significant contrast in stiffness [100,190]. In recent past, computational techniques have been implemented [100,101,191,192] for improved accuracy. Lattice approach involving discrete elements have been used for meso-scale simulations [193,194]. However, applicability of such technique is limited when large deformations are considered [194,195]. Finite element method has been proved to be very efficient under such scenario [195].

Herein, exploiting the superiority of finite element methods [195], we implement a multiscale numerical framework to predict the fracture-response of iron-powder incorporated mortars. Numerical homogenization is performed at two different interactive length-scales to obtain effective constitutive response and fracture energy of iron powder-incorporated mortars. The numerical homogenization approach incorporates interfacial debonding at the matrix-inclusion interface using cohesive zone model (CZM) [196–198] and implements isotropic damage [96,97,130] in the matrix to simulate the composite post-peak response. In order to validate the multiscale numerical approach, macro-scale simulations for three-point-bend test of notched mortar beams are performed using extended finite element method (XFEM). The macro-model imports composite material properties obtained from multi-scale numerical homogenization as input, incorporates a maximum principal stress-based crack initiation criteria and a bilinear traction separation law coupled with concrete damage plasticity (CDP) [199–201] for propagation of crack to obtain macro-scale fracture parameters which are validated against experimental values obtained from DIC. Overall, the present study intends to investigate the influence of iron powder incorporation in the mortars as cement-replacement and demonstrate a multi-scale numerical approach to predict macroscopic fracture response of such cementitious composites facilitating microstructure-guided material design.
2. EXPERIMENTAL PROGRAM

2.1 Materials and mixture proportions

The cement used for the experiments on mortar is commercially available Type I/II ordinary Portland cement. The chemical composition of the oxides of each element in the aforementioned OPC conforming to ASTM C150 is mentioned in Table 1.

<table>
<thead>
<tr>
<th>Element</th>
<th>Si</th>
<th>Al</th>
<th>Fe</th>
<th>Ca</th>
<th>Mg</th>
<th>S</th>
<th>Na</th>
<th>K</th>
<th>Others</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxide%</td>
<td>21</td>
<td>3.61</td>
<td>3.47</td>
<td>63</td>
<td>3.26</td>
<td>3.04</td>
<td>0.16</td>
<td>0.36</td>
<td>2.13</td>
</tr>
</tbody>
</table>

Metallic waste iron powder is obtained from industrial shot-blasting facility in Phoenix, AZ. The iron powder consists of 88% Fe and atmospheric oxidation introduces 10% oxygen into it. Traces of Cu, Mn and Ca are also present. The sand used in the mortar has a $d_{50}$ of 600 µm while that of iron powder is 19 µm. The particle size distributions of OPC, sand and iron powder, obtained from laser diffraction analysis, are shown in Figure 1.

![Particle size distribution of OPC, Iron powder and sand.](image)

Four different mortar mixtures were prepared with by replacing 0% (control mortar), 10%, 20%, and 30% of OPC by volume. Other mix design parameters for all the mortars were similar with a mass-based water-cement ratio of 0.5 and a constant sand volume of 50% in the mortar. This study does not consider iron powder content higher than 30% as cement-replacement since the mixtures with iron powder content higher than 30% do not show desirable rheological properties. While the flexural strength tests used four replicate prismatic beams of size 250 (length) x 50 (width) x 50
(depth) mm for each mixture, four replicate notched beams of size 330 (length) x 25 (width) x 76 (depth) mm were used for each mixture to evaluate fracture response. For compressive strength test, 50 mm cubes were cast. All the beams and cubes were cast and were demolded after 24 hours followed by exposure to a moist environment with RH > 98% at a temperature of 23±2 °C for curing till the desired age of testing. For micro-structural examination, companion paste samples (iron powder in cement paste) were cast for each of the mixtures.

2.2 Compressive and Flexural Strength Evaluation

The 28-day compressive strengths were determined according to ASTM C109 and the flexural strengths were obtained after 28 days according to ASTM C293/C293M-10. The three-point-bend specimens of size 250 x 50 x 50 mm were supported with a span of 200 mm and were centrally loaded at a constant displacement rate of 0.004 mm/s.

2.3 Three-point bend test coupled with Digital Image Correlation (DIC) for evaluation of fracture behavior

For evaluation of fracture behavior, three-point-bend tests were performed on notched mortar beams of size 330 (length) x 76 (depth) x 25 mm (width) with a span of 304 mm and notch depth of 19 mm as shown in Figure 2. For each mixture, four replicate beam specimens were tested. A closed loop testing machine was employed under crack mouth opening displacement (CMOD)-controlled mode where the CMOD was measured by a clip gauge. An initial load control mode was first employed up to a load of 100 N beyond which CMOD-controlled mode was initiated. A CMOD value of 0.2 mm marked the termination point of the test. The above-mentioned three-point-bend test was coupled with digital image correlation (DIC) method for direct measurement of crack length and fracture properties. DIC is a speckle-tracking non-contact method to obtain displacement and strain fields on the specimen surface [27,185,186,202,203]. The surfaces of the specimens were first painted white and then random black speckles were made on the white surface using a black spray-paint to achieve a good contrast. During the test, the specimen surface was imaged every 5 seconds by a charge-coupled device camera (CCD). After the test, the images were correlated and a rectangular area of 120 x 60 mm above the notch (as shown in Figure 2) was analyzed to obtain the displacement fields using VIC-2D software™ [204]. The displacement fields, thus obtained from DIC, were used to obtain the fracture properties (fracture toughness and critical crack tip opening displacement) as detailed later in this paper.
2.4 Scanning Electron Microscopy

The companion paste samples with different dosage of iron powder were subjected to a microstructural evaluation. Small rectangular pieces (10 × 10 mm in size) were cut from the core of paste specimens using a diamond saw. Prior to polishing, the cut pieces were cleaned ultrasonically to remove the debris. Afterwards, the sample was impregnated in epoxy and vacuum-saturated followed by overnight curing. Several grinding/polishing steps were performed using SiC abrasives and finally the sample was polished using 0.04 µm colloidal silica suspension. The polished samples were imaged using Philips XL30 field emission environmental scanning electron microscope (FESEM) under backscattered mode for microstructural evaluations.

3. EXPERIMENTAL RESULTS AND DISCUSSIONS

This section presents the experimental observation of the influence of iron powder on the strength and fracture response of mortars. Flexural response of prismatic beams are used in an inverse analysis procedure to obtain uniaxial tensile behavior of mortars. While the flexural response of the prismatic beams and the extracted tensile parameters serve as input to the multiscale numerical model for prediction of fracture response of particulate-reinforced mortars, the fracture response obtained from notched beams are used to validate the findings from the numerical simulations as explained later in this paper.

3.1 Material Microstructure

The companion paste samples were subjected to microstructural analysis after 28 days of hydration. Such an analysis provides a deeper insight into the distribution of iron particulates. Figure 3 shows representative micrographs for the mortar containing 30% iron powder as cement-replacement. Distribution of bright (owing to higher density) elongated iron particulates are clearly visible in the backdrop of the gray phases indicating the reaction products and the black areas indicating pores in the BSE image. The elongated iron particles are likely to play a role in improving the fracture
performance by crack bridging/deflection mechanisms as explored in the forthcoming section. Some matrix cracks can be observed which are a result of sample preparation. An image analysis of several BSE images yielded an average aspect ratio of 12 for the elongated iron particles which is used later in this paper in the generation of representative unit cells for the microstructural analysis.

![Figure 3](image_url)

**3.2 Influence of particulate-reinforcement on compressive and flexural strength**

The compressive strengths of all the mixtures are found to be similar (38 ± 2.4 MPa) irrespective of volume fraction of iron powder. While the compressive strengths are similar for all the mixtures irrespective of iron powder content, a difference in flexural behavior is observed with increase in iron powder content. Figure 4(a) shows the load deflection behavior of the control and iron powder-incorporated mortars. With increasing iron powder content, the peak load and the slope of load-deflection curve increases indicating superior flexural performance and increase in Young’s modulus due to incorporation of iron powder. The flexural strengths of the specimens are shown in Figure 4(b). It is observed that the flexural strength follows an increasing trend with increasing iron powder content. A gain in flexural strength of around 15% is obtained with incorporation of 30% iron powder. This can be explained from the fact that significant amount of stress is transferred from matrix to the stiffer iron particles resulting in stress-relaxation in the matrix and increase in the flexural strength of the mortars with incorporation of iron powder. The aspect of influence of iron particles on the microstructural stress-distributions is explained using finite element analysis (FEA) later in this paper for detailed insight.
3.3 Influence of particulate-reinforcement on Flexural Fracture Response

While the previous section explained the influence of iron powder on flexural strengths, this section explains the impact of particulate reinforcement on the fracture response of mortars after 28 days of hydration. The fracture response of the mortars are characterized using Hillerborg's work-of-fracture [206,207] as well as two parameter fracture model (TPFM) [208].

3.3.1 Load-CMOD responses

The load-CMOD responses of control mortar and iron powder incorporated mortars are shown in Figure 5(a). The peak load increases with increase in the amount of iron powder included in the binder due to the reasons explained in the previous section. Additionally, the area under load-CMOD curve, which is a measure of the material toughness, increases significantly with increasing iron powder content signifying improved toughness of the material. Figure 5(b) shows the size-dependent fracture energy (\(G_{1C}\)), calculated using Hillerborg's work-of-fracture method as shown in Equation 1.

\[
G_{1C} = \frac{W_0 + 2P_w\delta_0}{(D-a_0)t}
\]  \[3-1\]

Where \(W_0\) is the area under load-CMOD curve for specimen of self-weight \(P_w\) with depth D, width t and notch height \(a_0\) that can withstand a maximum CMOD \(\delta_0\). Since similar specimens are used for each set of experiments, the otherwise size-dependent \(G_{1C}\) can be used for comparing the relative gain in performance with increasing volume fraction of iron powder. Figure 5(b) shows an increasing trend of work of fracture with increasing iron powder volume fraction indicating
improved dissipation potential. About 42% increase in fracture energy is observed with incorporation of 30% iron powder as cement-replacement. These results serve as a motivation to study the fracture behavior of such systems in more depth, as elucidated in the following subsections.

Figure 3.5 (a) Load-CMOD responses and (b) work of fracture for iron incorporated mortars with different iron powder contents

3.3.2 Application of DIC towards fracture response

This sub-section applies DIC to obtain TPFM parameters ($K_{IC}$ and $CTOD_{C}$). As explained earlier, images obtained after the test are correlated to obtain displacement field using VIC-2D software [204]. Figure 6(a) shows a schematic representation of a 3D surface plot showing the horizontal displacement field. The crack tip opening displacement (CTOD) is computed from the displacement field as displacement-jump at the tip of the notch (see Figure 6(a)). Crack-extension ($\Delta a$) is measured as the extent of the displacement-jump as shown in Figure 6(a). Displacement-jumps only above 0.005 mm were considered significant enough so as to contribute to crack extension in this study. Similar approach was successfully incorporated in [27,38,185,190,209]. The critical values of the fracture parameters $K_{IC}$ and $CTOD_{C}$ correspond to a load of 95% of the peak load in the post-peak regime. At that point of loading, $CTOD_{C}$ is directly obtained from DIC and TPFM model yields the $K_{IC}$ using Equations 2a and 2b [210].

$$K_{IC} = \frac{PL}{bd^{3/2}} F\left[\frac{a_{eff}}{d}\right]$$  \[3-2a\]
\[ F \left[ \frac{a_{\text{eff}}}{d} \right] = \left[ 2.9 \left( \frac{a_{\text{eff}}}{d} \right)^{\frac{1}{2}} - 4.6 \left( \frac{a_{\text{eff}}}{d} \right)^{\frac{3}{2}} + 21.8 \left( \frac{a_{\text{eff}}}{d} \right)^{\frac{5}{2}} - 37.6 \left( \frac{a_{\text{eff}}}{d} \right)^{\frac{7}{2}} + 38.7 \left( \frac{a_{\text{eff}}}{d} \right)^{\frac{9}{2}} \right] \]  

(3-2b)

Where the effective crack length \( a_{\text{eff}} = a_0 + \Delta a \) at the 95% of the peak load in the post-peak regime. Figure 6 (b) shows a representative digitally correlated image (for the control mortar) corresponding to 95% of the peak load in the post-peak regime for obtaining the crack-extension (\( \Delta a \)) from horizontal \( u \)-displacement fields.

Figure 3-6 (a) schematic 3D surface plot showing correlation between displacement fields and fracture parameters and (b) the experimental result obtained to calculate crack growth.

Figure 7 shows the two fracture parameters \( K_{\text{IC}} \) and \( \text{CTOD}_C \) for all the mixtures. About 36% increase in \( K_{\text{IC}} \) is observed with incorporation of 30% iron powder. As can be observed in, The elongated iron particles (see Figure 3) serve as micro-reinforcements to facilitate crack bridging that improves the fracture response of such systems drastically. \( \text{CTOD}_C \) signifies the threshold limit beyond which unstable crack propagation starts. \( \text{CTOD}_C \) also increases significantly with increase in iron powder content thus indicating improved crack resistance of iron powder-modified mortars.
3.3.4 Extraction of tensile parameters of composite mortars

While the previous sub-section elucidated the influence of iron powder inclusion on the fracture response of mortars, this section uses the load-deflection behavior obtained from prismatic beam sections (shown in Figure 4(a)) towards a moment-curvature-based inverse analysis approach [205] to extract uniaxial tensile parameters (tensile strength $f_t$, the modulus of elasticity $E$, the peak strain $\epsilon_D$ and the strain near failure $\epsilon_{tu}$) for the mortars, which are otherwise difficult to obtain experimentally. The inverse analysis approach has been successfully incorporated in [185] and is adequately detailed in [211]. Table 2 quantifies the tensile parameters as a function of iron powder content for the mortars. An increasing trend of tensile strength for mortars is observed with increasing volume fraction of iron powder which is in line with the flexural strength observations. The Young’s modulus ($E$) increases with increase in iron powder content since iron powder has a higher $E$ than the cement it replaces. The $f_t$ and $\epsilon_{tu}$ also increases with increasing iron powder content signifying the higher toughness of the particulate reinforced composites. The values of $\epsilon_D$ are fairly consistent for all the specimens. The tensile parameters, thus obtained, serve as input to multiscale numerical models for prediction of fracture response as explained in the forthcoming section.
Table 3-2. Extracted tensile parameters of mortar as a function of iron powder content

<table>
<thead>
<tr>
<th>Iron powder %</th>
<th>$f_t$ (MPa)</th>
<th>$\epsilon_{D_0}$</th>
<th>E(GPa)</th>
<th>$\epsilon_{tu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.12</td>
<td>0.00013</td>
<td>23.9</td>
<td>0.000295</td>
</tr>
<tr>
<td>10</td>
<td>3.79</td>
<td>0.00013</td>
<td>29.1</td>
<td>0.000305</td>
</tr>
<tr>
<td>20</td>
<td>4.26</td>
<td>0.00014</td>
<td>34.1</td>
<td>0.000310</td>
</tr>
<tr>
<td>30</td>
<td>4.73</td>
<td>0.00014</td>
<td>39.8</td>
<td>0.000315</td>
</tr>
</tbody>
</table>

4. MULTISCALE NUMERICAL SIMULATION

While the previous section elucidated experimental evaluation of flexural strength and fracture behavior of particulate-reinforced mortars, this section is aimed towards simulation of fracture behavior of such systems. In order to encompass the complex heterogeneity of cementitious systems that contains random microstructure at different length scales, the numerical simulation framework, presented here, performs numerical homogenization at different length scales involving continuum micromechanics so as to obtain homogenized constitutive behavior of the material that serves as input to macro-scale model. Such an approach involves representation of the geometrical configuration of the different phases in the form of representative volume element (RVE) at different length scales. In this study, two interactive length scales at the paste level and mortar level are used to predict the fracture behavior of the iron powder-modified mortars which is validated with the experimental observations presented earlier in this paper. The forthcoming sub-sections explain the numerical simulation approach and apply the framework towards prediction of fracture response of particulate-reinforced mortars.

4.1 Multiscale Numerical Simulation Approach for prediction of effective constitutive response and Fracture behavior

The framework aims to elucidate the influence of addition of particulate inclusions on the macroscale fracture response of inclusion modified heterogenous system. The numerical framework implements cohesive zone model (CZM)-based debonding using continuum damage approach [136,154] at the matrix-inclusion interfaces and an isotropic damage model in the matrix [97,130,154] of the RVEs towards achieving the effective constitutive response in the post-peak
regime. The effective tensile constitutive response, thus predicted, is used to simulate three-point-bend test of notched beams to obtain TPFM parameters.

4.1.1 Prediction of Effective Constitutive Response

Prediction of effective constitutive response involves generation of RVE based on known microstructural features of the material, application of appropriate boundary conditions on the RVE, meshing the RVE and application of uniaxial strain to obtain stress-response. The current study incorporates debonding at the matrix-inclusion interfaces by incorporating cohesive zero thickness interface elements and interfacial debonding is implemented using a continuum approach coupled with CZM [154]. Similar approach was successfully implemented to evaluate electromechanical response of self-sensing structural materials in [136]. The current approach also implements isotropic damage in the matrix so as to obtain the post-peak effective constitutive response of the composite. Figure 8 shows a schematic representation of the numerical homogenization approach and the forthcoming sub-sections elucidate different components of the approach.

![Schematic representation of the numerical homogenization approach](image)

**Figure 3-8** schematic representation of the numerical homogenization approach

4.1.1.1 Generation of unit cell: general schematic

The unit cells are generated here using the Lubachhevsky-Stillinger algorithm [103,104]. This algorithm employs a hard contact model and hence particle overlaps are not allowed. Finally, the obtained microstructural information is implemented via a python language script to enable it to be
imported to a commercial finite element software. The unit cell generation algorithm has been successfully implemented in [101] and adequately detailed in [136].

4.1.1.2 Boundary conditions

Once the unit cell is generated, it is meshed using the python script and periodic boundary conditions (PBC) [110,136] are applied. PBCs ensure a continuity of displacement and traction across boundaries of neighboring unit cells. PBCs have been applied successfully towards FE analysis of random heterogenous materials [106]. PBCs are shown to be computationally efficient even with smaller size of unit cells facilitating faster convergence[101]. More details on the PBC can be found in [100,102]. The meshed RVE with PBC is subjected to uniaxial tensile strain to simulate a displacement-controlled test scenario. In order to incorporate interfacial debonding and the damage-in the matrix, the numerical homogenization approach implements CZM-based damage at the interface and isotropic damage in the matrix as detailed in the forthcoming subsections.

4.1.1.3 CZM damage for interfacial debonding

Interfacial debonding is implemented here using CZM coupled with continuum damage. Here, a continuity in displacement is ensured by implementation of zero-thickness interface elements. Such zero-thickness interface elements have been implemented successfully to model relative slip or separation on a predetermined surface in [136,154]. The CZM implements Mode I fracture when the stress state reaches the tensile strength of the matrix. Traction separation law which governs the propagation of damage is characterized here using an equivalent interface opening, $\lambda$ (Equation 3(a)) and equivalent traction, $\sigma_c$ (defined in Equation 3(b)) [136,154,197].

$$\lambda = \sqrt{\langle [u_n] \rangle^2 + [u_t]^2} \quad [3-3a]$$

$$\sigma_c = \begin{cases} 
K_p \lambda, & \lambda < \lambda_0 \\
 f_t \exp \left( -\frac{f_t(\lambda - \lambda_0)}{G_F} \right), & \lambda \geq \lambda_0 
\end{cases} \quad [3-3b]$$

Where $u_n$ and $u_t$ are normal and tangential displacement jumps, $\lambda_0$ is the threshold limit [136,154] defined by $\frac{2G_f}{f_t}$ ($G_f$ is initial fracture energy) up to which the $\sigma_c$ increases with $\lambda$ with a linear coefficient $K_p$ (penalty stiffness), $f_t$ is tensile strength, $G_F$ is total fracture energy. Equivalent normal traction $t_{cn}$ and tangential traction $t_{ct}$ are obtained by partially differentiating the volume integral of $\sigma_c$ with respect to $u_n$ and $u_t$ respectively. The mechanical tangent material matrix $C_C^t$ can be expressed as partial derivatives of the resulting traction with respect to displacement jump as shown in Equation 4 [136,154].
The tangent material matrix $C_c$ is transformed to the local co-ordinate system to obtain mechanical stiffness matrix of each cohesive element. While the penalty stiffness governs the traction-separation law with increase in $\lambda$ when $\lambda < \lambda_0$, the mechanical stiffness matrix is modified at every iteration with increasing $\lambda$ based on phenomenological damage model when $\lambda \geq \lambda_0$ [154]. Here, progressive debonding has been characterized with increasing $\lambda$ using a scalar interface damage parameter $D_c$ which is defined as follows [136]:

$$D_c = \frac{\lambda}{\lambda_{cr}}$$

Where $\lambda_{cr}$ corresponds to equivalent interface opening at very low traction values in the post-peak regime of the traction-separation behavior, generally computed at 0.1 $f_t$ in the post-peak regime. The numerical simulation is implemented using user defined subroutine in ABAQUS™ and it requires initial fracture energy ($G_f$), total fracture energy ($G_F$) and tensile strength of matrix ($f_t$) as input [136,214].

### 4.1.1.4 Isotropic damage in matrix

Isotropic damage is implemented in the simulation framework to quantify the stiffness loss for a strain state beyond cracking strain ($\varepsilon_{D_0}$). Assuming isotropic stiffness degradation, the damage variable, $D$ is given as [96,97,130,136]:

$$\sigma = (1 - D) \mathbf{C} : \varepsilon$$

Where the effective stress tensor is denoted by $\sigma$, $\mathbf{C}$ denotes fourth order tensor of elasticity and $\varepsilon$ is the strain tensor. The value of damage, $D$ ranges from 0 (undamaged) to 1 (completely damaged). The damage rate denoted by $\dot{D}$ assumes only zero or positive values [82]. A non-local equivalent strain $\bar{\varepsilon}$ is used to obtain the damage, $D$ which is defined as [96].

$$\bar{\varepsilon} = \sqrt{\sum_i < \varepsilon_i >_+^2}$$

Where $< \varepsilon_i >_+$ is the positive part of the principal strain. The damage $D$ evolve as a function of $\bar{\varepsilon}$ as per the Equation 8 for uniaxial tensile strains:

$$D(\bar{\varepsilon}) = 1 - \frac{\varepsilon_{D_0}(1-A_t)}{\bar{\varepsilon}} - \frac{A_t}{\exp[B_t(\bar{\varepsilon}-\varepsilon_{D_0})]}$$
Where $\varepsilon_{D_0}$ is damage initiation threshold defined as

$$\varepsilon_{D_0} = \frac{f_t}{E} \tag{3-9}$$

Thus, the isotropic damage model requires the tensile strength ($f_t$) of the matrix and the damage propagation parameters $A_t$ and $B_t$ (see Equation 8) to fully characterize the post peak tensile constitutive response at strains exceeding $\varepsilon_{D_0}$. The isotropic damage is implemented here using user defined subroutine in ABAQUS™. The tensile constitutive response and the isotropic scalar damage variable $D$ can be used to obtain fracture energy $G_F$. Isotropic damage has been used successfully [194,215] to correlate $f_t$ and fracture energy $G_F$ for stiffer inclusions embedded in a softer matrix and the relationship is defined as shown in Equation 10 [194].

$$\left(1 - D\right)\varepsilon = \varepsilon_{D_0}\exp\left(-\frac{dbfsf_{t}}{G_F}\right) \tag{3-10}$$

Where $D$ is damage variable expressed in Equation 8, $\varepsilon$ is the strain response of the tensile constitutive relation with its value being $\varepsilon_0$ corresponding to the tensile strength $f_t$; $h$ is a mesh dependent parameter defining the mean distance between centroids of adjoining elements and $G_F$ is fracture energy. In multiscale simulations of particulate-reinforced mortars, $G_F$ obtained for microscale (inclusion modified hardened cement paste), is used as input to the CZM-damage debonding model at the matrix–inclusion interfaces in the mesoscale (mortar). Thus, the procedure explained herein, can be invoked for translating mesoscale damage to macroscale fracture energy analysis.

4.1.1.5 Post-processing and Effective Constitutive Response

The analysis is implemented using ABAQUS™ solver to obtain stress distributions, debonding status as well as isotropic damage parameter $D$ in the RVE. A post-processing module coded in MATLAB® implements a volume computation thereby yielding a volume averaged stress-strain relation thus providing the effective constitutive tensile response.

4.1.2 Upscaling to macro-scale Fracture Response

The effective constitutive tensile response as well as the fracture energy, mentioned in the previous sub-section, is obtained at different length scales to finally provide input to a macro-scale analysis of three-point-bend test on notched beams. The macro-scale simulation is performed using extended finite element method (XFEM) which incorporates a maximum principal stress-based damage initiation criteria and a bilinear traction-separation law coupled with a damage plasticity model for propagation of damage.
The XFEM-based damage model initiates damage if the maximum principal stress exceeds the tensile strength. A bilinear traction-separation law [214] coupled with concrete damage plasticity model [200] is used for damage propagation. In this model, isotropic damage is represented as:

\[
\mathbf{\sigma} = (1 - d) \mathbf{D}_0^{el} : (\mathbf{\varepsilon} - \mathbf{\varepsilon}^{pl}) = \mathbf{D}_0^{el} : (\mathbf{\varepsilon} - \mathbf{\varepsilon}^{pl})
\]  \[3-11\]

where \( \mathbf{\sigma} \) is the Cauchy stress tensor, \( d \) is the scalar stiffness degradation variable, \( \mathbf{\varepsilon} \) is the strain tensor, \( \mathbf{\varepsilon}^{pl} \) is the plastic strain, \( \mathbf{D}_0^{el} \) is the initial elastic stiffness of the material, and \( \mathbf{D}_0^{el} \) is the degraded elastic stiffness tensor. The effective stress tensor \( \mathbf{\bar{\sigma}} \) is given as:

\[
\mathbf{\bar{\sigma}} = \mathbf{D}_0^{el} : (\mathbf{\varepsilon} - \mathbf{\varepsilon}^{pl})
\]  \[3-12\]

The plastic flow is given as [200]:

\[
\dot{\mathbf{\varepsilon}}^{pl} = \dot{\lambda} \frac{\partial G(\mathbf{\bar{\sigma}})}{\partial \mathbf{\bar{\sigma}}}
\]  \[3-13\]

where, the flow potential, \( G \) is given using a Drucker-Prager hyperbolic function as:

\[
G = \sqrt{(f_c - m f_t \tan \beta)^2 + p^2} - \rho \tan \beta - \sigma
\]  \[3-14\]

Here, \( f_t \) is the tensile strength and \( f_c \) is the compressive strength, \( \beta \) is the dilation angle and \( m \) is the eccentricity of the plastic potential surface, \( p \) is the effective hydrostatic stress and \( q \) is the Mises equivalent effective stress. The CDP model uses a yield condition based on loading function:

\[
F = \frac{1}{1 - \alpha} (q - 3 \alpha p + \theta(\mathbf{\varepsilon}^{pl}) \langle \mathbf{\bar{\sigma}}_{max} \rangle - \gamma(-\mathbf{\bar{\sigma}}_{max}) - \mathbf{\sigma}, (\mathbf{\varepsilon}^{pl}))
\]  \[3-15\]

where the function \( \theta(\mathbf{\varepsilon}^{pl}) \) is given as:

\[
\theta(\mathbf{\varepsilon}^{pl}) = \frac{\bar{\sigma}_c(\mathbf{\varepsilon}^{pl})}{\bar{\sigma}_t(\mathbf{\varepsilon}^{pl})} (1 - \alpha) - (1 + \alpha)
\]  \[3-16\]

The parameter \( \alpha \), a function of biaxial compressive strength \( (f_{b0}) \) and uniaxial compressive strength \( (f_c) \), is defined as follows:

\[
\alpha = \frac{(f_{b0}/f_c) - 1}{2(f_{b0}/f_c) - 1}
\]  \[3-17\]
The CDP model [200,201] requires input parameters $\beta$, $m$, $\gamma$ (determines the shape of the loading surface in deviatoric plane) and $\alpha$. To calculate fracture toughness $K_{IC}$, the crack-extension values, obtained from simulations at 95% peak load in the post-peak regime are used. Using the simulated crack-extension values $K_{IC}$ can be calculated using Equations 2(a) and 2(b) as explained earlier in this paper. While $K_{IC}$ can be obtained from Equation 2, CTOD$_C$ can be computed directly from the XFEM simulations as the horizontal displacement at the tip of the notch. Thus, the numerical simulation approach, presented here, links different interactive length-scales and obtains macro-scale fracture response facilitating microstructure-guided material design towards improved toughness. The forthcoming section elucidates application of the multiscale numerical simulation approach towards prediction of macro-scale fracture parameters of iron powder-modified mortars.

4.2 Multiscale Numerical Simulation of fracture response in particulate-reinforced mortars

The numerical simulation of fracture response in particulate-reinforced mortars involves three interactive length scales at the cement paste scale, mortar scale and macro-scale (simulation of three-point-bend test) as shown in Figure 9 for a representative mixture containing 10% iron powder. The constitutive response and fracture energy obtained for particulate-reinforced hardened cement paste (Figure 9(a)) are assigned as the matrix property in the mesoscale containing the homogenized matrix and sand particles (Figure 9(b)). The constitutive response and fracture energy extracted from mesoscale are used towards XFEM simulation (Figure 9(c)) of three-point-bend test of notched beams to obtain $K_{IC}$ and CTOD$_C$. Although the numerical simulation is performed for the control mixture as well as all the mixtures with different dosage of iron powder, the generated micrographs and matrix/interface damage are shown for a representative simulation of the mixture containing 10% iron powder. The results are plotted for all the mixtures for a comparative evaluation.
Figure 3-9 Interactive length scales representing the (a) micro-scale HCP with 10% iron powder; (b) meso-scale mortar with sand embedded in modified HCP (c) macro-scale mortar TPB notched beam

Implementation of interface damage and isotropic damage in the matrix requires inputs such as fracture energy and isotropic damage model parameters, as explained earlier in this paper. While the these parameters for hardened cement paste are available in the literature [131], the parameters for inclusion-modified matrices are not readily available. The numerical simulation approach, presented in this paper, uses the macro-scale tensile parameters of inclusion-modified mortars, extracted from the flexural response of the prismatic beams, as input to the multiscale numerical model to determine the parameters for isotropic damage model for iron-powder modified HCP (see Figure 9(a)). In this paper, the properties of the interface elements are assumed to be similar to those of the matrix owing to lack of data. Similar methodology was successfully adopted in [136,216]. Although the numerical simulation approach presented in this paper can incorporate 3D unit cells, here 2D unit cells are incorporated as a trade-off between computational efficiency and demand. 2D unit cells have been successfully implemented to evaluate damage in quasi-brittle materials in [136,217]. In order to determine the representative size of unit cells, a sensitivity study was performed and the representative size of the unit cells at different length scales are shown in Figure 9. Sizes of unit cells beyond these adopted edge lengths resulted in insignificant change in the constitutive response. Median size of inclusions, reported in Section 2.1, are adopted for numerical simulation. As can be observed from the microstructure in Figure 3, the shape of the iron
particulates in the powder are mostly elongated. Microstructural image analysis on several BSE micrographs yields an average aspect ratio of 12 which is used as a reference for generating iron particulate inclusions in the micro-scale. The following sub-sections elucidate the parameter identification for interface damage/isotropic damage model for the iron powder incorporated HCP, perform numerical homogenization at two different length scales and implement macro-scale XFEM analysis of three-point-bend test to obtain TPFM parameters of the particulate-reinforced mortars.

4.2.1 Material Properties for Numerical simulation and Parameter identification for interface damage/isotropic damage model

Damage model parameters ($f_t$, $\varepsilon_{D_0}$, $A_t$, $B_t$ and $G_F$) for iron powder-modified HCP are tuned in a way so that the simulated tensile constitutive response for particulate-reinforced mortars matches with the experimental tensile constitutive response, obtained through inverse analysis from flexural response of prismatic beam sections as explained in the Section 3.3.4. The identified parameters for all the mixtures are reported in Table 3. The parameters identified for the control HCP correlates well with the values reported in [96,131], thus validating the parameter identification approach presented here. The Young’s modulus for HCP, sand and iron particulates are considered 20 GPa, 70 GPa and 200 GPa [101,136]. A constant Poisson’s ratio of 0.2 is used for all the simulations presented in this paper since variation of Poisson’s ratio in the range of 0.17-0.22 has been shown to result in insignificant changes in the results [106,218]. $G_t$ is assumed to be 0.6 times that of $G_F$. Similar value of $G_t$ with respect to $G_F$ has been successfully implemented for quasi brittle materials in [207].

Table 3 - Material properties and parameters for iron powder modified HCP

<table>
<thead>
<tr>
<th>Iron Powder %</th>
<th>$f_t$ (MPa)</th>
<th>$\varepsilon_{D_0}$</th>
<th>$A_t$</th>
<th>$B_t(10^4)$</th>
<th>$G_F$ (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Micro-scale</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(HCP-iron powder composite)</td>
<td>0</td>
<td>1.78</td>
<td>0.000100</td>
<td>0.98</td>
<td>1.15</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.16</td>
<td>0.000105</td>
<td>0.99</td>
<td>1.18</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>2.43</td>
<td>0.000110</td>
<td>1.00</td>
<td>1.21</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>2.7</td>
<td>0.000115</td>
<td>1.01</td>
<td>1.24</td>
</tr>
</tbody>
</table>
4.2.2 Multi-scale effective constitutive response

This section reports the multiscale numerical homogenization results. First, numerical homogenization is performed in micro-scale (refer to Figure 9(a)). The meshed unit cell, shown in Figure 9(a) is subjected to periodic boundary conditions and a uniaxial tensile strain along X direction as explained earlier in this paper. The fracture energy and the isotropic damage parameters, reported for control HCP in Table 3 are adopted since the matrix remains same (HCP with same mass-based water-to-cement ratio of 0.5) irrespective of the dosage of iron powder. The analysis is performed using ABAQUS™ solver and the simulation yields progressive interface damage and damage in the matrix as shown in Figure 10.

Figure 10 Progressive interface damage and damage in iron particulate-reinforced HCP containing 10% iron powder for applied strain of (a) 0% (undeformed), (b) 0.004%, (c) 0.0106% and (d) 0.012%.

While Figure 10(a) correspond to undeformed configuration (no applied strain), Figures 10(b), (c) and (d) correspond to applied uniaxial strain of 0.004%, 0.0106% and 0.012% respectively. Interfacial debonding sets in at a strain lower than the peak strain and it keeps on propagating resulting in progressive increase in stress in the matrix. The debonding stops propagating once the matrix stresses reach the tensile strength, beyond which progressive damage in the matrix begins initiating the post-peak response. These are clearly reflected in Figure 10. Figure 11 shows the generated tensile constitutive response of iron particulate-reinforced HCP with different dosage of
iron powder. Incorporation of iron powder leads to a higher tensile strength that corroborates the gain in fracture toughness.

![Simulated tensile constitutive response of control HCP as well as iron powder-modified HCP containing various dosage of iron powder](image)

Figure 3-11 Simulated tensile constitutive response of control HCP as well as iron powder-modified HCP containing various dosage of iron powder

The homogenized tensile constitutive response for particulate-reinforced HCP along with the damage model parameters and $G_F$ are assigned to the matrix in the mortar scale (see Figure 9(b)). Figure 12 presents the progressive interface damage and damage in iron particulate-reinforced mortar containing 10% iron powder. While Figure 12(a) corresponds to undeformed configuration for the meso-scale showing undeformed matrix and sand inclusions, Figures 12(b), (c) and (d) present the interface damage parameter as well as the matrix damage variable (D) under applied strain of 0.005%, 0.017% and 0.03% respectively. General trend in progressive interface debonding and damage in the matrix remains similar to that observed in the micro-scale. Figure 13 shows the computed tensile constitutive response for control mortar as well as iron powder-modified mortars. $G_F$ for the mortars are obtained from simulated tensile softening responses using Equation 10 and the values are found to be 0.034, 0.038, 0.043 and 0.048 N/mm for control mortar and mortars containing 10%, 20% and 30% iron powder respectively. $G_F$ values are adopted as 0.6 times that of $G_F$ [207] as explained earlier. The simulated tensile constitutive responses and fracture energies, thus obtained using numerical homogenization, serve as input to simulate macro-scale three-point-bend tests as explained in the forthcoming section.
Figure 3.12 Progressive interface damage and damage in iron particulate-reinforced mortar containing 10% iron powder for applied strain of: (a) 0% (undeformed), (b) 0.005%, (c) 0.017%, and (d) 0.03%.

Figure 3.13 Simulated tensile constitutive response of control mortar as well as mortars containing iron powder-modified matrix

4.2.3 Macro-scale fracture responses

The macro-scale simulation of a three-point-bend test incorporates the material properties of the mortars, obtained from numerical homogenization, and performs the analysis using XFEM-based framework implementing CDP to obtain TPFM parameters. The notched beam model is shown in Figure 9 (c). Three-point-bend model in ABAQUS™ simulates a displacement controlled test. A
A mesh sensitivity study was performed and a mesh containing 1027 CPE4R elements provided converged solution. Under the application of center-point displacement, the crack initiates when the stress reaches the tensile strength beyond which the propagation of crack is governed by traction-separation law (defined by initial fracture energy ($G_I$), total fracture energy ($G_F$) and tensile strength of matrix ($f_t$)) coupled with CDP. The values for the CDP parameters $\beta$, $m$, $\gamma$ and $f$ are $38^\circ, 1, 0.67$ and $1.12$ respectively which are adopted from [200]. While these parameters are provided for concrete in [200], they are used in this study for mortars also, for lack of better experimental data on these parameters. Similar approach was successfully adopted in [219].

Figure 14 shows the load-CMOD responses obtained from XFEM simulation for control mortar as well as the mortars with varying iron powder content. As can be seen in the figure, the peak load increases with increase in iron powder content. The points P-1, P-2 and P-3 for the representative mortar containing 10% iron powder correspond to 85% of peak load (pre-peak), 95% of peak load (post-peak) and a load that yields CMOD near ultimate failure respectively. The load-CMOD responses, thus obtained, are used later in this section to quantify TPFM parameters of these mortars.

![Figure 14](image.png)

**Figure 14** Simulated load-CMOD results for control and iron powder incorporated mortars with P1, P2 and P3 at 85% of peak load in pre-peak regime; P2 at 95% of peak load in post-peak regime; P3 at near ultimate failure.

Figure 15 shows the maximum principal stress contours (for the representative mortar containing 10% iron powder) at three different stages of the simulated load-CMOD response. These stages correspond to points P-1 (Figure 15(a)), P-2 (Figure 15(b)) and P-3 (Figure 15(c)) as shown in Figure 14. The figure corresponding to point P1 doesn’t show crack formation since the maximum
principal stress failure criterion is not met. On the other hand, the figure corresponding to point P2 show a single crack that have grown with a stress concentration at the tip of the crack. The figures corresponding to P3 depict that the crack have propagated almost completely leading to failure.

Figure 3.15 Maximum principal stress contours for mortar beams with 10% iron powder (a) P1 (b) P2 and (c) P3

From the load-CMOD response and crack-extension values obtained from XFEM, TPFM parameters are obtained using equation 2(a) and 2(b) as explained in sub-section 3.3.2. Table 4 shows the simulated TPFM parameters along with those experimentally obtained from DIC.

Table 3.4 TPFM parameters for varying iron powder containing mortars obtained by DIC experiments and XFEM simulations

<table>
<thead>
<tr>
<th>Fracture Toughness ($K_{IC}$) [MPa.mm$^{0.5}$]</th>
<th>Crack tip opening displacement, CTOD, (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron Powder %</td>
<td>0</td>
</tr>
<tr>
<td>XFEM</td>
<td>21.41</td>
</tr>
<tr>
<td>Experimental (DIC)</td>
<td>21.92±2.15</td>
</tr>
</tbody>
</table>

The fracture parameters ($K_{IC}$ and CTOD$_C$) obtained from multiscale numerical simulation are found to be in very good agreement with those directly obtained from DIC for control mortar as well as
mortars with varying iron powder content signifying efficacy of the multiscale numerical simulation approach presented in this study.

5. CONCLUSION
This study involves combined experimental and numerical evaluations to provide insight into the fracture response of waste iron powder-incorporated mortars. Experimental evaluations using CMOD-controlled three-point-bend test coupled with DIC showed superior flexural fracture response of modified cementitious systems when waste iron powder is used to replace cement. While experimental evaluations established beneficial impact of iron powder when added as cement-replacement (up to 30% by volume), the multiscale numerical approach, presented in this paper, is aimed towards development of a predictive tool that can help develop design strategies for efficient performance of these particulate-reinforced systems. The multiscale numerical simulation approach performs numerical homogenization at different length scales. The numerical homogenization approach incorporates interfacial debonding using CZM-based interface damage approach and implements isotropic damage in the matrix to obtain post-peak response. The homogenized constitutive response, thus obtained from numerical homogenization, serves as input to the macro-scale XFEM simulation of three-point-bend test on notched beams. The macro-model uses a maximum principal stress-based crack initiation criteria and implements bilinear traction-separation law coupled with CDP as crack propagation criteria to obtain $K_{IC}$ and $CTOD_c$ values for iron particulate-reinforced mortars. The simulated values of $K_{IC}$ and $CTOD_c$ are found to be in good agreement with the experimental values obtained from DIC for varying dosage of iron powder signifying efficacy of the multiscale numerical simulation approach. Thus the multiscale numerical simulation framework, presented in this study, successfully links the material structure at different length scales to obtain macro-scale mechanical response of particulate-reinforced mortars facilitating microstructure-guided material design. Although the simulation approach is specifically applied in this paper towards particulate-reinforced mortars, it can also potentially provide efficient means to tailor the microstructure of a large class of inclusion-modified cementitious composites which needs further investigation.
Chapter 4

Predicting the fracture response of particulate reinforced cementitious composites
using state based peridynamics

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Abstract

This paper presents a peridynamics-based micromechanical analysis framework that can efficiently handle material failure for random heterogeneous structural materials. In contrast to conventional continuum-based approaches, this method can handle discontinuities such as fracture without requiring supplemental mathematical relations. The framework presented here generates representative unit cells based on microstructural information on the material and assigns distinct material behavior to the constituent phases in the random heterogeneous microstructures. The framework incorporates spontaneous failure initiation/propagation based on the critical stretch criterion in peridynamics and predicts effective constitutive response of the material. The current framework is applied to a metallic particulate-reinforced cementitious composite. The simulated mechanical responses show excellent match with experimental observations signifying efficacy of the peridynamics-based micromechanical framework for heterogenous composites. Thus, the multiscale peridynamics-based framework presented in the study can efficiently facilitate microstructure guided material design for a large class of inclusion-modified random heterogeneous materials.

Keywords: state based peridynamics; micromechanical modeling; critical stretch; random heterogeneous structural materials; particulate reinforced cementitious composites.
1. INTRODUCTION

The classical theory of solid mechanics, because of its reliance on partial differential equations, is inherently limited when applied to failure of materials [40–42]. The non-existence of the spatial derivatives at the crack tips introduces singularity, which is alleviated with supplemental relations for stable numerical modeling. This necessitates a reformulation of the fundamental equations of continuum mechanics for universal application regardless of discontinuities arising from deformations. To address this, an alternative approach called peridynamics has been proposed, which uses integral equations and maintains the integrity of the mathematical structure in the event of a discontinuity [43–45].

In peridynamics, any failure is treated as a natural outcome of the deformation arising out of the equations of motion and the constitutive model [41]. This eliminates the need for supplemental kinetic relations which would otherwise be necessary in fracture mechanics to define crack initiation and propagation [48,49]. Thus, peridynamics has been gaining traction owing to its ability to handle multiple scales with long-range forces that can be efficiently integrated in a constitutive model. In contrast to contact forces in classical methods, peridynamics considers the forces between particles beyond the immediate neighbor, as though they act across a finite distance. This non-locality contributes to the robustness of peridynamics in handling multiple interactive scales [46,47].

Broadly, peridynamics can be classified into bond-based and state-based models. Bond-based peridynamics was initially developed [44,220] which was restricted to only central force loading and a Poisson’s ratio of ¼ [40,221]. A more robust formulation was later introduced in the form of state based peridynamics [40,222] that can capture volume changes thereby overcoming the limitations posed by the bond-based theory. In the state-based peridynamics, the forces between the peridynamic nodes are not only governed by those particles but also by the surrounding bonds. Additionally, the introduction of force and deformation states in the state-based model allows easier correlation with classical continuum mechanics and easy import of classical constitutive relationships into the framework, thereby reconciling the peridynamic theory with classical mechanics [223]. The wide applicability of peridynamic formulation is exemplified by its usage for modeling fiber reinforced composites [224–226], polycrystals [224,227,228] and macro-scale concrete structures [47,229].

While the previous studies mostly correspond to macro-scale analysis of such materials, the current study implements a multiscale state-based peridynamic framework towards effective property computation in random heterogeneous structural materials. Towards that end, a numerical
simulation framework is proposed in the current study involving multi-phase random microstructures which are assigned peridynamic material models and solved at different interactive length scales. In order to predict the constitutive behavior and fracture response of highly heterogeneous structural materials, the challenge lies in establishing techniques that can handle more than the phase volume fractions. Analytical homogenization techniques [187–189] resulting in closed form solutions are often incapable of post-peak response prediction and are rendered ineffective while handling distinct phases with significant stiffness contrasts [100,190]. Lately, computational techniques towards enhanced accuracy have been implemented [100,101,191,192]. Such techniques include Lattice approach demonstrating meso-scale simulations [193–195] with discrete elements and Finite element method (FEM) involving additional kinetic relations for failure initiation and propagation [230,231]. The peridynamic formulations eliminate the need for such explicit relations. In addition, in case of modelling of interfacial characteristics in heterogeneous systems, FEM-based cohesive zone models (CZM) are often plagued by mathematical and physical limitations apart from constraints on cohesive laws and loss of accuracy at crack tips in extended finite element method (XFEM) that explicitly define the nature of crack initiation and propagation [232–234]. The implementation of peridynamics not only does away with such ad hoc postulations used in classical approach but also enables a mesh-free discretization thereby eliminating the need for computationally expensive meshing algorithms.

This study applies the proposed peridynamics-based multiscale framework towards prediction of effective mechanical response of a metallic particulate incorporated cementitious composite. The predicted responses are compared with macro-scale experimental results to assess the effectiveness of the proposed framework. Thus, the proposed peridynamics-based framework is expected to enable efficient design of a sizable class of inclusion-reinforced random heterogeneous cement-based composites for various applications which is the ultimate objective of this research work.

2. PERIDYNAMICS BASED NUMERICAL SIMULATION FRAMEWORK

This section elaborates the peridynamics-based numerical simulation framework. The framework involves generation of discretized unit cells accurately representing the multi-phase material microstructure followed by a peridynamics-based micromechanical analysis. The material definitions and damage models are implemented in the discretized domain and an explicit solver in the open source code Peridigm [222] is used to obtain the engineering stresses and strains. A post-processing module enables visualization of the deformed unit cells and the computation of effective constitutive response. The surface effects observed in such simulations are eliminated by the
implementation of influence functions in the force state that can effectively incorporate the presence of interfaces and boundaries. A schematic for the numerical simulation framework is shown in Figure 1.

![Schematic Diagram](image)

Figure 4-1 A schematic framework for peridynamics-based micromechanical modeling

### 2.1 Generation of representative unit cells

The representative unit cell generation is carried out using Lubachevsky-Stillinger algorithm [101,103,104]. The algorithm implements random packing of rigid particles which are not allowed to overlap owing to hard contact model. Random positions and velocities are assigned to the particles with zero initial radius. At time \( t = 0 \), the initial velocities of the infinitesimal points have randomly distributed components between \(-1\) and \(+1\). As the points begin to grow into particles, their sizes at any instant of time are governed by a continuous nondecreasing function of the growth rate \( g_i \) for every \( i^{th} \) particle. The growth of the particles results in collisions, which in turn determines the subsequent velocities of the particles. In an iterative framework, the frequency of such collisions increases with increase in the size of the particles. The formulations of the iterative framework that terminates at a target volume fraction, as presented in [235], places the particles at various positions in the bounding box, which thereafter collide and grow so as to achieve the target volume fraction [102]. The iterative algorithm is terminated as the inclusions occupy the target volume fraction. As the terminating criterion is met, the positions and velocities of the particles are frozen. Thus, the final states of the particles in the representative geometry are obtained. The representative unit cells are periodic in nature [107–110,236] implying material continuity at the boundaries. The information pertaining to the final particle radii and their locations along with their orientations are passed as input parameters to the discretization module. The formulation is implemented in a python script that outputs the final states of the particles in the generated unit cell.
2.2 Discretization module and boundary conditions

The microstructural information obtained from the unit cell generation framework is passed on to the discretization module. The numerical implementation of the discretization procedure commences with the definition of a bounding box with dimensions equal to that of the unit cell. Thereafter, the module discretizes the unit cell domain into nodes, each with a known volume, that serves as the reference configuration for the ensuing Peridynamics framework. This discretization method is meshfree [41] as there are no elements or geometrical connections between the nodes. Such a discretization method enables efficient computation of forces at a node in the Peridynamics-based framework where the influence of only the surrounding nodes lying within the horizon are considered. The nodes in the discretized unit cell domain are assigned different sets of materials IDs so as to represent the shapes and orientations of the different component phases in the generated representative unit cell (section 2.1) effectively. This facilitates application of relevant material and damage models to various phases in a random heterogenous microstructure in the Peridynamics code. The meshfree discretization is performed using a python script. The generated meshfree representative unit cell is used in the Peridynamics code.

The boundary conditions of the unit cell are imposed on a volume of boundary layers equaling the horizon. In order to implement periodic boundary conditions, a necessary condition is to ensure the continuities of displacement and traction. Along the boundary of the material region, the displacement boundary conditions are implemented on the boundary layer (with a depth equaling horizon as mentioned earlier). In the boundary layer, constraints are assigned to the material points in the region. The displacements thus assigned to the layer are linear approximations of the boundary displacement (as applied on the unit cell). Traction conditions can be similarly enforced, which in the present scenario is zero and can be implemented naturally. In order to ensure the continuity of both displacement and traction at surfaces defining the unit cell, the family of material points are generated in a periodic array. Once the boundary is encountered at a corner or surface, a cut-off procedure is adopted and the surplus material points are impressed on the opposing face or corner. The periodic conditions are thereafter adopted by constraining the mapped points on opposite faces or corners. The uniaxial response prediction is implemented by imposing a relative displacement between two such points (in a plane perpendicular to the direction of loading) lying on opposite faces.

2.3 Peridynamics-based micromechanical modeling

The state-based generalization of the peridynamics is used in this paper. In this state-based framework, the response of a material at a point depends collectively on the deformation of all
bonds connected to the point which is ensured by defining mathematical objects called deformation state and force state. While the deformation state contains the deformed configurations of the bonds, the force state contains the forces in all these bonds. The constitutive material model relates the deformation and force states. The kinematics of the peridynamic method are captured in a discretized domain (See Figure 2). Each material point \( \mathbf{x} \) in the discretized domain has a finite volume. It interacts with other points \( \mathbf{x}' \) which are located within a specific region \( H_x \) (family of \( \mathbf{x} \)). This region is considered to be a sphere centered at point \( \mathbf{x} \) with a radius \( \delta \), referred to as the horizon. The position vector state \( \mathbf{X} \), also referred to as the bond between the particles \( [40,237] \), captures the relative positions of the interacting particles in the undeformed configuration. The position vector state corresponding to the bond \( \mathbf{x}' - \mathbf{x} \) is denoted by \( \mathbf{X}(\mathbf{x}' - \mathbf{x}) \). Once the deformation sets in, the relative displacements between the two points is defined by \( \eta \) (refer to Equation 1(a)). Thereafter the deformation vector state \( \mathbf{Y}(\mathbf{x}' - \mathbf{x}) \) is defined as the sum of \( \mathbf{X}(\mathbf{x}' - \mathbf{x}) \) and \( \eta \) (see Equation 1(b)).

\[
\begin{align*}
\eta &= \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t) \quad [4-1a] \\
\mathbf{Y}(\mathbf{x}' - \mathbf{x}) &= \mathbf{X}(\mathbf{x}' - \mathbf{x}) + \eta \quad [4-1b]
\end{align*}
\]

Where \( \mathbf{u} \) is the displacement vector field. The peridynamics-based simulations are governed by the equation of motion, derived from the conservation of linear momentum \([40,48]\), as shown in Equation 2 \([41]\).

\[
\begin{align*}
\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) &= \int_{H_x} \{ \mathbf{T}[\mathbf{x}, t](\mathbf{x}' - \mathbf{x}) - \mathbf{T}[\mathbf{x}', t](\mathbf{x} - \mathbf{x}') \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \quad [4-2]
\end{align*}
\]

Where \( \rho \) is the local density, \( \ddot{\mathbf{u}}(\mathbf{x}, t) \) is the acceleration of point \( \mathbf{x} \) at time \( t \), \( \mathbf{b} \) is the external body force density, \( dV_{\mathbf{x}'} \) is an infinitesimal volume around \( \mathbf{x}' \) and \( \mathbf{T} \) is the force vector state that describes interaction between points. The force state \( \mathbf{T}[\mathbf{x}, t] \) at a point \( \mathbf{x} \) at time \( t \) is a function that associates a force density to the bond \( \mathbf{x}' - \mathbf{x} \) acting at \( \mathbf{x} \). The force density arises due to the internal forces generated by deformation of family of \( \mathbf{x} \) (points within the horizon of \( \mathbf{x} \) in the reference configuration) relative to \( \mathbf{x} \). Since \( \mathbf{T}[\mathbf{x}, t] \) depends only on the deformation of the family of \( \mathbf{x} \), it assumes a zero value for any bond beyond the horizon. The forthcoming subsections elaborate the peridynamic formulations in the context of material properties.
2.3.1 Material model

For an ordinary state-based peridynamic formulation [40], a material is ordinary if the force state $T$ for any deformation has the same direction as that of the deformation state $Y$ as shown in Equation 3.

$$T(x' - x) = C\frac{Y(x' - x)}{||Y(x' - x)||} \quad [4-3]$$

Where $C$ is a scalar force state and $\frac{Y(x' - x)}{||Y(x' - x)||}$ is the unit vector that points from the deformed position of $x$ towards the deformed position of $x'$. For ordinary state-based model, Equation 3 is valid for $||Y(x' - x)|| \neq 0$. Otherwise, a zero value is considered for $T(x' - x)$. Thus, in an ordinary material the direction of $T$ matches with the direction of $Y$ for any bond where $C \neq 0$ (undamaged configuration). For an elastic material, a differentiable scalar valued function $W$ exists as shown in Equation 4.

$$T = \bar{T}(Y) = \nabla W(Y) \quad [4-4]$$

where $\nabla W(Y)$ is the Frechet derivative of the scalar differentiable function $W$, which is the strain energy density function of the elastic material. Note that the deformation state $Y$ considers material dependence on volume changes and shears. The following definitions (Equation 5) of extension scalar state ($e$), influence function ($\omega$), weighted volume ($m$) and scalar valued function dilatation ($\theta$) are used towards that end.

$$e = |Y| - |X| \quad [4-5a]$$

$$m = (\omega |X|) |X| \quad [4-5b]$$
\[ \theta = \frac{3}{m} (\omega |X|) \cdot e \] [4-5c]

Where \( e \) signifies the change in bond length due to deformation; the influence function \( \omega \) is a scalar state and \( \theta \) is considered equal to the volumetric strain at small deformations obtained by the trace of linearized strain in classical theory. Thereafter, \( e \) can be decomposed into isotropic part \((e^i = \theta |X|/3)\) and deviatoric part \((e^d = e - e^i)\). Thus, \( C \) can be obtained from the partial derivatives of \( W \) w.r.t. \( e^i \) and \( e^d \) as shown in Equation 6.

\[ C = \frac{\partial W}{\partial \theta} \frac{\partial \theta}{\partial e^i} + \frac{\partial W}{\partial e^d} \] [4-6]

For a linear peridynamic solid, the strain energy density function \( W(\theta, e^d) \) is defined as follows [40].

\[ W(\theta, e^d) = \frac{K \theta^2}{2} + \frac{15G}{2m} (\omega e^d) \cdot e^d \] [4-7]

Where \( K \) and \( G \) are bulk and shear moduli of the material. Substituting \( W(\theta, e^d) \) (Equations 7) in Equation 8, the force scalar state is obtained as shown in Equation 8.

\[ t = \frac{3K \theta}{m} \omega |X| + \frac{15G}{m} \omega e^d \] [4-8]

Since the force scalar state determines the constitutive model shown in Equation 3, the choice of influence function \( \omega \) can handle interfaces and free surfaces effectively. For a point \( x \) located near the boundary, the influence function is so chosen that it vanishes at all points in the horizon that lie outside the body. If the point \( x \) is near the interface of two different materials, two different influence functions can be chosen. The implementation of influence functions eliminates the surface effects observed in peridynamics [238]. The forthcoming subsection details the incorporation of damage in simulation framework.

### 2.3.2 Damage model

In peridynamics, material damage is introduced when interactions between material points are terminated. The existence of micro-potentials (interactions) is terminated between the material points when the bond between them is stretched beyond a threshold value. Such termination of interactions represents formation of a crack. In the peridynamic formulations, the breakage of a bond occurs independently among different bond lengths and orientations for a given particle. Thus, the initiation and growth process of cracks occurs without reference to any supplemental kinetic relation that controls crack growth. From this perspective, the fracture modeling is autonomous in
such formulations in contrast to conventional methods [46]. In order to calculate the critical stretch that serves as the threshold for bond stretch beyond which damage initiates, the total work required to eliminate all interactions across the new surface is equated to the critical energy release rate. The critical stretch $s_c$ thus obtained is shown in Equation 9 [239].

$$s_c = \sqrt{\frac{G_c}{\frac{6G}{\pi} + \frac{16(K-2G)}{9\pi^2}}} \delta$$

[4-9]

Where $G_c$ is the critical energy release rate; $K$ and $G$ are the bulk and shear moduli respectively and $\delta$ is the horizon. The critical stretch is a function of the horizon $\delta$ which brings in the effect of physical material characteristics, nature of loading, length scale and computational cut-off radius. While $s_c$ serves as the damage initiation criterion, a history dependent scalar-valued function $\mu$ stores the damage states of such bonds. $\mu$ is defined as shown in Equation 10.

$$\mu(x' - x, t) = \begin{cases} 1 & \text{if bond stretch} < s_c \\ 0 & \text{otherwise} \end{cases}$$

[4-10]

The function $\mu$ modifies the force state $T$ to zero as the failure criterion is met which implies initiation of damage. Thus, the solution process involves iterative computation of displacements at each point followed by corresponding stretches between interacting points which terminates by assigning a zero value to $\mu$ as the stretch exceeds $s_c$. The implementation of the history-dependent scalar function $\mu$ enables quantification of local damage at a point as shown in Equation 11 [222].

$$\varphi(x, t) = 1 - \frac{\int_{H_x} \mu(x' - x, t) dV_{x' - x}}{\int_{H_x} dV_{x' - x}}$$

[4-11]

Where $\varphi(x, t)$ defines local damage at point $x$ as the weighted ratio of the number of eliminated interactions to the total number of initial interactions of the material point $x$ with its family in $H_x$. $\varphi$ can range from 0 to 1 with 0 signifying that all the interactions are intact while 1 signifies termination of all such interactions. The local damage is an indicator of possible crack formation. Similar critical stretch-based failure criteria in peridynamic formulations has been successfully implemented and validated with experimental observations in [240]. The following sub-section elaborates the numerical implementation of the material and damage modules in a discretized framework.

In this paper, the peridynamic formulations are implemented in an open source program called Peridigm [222] developed at Sandia National Laboratories. The input file to Peridigm includes the discretization, block definition as described in Section 2.2; definition of material and
damage models corresponding to blocks as described in Section 2.3.1 and 2.3.2 respectively followed by initialization of relevant boundary conditions at nodes and invoking the quasi-static solver. The solutions are passed on to the post-processor. Thereafter, it enables visualization in an open source visualization tool ParaView [241] and computes the engineering stresses and strains. The fundamental considerations for micromechanical analyses involving unit cells are dictated by the solution of the displacement field being its volume average in the unit cell, as shown in Equation 12.

\[
\bar{u} = \frac{1}{V} \int_{V} u \, dV
\]

Where \( \bar{u} \) is the displacement field in a higher scale with its representative unit cell embodying displacement \( u \) throughout the unit cell volume \( V \). The displacement in the unit cell and its corresponding strain can be decomposed into averaged and fluctuation parts. The response in a macroscopically uniform deformation gradient can be obtained by unit cell response under equivalent loads. For uniaxial loading scenarios, the equivalent loads induce unit average strain thus enabling computation of the response of the unit cell which can thereafter characterize the constitutive response of the homogenized material at a higher scale. The uniqueness of the periodic conditions helps in simplification of the problems by ensuring equality between the fluctuating components on opposite faces.

3. APPLICATION OF THE FRAMEWORK TO PARTICULATE REINFORCED CEMENTITIOUS COMPOSITES

This section applies the aforementioned peridynamics-based framework towards performance-prediction of particulate-reinforced cementitious composite. Incorporation of waste iron powder replacing cement not only improves sustainability credentials of cementitious composite (due to reduction in cement-consumption) but also contributes towards enhanced mechanical behavior [235,242]. EAF (electric arc furnace) method of steel production and shot-blasting of structural steel sections generate a vast amount of the aforementioned waste iron powder which are landfilled at enormous environmental costs. Use of analytical homogenization techniques resulting in closed form solutions to predict constitutive relationships for such heterogenous systems is rendered ineffective owing to the stiffness contrasts in the component phases. Herein, employing peridynamics leads to a non-local method well suited for modeling solid bodies with stiffness-mismatch. Unlike FEA, spatial integral equations (sum of bond forces) are used in the peridynamic method which are defined even at discontinuities thereby reducing mathematical complexities. Thereby a multiscale numerical framework on iron powder modified mortars is undertaken towards
prediction of effective constitutive response of such systems. Towards that end, peridynamics
governed numerical homogenization is carried out at two distinct scales. In both the interactive
length-scales, the homogenization technique implements interfacial damage at the matrix-inclusion
interface and enacts damage in the matrix thus capturing the composite constitutive behavior. A
validation to the described multiscale numerical approach is realized by the strength and elastic
parameters as compared with experimental observations. The upcoming sub-sections detail the
numerical simulation results enacted at multiple scales for effective property computations.

3.1 Effective constitutive response prediction: A multiscale numerical approach

The inherent heterogeneity of cementitious systems calls for an approach that can capture the
complex microstructural features in randomly generated virtual microstructures while conserving
the same across length scales of pastes and mortars. The numerical homogenization at the micro
scale predicts the composite constitutive behavior of the waste iron powder modified cement paste.
The homogenized constitutive behavior, thus obtained, serves as the matrix property for the meso-
scale mortar model with sand inclusions. Thus, the current approach facilitates reproduction of
microstructural information pertaining to various component phases as geometrical features in unit
cells at distinct scales. The generated unit cells are thereafter discretized and subjected to suitable
boundary conditions to simulate their effective constitutive response from a peridynamic
perspective. The forthcoming sub-sections elaborate the unit cell generation, discretization,
material and damage definitions and corresponding boundary conditions for each scale.

3.1.1 Generation of unit cell and discretization

The unit cells in both the length scales are obtained using the methodology described earlier in this
paper (refer to sections 2.1 and 2.2). The generated unit cells for cement paste scale and mortar
scale as shown in Figure 3(a) and (b) respectively for a characteristic mixture replacing 10% cement
with iron powder. The constitutive response of the micro-scale model (Figure 3(a)) is extracted and
assigned to the matrix of mesoscale model (Figure 3(b)). While the micro-scale geometry is
characterized by waste iron powder inclusions in cement paste, the mesoscale geometry contains
sand particles dispersed in the homogenized matrix (obtained from micro-scale). In the following
sections, the generated micrographs and matrix/interface damage simulations are shown for the
representative sample (10% iron powder replacing cement). The results from the microstructure
guided numerical simulations include those of the control specimens and varying iron powder
dosage. A comparative evaluation among the specimens has been presented thereafter. The median
inclusion sizes adopted from [235,242] are 20 𝜇m, 600 𝜇m for iron particulates and sand inclusions
respectively. The respective aspect ratios are 12 (iron particulates) and 1 (sand) [235,243]. The paste-sand interface is considered 20 μm thick [144–146,244]. The random locations and orientations of the inclusions in the periodic unit cells are obtained using the algorithm described earlier (See Section 2.1). The sizes of the unit cells are chosen to be 5 times the size of the inclusions which shows sufficient convergence [237]. The changes in constitutive response for sizes beyond the adopted unit cells are deemed insignificant.

Figure 4.3 Interactive length scales (a) Step I: 10% iron powder dispersed in HCP matrix at micro-scale; (b) Step II: sand embedded in homogenized iron powder- HCP at meso-scale (the homogenized material from (a) serves as matrix for (b))

The discretization technique discussed in Section 2.2 enables the distinction between various phases as shown in the zoomed pictures of Figure 3 for each scale which enables a block-based material definition as explained later. A judicious choice of the grid size and the resulting horizon results in a computationally efficient framework [245] with a stable solution. Here a grid size of 0.005 mm and 0.01 mm is chosen here for micro and meso-scale respectively. The horizons are taken to be 3.015 times the grid spacing to remove mathematical instabilities [237]. The grid spacing and horizon, adopted for each length scale, sufficiently represents the geometrical features and are found to yield convergence for the computed stress-strain curves. Although the framework presented in the paper can be effectively applied to 3D unit cells, a trade-off between computational demand and efficiency has been struck by analyzing 2D unit cells for the comparative evaluation. Such 2D unit cells have been successfully implemented in peridynamic formulations in [47].

3.1.2 Blocks: material and damage definition

The input code in Peridigm assigns material properties to each material block in the discretized domain corresponding to every phase of the microstructure. The material input properties required for formulations in Sections 2.2.1 and 2.2.2 are the bulk and shear moduli for defining the linear peridynamic solid and the critical energy release rate to initialize the damage criterion. The input
Young’s modulus for the cement paste matrix, sand and iron particulates are 20, 70 and 200 GPa respectively [101,136]. A constant Poisson’s ratio of 0.2 is considered for all the materials except the iron particles since a range of 0.17-0.22 for the same yields insignificant changes in the results [106,218]. A Poisson’s ratio of 0.3 is adopted for iron particulates [216,235]. Owing to lack of data, the matrix properties are assigned to the iron particulate-HCP interface elements as well. Similar properties have been successfully adopted in [136,216]. The bulk and shear moduli are thus computed from the Young’s modulus and the Poisson’s ratio for each phase of the micro-scale unit cell. The HCP matrix implemented in the micro-scale simulations have a critical energy release rate of 0.017 N/mm [235]. The constitutive response of the iron powder modified cement pastes (output from the micro-scale post-processor) characterizes the matrix properties of the meso-scale mortar model. The sand-matrix interface is considered to have elastic properties a third of the surrounding matrix [246]. To characterize the damage in the meso-scale, the following formulations are used to obtain the $G_c$ [194].

$$(1 - D)\varepsilon = \varepsilon_{D_0} \exp \left(- \frac{D h \varepsilon f_t}{G_c} \right)$$ \[4-13\]

Where $D$ is damage variable ($0 < D < 1$) relating stress tensor $\sigma$ with strain $\varepsilon$ in terms of elasticity tensor $E$ as $\sigma = (1 - D)E \varepsilon$; $\varepsilon$ is the tensile strain reaching $\varepsilon_{D_0}$ when tensile strength reaches $f_t$; $h$ is the centroidal mean distance of adjacent elements (here, grid spacing) and $G_c$ is strain energy release rate. Here, the value of $D$ is considered 0.9 and the corresponding strain $\varepsilon$ is adopted. The values of $\varepsilon_{D_0}$ and $f_t$ are obtained from the effective constitutive relation of the material. This enables definition of $s_c$ as per Equation 9. The identified material parameters for the micro-scale iron-powder modified cement pastes are presented in Table 2 for different dosages of waste iron powder. These parameters serve as input for the meso-scale simulations.

<table>
<thead>
<tr>
<th>% iron powder</th>
<th>E (GPa)</th>
<th>$f_t$ (MPa)</th>
<th>peak strain</th>
<th>$G_c$ (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Micro scale</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>20</td>
<td>1.77</td>
<td>0.000111</td>
<td>0.017</td>
</tr>
<tr>
<td>10</td>
<td>22.25279</td>
<td>2.15</td>
<td>0.000118</td>
<td>0.02</td>
</tr>
<tr>
<td>20</td>
<td>24.98885</td>
<td>2.42</td>
<td>0.000125</td>
<td>0.023</td>
</tr>
<tr>
<td>30</td>
<td>25.66295</td>
<td>2.69</td>
<td>0.000131</td>
<td>0.025</td>
</tr>
</tbody>
</table>

**3.1.3 Effective constitutive responses at multiple scales**

The results from the numerical homogenization carried out at multiple scales are reported in the current section. The procedure initiates with a microstructure guided numerical homogenization at
the micro-scale (See Figure 3(a)). A uniaxial tensile strain along X is applied to the discretized unit cell. This is implemented in the input file to Peridigm as a nodal displacement boundary condition that ensures a constrained left edge along X. The nodes are subjected to a velocity simulating a quasi-static strain rate. The material properties as reported in Section 3.1.2 for the hardened cement paste without any iron content are adopted. It is to be noted that the micro-scale matrix is HCP with a water-cement ratio of 0.5 by mass for all the digital specimens with varying iron powder contents. The analysis is carried out using the quasi-static solver and the simulation yields progressive damage as shown in Figure 4.

Figure 4 - Progressive damage observed in iron powder (10%) modified HCP corresponding to applied tensile strains of (a) 24 με, (b) 78 με, (c) 121 με and (d) 130 με

Figure 4 shows the progressive damage when the digital specimens are subjected to uniaxial strains of (a) 24, (b) 78, (c) 121 and (d) 130 με respectively. The damage initiates at the iron particulate-HCP interfaces and propagates with increasing strains. Beyond the peak strain, the damages along the interfaces coalesce thus initiating matrix damage. Thereafter, matrix damage continues to propagate with increasing strains. Figure 5 shows the constitutive response for tensile loading of iron powder modified cement paste for varying iron powder dosages clearly illustrating the gain in tensile strength with higher dosages.
The extracted tensile constitutive response of the pastes are thereafter applied as matrix properties in the mortars (see Figure 3(b)). A similar procedure of assigning material properties to the blocks followed by application of tensile strain is followed. The progressive interface and matrix damage for iron particulate (10%) modified mortars are presented in Figure 6.

Figure 4.5 Simulated tensile constitutive response of pastes with varying iron powder dosage in HCP

Figure 4.6 Progressive damage (interface/matrix) observed in iron powder (10%) modified mortar corresponding to applied tensile strains of (a) 52 με, (b) 105 με, (c) 153 με and (d) 208 με; (the interface damage is highlighted in zoomed pictures)

Figure 6 presents the interface damage and matrix damage under applied strain of (a) 52 με, (b) 105 με, (c) 153 με and (d) 208 με respectively. A weaker interface implies onset of damage much lower than the peak strain. As the interfacial damage propagates, the stress in the matrix keeps on increasing. The debonding brought about the interfacial damage terminates at the point of initiation.
of matrix damage which corresponds to the matrix tensile strength. For higher strains, the damage propagates in the matrix thereby characterizing the post-peak response. The tensile constitutive behavior of the simulated mortars are shown in Figure 7 with varying iron powder dosages.

The current framework effectively captures the heterogeneities in particulate modified cement pastes and predicts their constitutive responses with varying iron powder contents. The three-phase interactions involving stiff inclusions in a weak matrix surrounded by a weaker interface are enabled by peridynamic formulations with critical stretch-based failure. Progressive failure is captured in the interface and the matrix leading to accumulated damage in the representative unit cells.

3.2 Comparison with experimental observations

This section draws a comparison between the simulated responses and the experimental observations [235]. Here the experimental observations are obtained from a previous publication [235]. Figure 8 reports the comparison of (a) Young’s modulus, (b) tensile strength and (c) fracture energy respectively. Equation 13 enables calculation of fracture energy from the effective constitutive response as shown in Figure 7. The simulated responses show excellent match with the experimental observations for various dosage of iron powder. Such close correlation between the experimental and simulated responses signifies the efficacy of the peridynamics-based multiscale numerical simulation approach for random heterogenous structural composites presented in this paper.
4. CONCLUSIONS

The study elaborates a peridynamics-based micromechanical simulation framework for random heterogenous composites. The conclusions are mentioned herewith.

- The microstructural features of the composite are effectively captured into the framework by means of representative unit cells with multiple phases that are discretized into distinct blocks thus enabling material property application.
- The peridynamic formulations allows spontaneous damage initiation and propagation based on critical stretch criterion.
- The framework effectively integrates the phase separated microstructure in a peridynamic solver that applies a uniaxial strain to characterize the composite constitutive response for tensile loading. The framework is thereafter applied for random heterogenous microstructures of metallic particulate reinforced cement-based composites in a multiscale approach with a view to assess the capability of the numerical framework.
- The multiple length scales involve microscale simulations for iron inclusions embedded in cement paste, the properties of which are homogenized to form the input to the matrix of the meso-scale mortar with sand inclusions.
- Thereafter, the framework is applied in the meso-scale to obtain simulated effective constitutive responses of the mortars.
- The simulated Young’s modulus, tensile strength and fracture energy for iron powder-incorporated cementitious composites are compared with experimental observations which shows a close correlation thereby validating the framework.

Since the framework is peridynamics-based, it can handle discontinuities arising out of deformities in a robust and efficient computation that involves integral equations unlike the differential counterparts used in classical continuum mechanics. Additionally, the implementation of state based peridynamics provides extensibility to conventional constitutive material models and nano-scale molecular dynamic based simulations alike. The predictive tool thus developed potentially
provides an efficient means to customize the microstructure of a variety of inclusion-incorporated composites for optimized performance.
Chapter 5

Fracture behavior of metallic particulate reinforced alkali-activated slag

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Abstract

This paper presents fracture response of alkali-activated slag (AAS) mortars with up to 30% (by volume) of slag being replaced by waste iron powder which contains a significant fraction of elongated particles. The elongated iron particles act as micro-reinforcement and improve the crack resistance of AAS mortars by increasing the area of fracture process zone (FPZ). Increased area of FPZ signifies increased energy-dissipation which is reflected in the form of significant increase in the crack growth resistance as determined from R-curves. Fracture response of notched AAS mortar beams under three-point bending is simulated using extended finite element method (XFEM) to develop a tool for direct determination of fracture characteristics such as crack extension and fracture toughness in particulate-reinforced AAS mortars. Fracture response simulated using the XFEM based framework correlates well with experimental observations. The comprehensive fracture studies reported here provide an economical and sustainable means towards improving the ductility of AAS systems which are generally more brittle than their conventional ordinary portland cement counterparts.

Keywords: alkali activated slag; particulate reinforcement; fracture response; digital image correlation; extended finite element method
1. INTRODUCTION

Alkali activated ground granulated blast furnace slag (GGBFS) has emerged as a sustainable alternative to ordinary portland cement (OPC)-based binders primarily because of the fact that production of ground granulated blast furnace slag (GGBFS) results in lower energy and carbon footprints than OPC production [247–250]. Alkali silicates are the commonly used activating agent for slag. The main reaction product in these binders is calcium (alumino) silicate hydrate, C-(A)-S-H gel, similar to C-S-H gel in conventional portland cement-based binders [23,251]. The fresh and hardened properties of alkali activated slag (AAS) binders have been characterized in detail in various studies [252–257]. Although the flexural and compressive strengths of AAS binders have been reported in detail in several studies [258–261], limited studies exist on the fracture response of such binders, primarily because they are known to be generally very brittle. One of the means to reduce the brittleness of such mixtures is the use of metallic reinforcement, which is usually incorporated in the form of fibers. In this study, we report the use of a waste metallic powder as an additive to AAS mortars to enhance the crack resistance of such systems. A well-established two parameter fracture model (TPFM) [185,262] coupled with digital image correlation (DIC) [209] is used to quantify the beneficial effects of metallic waste power on the fracture performance of mortars.

The waste iron powder used in this study is a byproduct from the electric arc furnace (EAF) manufacturing process of steel and shot-blasting of structural steel [263,264]. This waste dust is primarily landfilled since recycling of iron from the dust is not economically feasible [265]. Several million tons of such waste iron dust is being landfilled all over the world at a great cost. Hence, potential use of this waste iron dust in AAS mortars as replacement of slag would reduce the demand of slag in these binders. Since ground granulated blast furnace slag (GGBFS) is a marketed commodity with no excess supply in the United States, reducing slag use is an economical means to produce durable concrete. However, it has been reported that alkali activated slag mixtures are much more brittle than conventional portland cement mixtures [266]. Here, we employ the use of metallic particulate reinforcement than the commonly used metallic fiber reinforcement to enhance the ductility of such systems. Moreover, the metallic particulate used here is a waste material from steel shot blasting, thereby providing the composite with sustainability benefits. We evaluate the fracture behavior of the waste iron powder-incorporated AAS mortars using compliance-based resistance curves (R-curves) [38,185,199,242,262] determined from three-point bending tests.

Fundamental characterization of fracture response in quasi-brittle materials also requires direct observation of fracture process zone (FPZ) which is denoted by the zone of strain localization near
the tip of the advancing crack. FPZ has been geometrically quantified using microscopy [267,268], photography [269] or a non-contact speckle-tracking method called digital image correlation (DIC) [27,262,270,271]. In DIC, the surface displacements and strain maps are obtained by correlating the images and the direct measurements of the crack extensions/FPZ are quantified from the displacement/strain maps. In order to shed more light into the fundamental difference in crack propagation and strain localization behavior imparted by iron particulates in AAS mortars, direct measurements of crack extension and fracture process zone are made using digital image correlation (DIC) technique. Furthermore, correlations are drawn between the FPZ characteristics and the crack growth resistance. We have also simulated the fracture response of notched AAS mortar beams under three-point bending using the extended finite element method (XFEM) [272,273] so as to predict crack extension and fracture toughness in particulate-reinforced AAS mortars. The paper thus combines experimental characterization of fracture response and the process zone along with numerical simulation to provide detailed insights into the fracture response of these systems.

2. EXPERIMENTAL PROGRAM

2.1 Materials and mixture proportions

The materials used in the experiments are commercially available Type I/II OPC complying with ASTM C 150 and ground granulated blast furnace slag (GGBFS) Type 100 complying with ASTM C 989. Table 1 shows the chemical composition of OPC and GGBFS along with their median particle sizes. The iron powder used in the experiments is a waste powder obtained from shot-blasting of structural steel sections, which is expensive and difficult to dispose. It has an iron content of 88% and oxygen content of 10% which is due to the atmospheric oxidation of iron apart from trace elements like copper, manganese and calcium. Four GGBFS mortar mixtures were prepared where the sand had an average particle size of 0.6 mm, and varying amounts of iron powder waste (0, 10, 20, 30%) by volume replaced slag. The volume of sand in the mortar was kept at 50%. Potassium silicate activator solutions were proportioned based on the K₂O-to-slag (binder) ratio (n) and the silica modulus of the activator (molar SiO₂-to-K₂O ratio) (Mₛ). A K₂O-to-slag (binder) ratio (n) of 0.05 was adopted here based on previous studies [209]. The potassium silicate solution has a solids content of 44% and a molar Mₛ of 3.29. KOH was added to bring the activator Mₛ down to 1.5 which has been shown to provide strength equivalent to hardened cement paste [274,275]. A constant liquid-to-slag ratio of 0.50 by mass was maintained. For compressive strength tests, 50 mm mortar cubes were used. For flexural strengths, prismatic mortar beams of size 250 mm x 50 mm x 50 mm were used. For fracture tests, 330 mm long notched beams with a
cross section of 25 mm x 75 mm were used. Four replicates were used in all the mechanical property tests. Each sample was demolded after 24 hours and exposed to a moist environment with relative humidity greater than 98% and the curing temperature was maintained at 23±2°C. The samples used for microstructural analysis by mercury intrusion porosimetry and scanning electron microscopy were kept sealed in containers.

<table>
<thead>
<tr>
<th>Material</th>
<th>Oxide composition (% by mass)</th>
<th>d_{50} (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CaO</td>
<td>SiO\textsubscript{2}</td>
</tr>
<tr>
<td>OPC</td>
<td>63</td>
<td>21</td>
</tr>
<tr>
<td>GGBFS</td>
<td>37.1</td>
<td>41.8</td>
</tr>
</tbody>
</table>

2.2 Mercury Intrusion Porosimetry (MIP)

The pore structure of the mortars was evaluated using mercury intrusion porosimetry (MIP). The low pressure run includes gas evacuation and exposing the sample to 345 kPa whereas the high pressure run exposes the sample to 414 MPa. The Washburn equation \[276-279\] was used to determine the pore diameter. The surface tension of mercury was taken as 0.485 N/m while the contact angle between mercury and the pore wall was considered 130°. Although the pore-structure information obtained using MIP cannot be used for exact quantitative measurements \[280\], it is suitable for qualitative comparisons \[262\].

2.3 Scanning electron microscopy for microstructural evaluation

The sample preparation for the microstructural analysis involved cutting the sample into a cube of 2 mm edge length with a diamond saw followed by ultrasonic cleaning and alcohol rinsing to remove debris. The sample was then impregnated with epoxy by vacuum impregnation technique and cured overnight. Suitable grinding and polishing techniques were adopted to achieve a planar surface suitable for microscopic analysis. SiC discs were used to polish using successively finer abrasives. Finally the sample was polished with 0.04µm colloidal silica suspension and subjected to backscattered mode imaging in a Philips XL30 field emission environmental scanning electron microscope (FESEM).

2.4 Three Point Bending Test

The experimental setup for three-point-bending tests is shown in Figure 1. Notched mortar beams of size 330 mm (effective span 305 mm) x 25 mm (width) x 75 mm (depth) were used. The notch
depth was chosen as a quarter of the total depth as shown in Figure 1. The test was performed under crack mouth opening displacement (CMOD)-controlled mode, with the CMOD monitored using a clip gauge. The test was carried out under load-controlled mode till a load of 100 N, beyond which CMOD-controlled mode was initiated. CMOD-controlled stage was terminated at a CMOD value of 0.38 mm following which unloading was initiated using load-controlled mode. The unloading rate was 556N/m, and was terminated at a load of 50 N. Next, CMOD-controlled mode was again implemented in the reloading cycle followed by load-controlled unloading cycles until a CMOD of 0.18 mm is reached. The loading-unloading cycles, thus implemented in the load-CMOD response, are used in a compliance-based technique to obtain crack growth resistance values which is explained in detail later.

2.5 Digital Image Correlation (DIC)

Digital image correlation (DIC) is a non-contact optical method that tracks speckles to measure displacements on the surface of the specimen. A correlation is drawn between images of undeformed and deformed states to calculate displacement fields [184,202,203,270,281–284]. In this study, the beam surfaces were first painted white, and random black speckles were sprayed on them. A CCD camera was used to capture images every 5 seconds during the CMOD-controlled three-point-bending test using VIC-snap software from Correlated Solutions [17,18]. Once the images were obtained, commercially available software VIC-2D was used to obtain the displacement and strain fields [262]. The displacement/strain maps are used here to characterize the fracture process zone (FPZ) and crack propagation behavior.

3. RESULTS AND DISCUSSIONS

3.1 Pore- and Microstructure

A microstructural analysis of the polished samples after 28 days yields distribution of various component phases in the alkali-activated slag paste. Figure 2(a) shows a back scattered (BSE)
image of hardened alkali-activated slag paste with 30% iron powder by volume. The bright (dense) elongated iron particles are clearly visible in the micrograph. The elongated shape of iron particles likely contributes towards improvement of fracture response through mechanisms such as crack bridging and crack deflection which are explored in detail in this paper.

Figure 2(b) shows the total porosity and average pore diameters, extracted using MIP, for the control AAS mortar as well as mortars containing various dosage of iron powder after 28 days. The total porosity and average pore diameters are not found to vary significantly with iron powder content. The similar liquid-to-slurry ratio in all mixtures along with the fact that iron powder is an inert filler in the highly alkaline environment contributes to this response.

Figure 2: (a) BSE micrograph showing distribution of iron particulates in alkali-activated slag paste containing 30% iron powder by volume; (b) porosity and average pore diameter of the pastes with varying volume fraction of iron powder.

3.2 Compressive and Flexural Strengths

Figure 3 shows the compressive and flexural strengths of mortars after 28 days of curing. The compressive strengths are similar for all the mortars irrespective of iron powder content which can be attributed to the similar pore-structure features for these mortars as shown in Figure 2(b). However, the flexural strength shows an improvement with the increasing iron powder content, attributable to the elongated shape of iron particles as observed in Figure 2(a). These elongated iron particles act as micro-reinforcement to the matrix. Overall the strength results indicate that the waste iron powder can be safely incorporated to AAS mortar systems without compromising mechanical properties.
3.3 Effect of Particulate-reinforcement on Fracture Behavior

While the previous section reported the strength and pore-structure of metallic particulate-reinforced AAS mortars, this section focusses on the influence of particulate reinforcement on the fracture response of AAS mortars.

3.3.1 Load-CMOD Responses

The load-CMOD responses of control and iron particle-incorporated AAS mortars are shown in Figure 4. Multiple loading-unloading cycles are implemented in the load-CMOD response in the post-peak regime in order to calculate unloading compliances corresponding to each cycle which are used to calculate compliance-based resistance curves as explained later in this paper. The peak load increases with increase in the amount of iron powder in the binder due to the micro-reinforcing effect of the elongated iron particulates. The area under the load-CMOD curve is a measure of the material toughness. An increase in the area under load-CMOD curve with increasing iron content indicates improved toughness of the material.
3.3.2 Crack Growth Resistance

The fracture response of particulate-reinforced AAS mortars is quantified here using compliance-based crack growth resistance curves. The basic assumption behind the development of the compliance-based R-curves is that the compliance increases as the crack propagates. The total crack growth resistance \( G_R \) contains an elastic part that is calculated from the elastic compliance while the inelastic part is based on the inelastic CMOD. The crack growth resistance can be expressed as [262,285,286]:

\[
G_R = G_{elastic} + G_{inelastic} = \frac{P^2}{2t} \frac{\partial C}{\partial a} + \frac{P}{2t} \frac{\partial (CMOD_{inelastic})}{\partial a}
\]  

Where \( C \) is the unloading compliance, \( t \) is the thickness of specimen, \( P \) is the load and \( a \) is the crack length. The crack extension values are obtained from unloading compliances as explained in [262]. The relationships between unloading compliances or the inelastic CMOD values and crack extensions are differentiated with respect to crack extension to obtain the rate terms of Equation 1 as explained in [262].

Figure 5 shows \( G_R \) as a function of crack extension for all the mortars. The crack growth resistance increases with crack extension culminating in a relatively constant portion signifying that the fracture process zone has almost fully developed. It can be noticed from this figure that the crack growth resistance increases with increase in iron particulate content which is attributed to the crack bridging/deflection effect of the elongated iron particles as shown in the micrograph in Figure 2(a). The crack growth resistance is enhanced by about 50% through the addition of 30% iron powder in the mixture. It can also be observed from Figure 5 that the values of crack extension at which the plateau is reached decreases with increasing iron powder content which can be explained by the crack deflection effect of elongated iron particles. Such elongated iron particulates increase the tortuosity of the micro-cracks in the FPZ and dissipate a significant amount of energy resulting in
achievement of a steady-state crack propagation at a lower value of crack extension in the presence of iron powder.

Figure 5: Crack growth resistance as a function of iron powder volume fraction

3.3.3 Evaluation of Fracture Process Zone (FPZ)

While the previous section evaluated the fracture response of the mortars through indirect quantifications, this section presents direct measurements of FPZ to shed more light on the influence of iron powder on the fracture response of AAS mortars. Direct characterization of the fracture process zone features including length, width and area is essential to elucidate the fundamental differences imparted by the iron particulates in terms of the crack extension and strain localization response. The geometric properties of FPZ are determined by DIC as explained in detail elsewhere [38,185,262].

Figure 6 shows the Lagrangian strain fields for control AAS mortar as well as AAS mortars with varying iron powder contents at 95% of the peak load in the post-peak region. It can be seen that the length of FPZ increases with increase in iron powder content whereas the width of FPZ almost remains unchanged. At a location 4 mm above the tip of the notch, the quantified measurements of the FPZ at 95% of peak load in post-peak regime are shown in Figure 7, as a function of the iron powder volume fraction. The length of FPZ increases significantly with increasing iron powder content, indicating energy dissipation by various mechanisms such as micro-cracking, crack arresting and crack deflection due to the presence of elongated metallic particles. On the contrary, the width of the FPZ remains fairly constant irrespective of the iron powder content due to the fact that the inelastic component of crack growth resistance is not expected to change with inclusion of stiff particulates for the volume fractions considered here. Figure 7(b) shows the area of FPZ as a
function of the iron powder content. The area of FPZ increases significantly with increasing iron powder content which is reflected in the form of overall increase in crack growth resistance shown in Figure 5. To shed more light, the forthcoming section correlates the directly measured FPZ features to the crack growth resistances, calculated indirectly using compliance-based approach.

Figure 5.6: Lagrangian strain fields at 95% of the peak load in post-peak regime for: (a) control AAS mortar, and AAS mortars with: (b) 10%, (c) 20% and (d) 30% waste iron powder as slag-replacement.

Figure 5.7: Relation between volume fraction of iron powder and: (a) FPZ geometry (b) FPZ area

3.3.4 Correlation between Crack Growth Resistance and FPZ

While it was mentioned in the previous section that the FPZ characteristics influence the energy dissipation in these mortars, this section quantifies such relationships. The FPZ characteristics are plotted against the crack growth resistances in order to draw a correlation between the two. The FPZ parameters correspond to 0.95Pmax in the post-peak regime for the control AAS mortar as well as mortars with varying iron powder contents. Figure 8(a) shows that the crack growth resistance increases with increase in the FPZ area, attributable to the increased area of energy dissipation with
incorporation of iron powder. Figure 8(b) depicts the correlation between FPZ length and elastic component of crack growth resistance. As the volume fraction of iron powder increases in AAS mortar, the elastic component of the crack growth resistance also increases linearly with increase in the FPZ length. Incorporation of iron powder in AAS mortars facilitates microstructural strengthening and toughening of the mortar matrix through various mechanisms such as micro-cracking, crack-arresting and crack-deflection in the direction of the crack-driving force as described earlier. This microstructural strengthening and toughening mechanisms result in significant increase in the length of FPZ and consequently the elastic component of the crack growth resistance increases with incorporation of iron powder. Thus, this study has shown that metallic waste iron powder can be incorporated in AAS mortars as partial replacement of slag without compromising the strength, yet providing significant enhancement in the fracture response.

![Figure 5-8: Relationships between: (a) FPZ area and crack growth resistance; (b) FPZ length and elastic components of crack growth resistance](image)

3.3.5 Numerical simulation towards predicting the fracture behavior of mortars

While the previous section elucidated experimental evaluation of fracture behavior of particulate-reinforced AAS, this section is aimed towards prediction of fracture behavior of such systems using extended finite element method (XFEM). Crack-growth analysis using XFEM eliminates the need for re-meshing and thus provides an efficient solution[272,273,287–289]. Brief description of the formulations related to damage model and the prediction results are shown in the forthcoming subsections as follows:

3.3.5.1 XFEM for damage prediction in quasi-brittle materials:

Extended finite element method (XFEM) is a versatile tool for the analysis of problems characterized by discontinuities, singularities, localized deformations and complex geometries. In
XFEM, local enrichment functions are incorporated in the FE approximation to model the crack (discontinuities) in an efficient manner. The enriched functions have additional degrees of freedom and simulate path-independent crack initiation and propagation based on the damage criteria provided. The approximation of displacement vector function with the partition of unity enrichment is given as [290,291]:

\[ u = \sum_{i=1}^{N} N_i(x)[u_i + H(x)a_i + \sum_{a=1}^{d} F_{a}(x)b_{a}^{q}] \]  \[5-2\]

where, \( N_i(x) \) are the conventional nodal shape functions at node I, \( u_i \) is the nodal displacement vector associated with the continuous part of the finite element solution; \( a_i \) is the nodal enriched degree of freedom vector, \( H(x) \) is the Heaviside function; \( b_{a}^{q} \) is the product of nodal enriched degree of freedom vector, and \( F_{a}(x) \) are the associated elastic asymptotic crack-tip functions. \( H(x) \) is given as:

\[ H(x) = 1 \text{ if } (x - x^*) \cdot n \geq 0 \]  \[5-3\]

If Equation 3 is not satisfied, it is equal to -1. Here, \( x \) is a sample Gauss point, \( x^* \) is the point on the crack closest to \( x \), and \( n \) is the unit outward normal to the crack at \( x^* \). The asymptotic crack tip functions \( F_{a} \) are given as [291]:

\[ F_{a}(x) = \left[ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \theta, \sin \frac{\theta}{2}, \sqrt{r} \sin \theta, \cos \frac{\theta}{2} \right] \]  \[5-4\]

where the crack tip is at the origin of the polar coordinate system and \( \theta = 0 \) is the tangent to the crack tip. The XFEM damage model requires appropriate damage initiation criteria. The maximum principal stress criterion is adopted in this study and the crack is considered to be initiated if the maximum principal stress exceeds the tensile strength of the mortar. A bilinear traction-separation law [292,293] is used for damage propagation, as shown in Equations 5a and 5b. The fracture energy \( (G_{F}) \) is the area under the entire traction-separation curve, given as:

\[ G_{F} = \int_{0}^{\infty} f(w)dw \]  \[5-5a\]

\[ f(w) = \begin{cases} f_{t} - (f_{t} - f_{1}) \frac{w}{w_{1}} & \text{for} \ w \leq w_{1} \ and \ \left| f_{1} - f_{1} \left( \frac{w}{w_{c} - w_{1}} \right) \right| \text{for} \ w_{1} > w \end{cases} \]  \[5-5b\]

where \( f_{t} \) is the tensile strength of the material, \( w_{c} \) is the critical crack tip opening displacement, and \( f_{1} \) and \( w_{1} \) are the stress and opening displacement corresponding to the kink in the bilinear traction-separation curve.
The numerical simulation framework incorporates the Concrete Damage-Plasticity (CDP) model [200] beyond the linear elastic regime for fracture simulation. CDP is a material model based on a combination of damage and plasticity theory. Plasticity theory is used to describe both the compressive and tensile response of concrete, while the damage theory is used for the cyclic and unloading characteristics. In this model, isotropic damage is represented as:

\[
\sigma = (1 - d)D^e_0 : (\varepsilon - \varepsilon^{pl}) = D^e : (\varepsilon - \varepsilon^{pl})
\]  

[5-6]

where \( \sigma \) is the Cauchy stress tensor, \( d \) is the scalar stiffness degradation variable, \( \varepsilon \) is the strain tensor, \( \varepsilon^{pl} \) is the plastic strain, \( D^e_0 \) is the initial elastic stiffness of the material, and \( D^e \) is the degraded elastic stiffness tensor. The effective stress tensor \( \bar{\sigma} \) is given as:

\[
\bar{\sigma} = D^e_0 : (\varepsilon - \varepsilon^{pl})
\]  

[5-7]

Damage states in tension and compression are characterized independently by two hardening variables which are the equivalent plastic strains in compression and tension respectively. The plastic flow is given as [200]:

\[
\dot{\varepsilon}^{pl} = \dot{\lambda} \frac{\partial G(\bar{\sigma})}{d\bar{\sigma}}
\]  

[5-8]

where, the flow potential, \( G \) is given using a Drucker-Prager hyperbolic function as:

\[
G = \sqrt{(f_c - m.f_t \tan \beta)^2 + \bar{q}^2 - \bar{p} \tan \beta - \sigma}
\]  

[5-9]

Here, \( f_t \) is the tensile strength and \( f_c \) is the compressive strength, \( \beta \) is the dilation angle and \( m \) is the eccentricity of the plastic potential surface, \( \bar{p} \) is the effective hydrostatic stress and \( \bar{q} \) is the Mises equivalent effective stress. The CDP model uses a yield condition based on loading function:

\[
F = \frac{1}{1 - \alpha} (\bar{q} - 3.\alpha \bar{p} + \theta(\varepsilon^{pl})(\bar{\sigma}_{\text{max}} - \gamma(-\bar{\sigma}_{\text{max}})) - \bar{\sigma},(\varepsilon^{pl})
\]  

[5-10]

where the function \( \theta(\varepsilon^{pl}) \) is given as:

\[
\theta(\varepsilon^{pl}) = \frac{\hat{\sigma}_c (\varepsilon_c^{pl})}{\hat{\sigma}_t (\varepsilon_t^{pl})} (1 - \alpha) - (1 + \alpha)
\]  

[5-11]

The parameter \( \alpha \), which is based on the ratio of biaxial compressive strength \( (f_{b0}) \) to uniaxial compressive strength \( (f_c) \), is defined as:

\[
\alpha = \frac{f_{b0}}{f_c}
\]
3.3.5.2 Simulation of three point bending tests of notched mortar beams:

The notched beam used for fracture experiments, explained in earlier sections, is modeled here using ABAQUS™ as shown in Figure 9.

![Assembly of a meshed notched beam in ABAQUS](image)

Figure 5-9 Assembly of a meshed notched beam in ABAQUS

The two pin supports have been modelled as analytical rigid bodies. The analytical rigid punch has been placed centrally with the displacement being applied on it using a reference point. Implementation of traction-separation law for propagation of cracks requires fracture energy and tensile strength of mortars. Here, fracture energies for all the mortars are calculated from the load-CMOD responses and the tensile strength values are obtained through a moment-curvature-based inverse analysis approach [205] that uses flexural load-deflection behavior to obtain uniaxial stress-strain behavior. The inverse analysis procedure in described in detail elsewhere [185,205,294–296]. The fracture energy and tensile strength values, obtained for different mortars with varying iron powder content, are shown in Table 2. The maximum tensile strength-based criteria is used for damage initiation, and the propagation of crack is modeled using a bilinear traction-separation law [198] as explained earlier. A mesh-sensitivity study was performed and a mesh containing 1030 CPE4R elements and 1079 nodes provided convergence.

The CDP model [199–201] parameters are $\beta$ or dilatation angle at high confining pressure, $m$ or eccentricity of the plastic potential surface, $\gamma$ that determines the shape of the loading surface in deviatoric plane and $s$ or the ratio of biaxial compressive strength to uniaxial compressive strength of concrete. The values for the above-mentioned parameters are adopted from [200] and shown in Table 2. While these CDP parameters are provided for concrete in [200], they are used in this study for mortars also, for lack of better experimental data on these parameters. Similar values of the parameters were successfully implemented for mortars in [219] and the fracture simulations were found to be not very sensitive to the CDP parameters. The fracture energies and elastic moduli for the different mortars with varying iron powder content is provided in Table 2 while the Poisson’s ratio used for simulation is 0.2.
Table 5.2 CDP and elastic parameters for mortars with iron inclusions

<table>
<thead>
<tr>
<th>CDP model parameters [58]</th>
<th>Iron (%)</th>
<th>0</th>
<th>10</th>
<th>20</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>β, m, γ, f, E (GPa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>38°, 1, 0.67, 1.12, 21</td>
<td>0</td>
<td>25.3</td>
<td>28.7</td>
<td>31.6</td>
<td></td>
</tr>
</tbody>
</table>

3.3.5.3 Numerical Simulation Results:

The XFEM models with the aforementioned inputs were used to yield elastic and fracture outputs. While the load deflection behavior depicts the elastic and post elastic behavior of the mortars with inclusions, the fracture parameters are obtained by their load-CMOD responses, the values of which are further used to calculate the fracture parameters. These fracture parameters when correlated with the experimentally obtained values can provide a clear insight as to the applicability of XFEM model incorporating CDP for studying the influence of cracks and their propagation in quasi-brittle materials like mortars.

Figure 10 (a) Load deflection curves obtained from XFEM analysis. The load-deflection plots show an elastic behavior followed by a non-linear post peak behavior which is a function of the plastic and damage parameters. These graphs depict the predicted behavior for the mortars which, with increasing iron content, show better load carrying capacities, similar to the experimental observations as explained earlier. Figure 10(b) shows the load-CMOD responses obtained from XFEM analysis for control AAS mortar as well as the mortars with varying iron

Figure 10 (a) shows the load deflection curves obtained from XFEM analysis. The load-deflection plots show an elastic behavior followed by a non-linear post peak behavior which is a function of the plastic and damage parameters. These graphs depict the predicted behavior for the mortars which, with increasing iron content, show better load carrying capacities, similar to the experimental observations as explained earlier. Figure 10(b) shows the load-CMOD responses obtained from XFEM analysis for control AAS mortar as well as the mortars with varying iron

Figure 10 (a) Load deflection and (b) Load CMOD curves indicating P1(pre-peak) at 85% of peak load, P2(post-peak) at 95% of peak load and P3 (near ultimate failure) at 0.125mm CMOD from XFEM model of mortars containing no iron powder, and 10%, 20%, or 30% iron powder,

and 10%, 20%, or 30% iron powder.
powder contents. As seen in the figure, the load carrying capacity increases with the iron content. The points P-1, P-2 and P-3 for the mortar containing 10% iron powder as slag-replacement correspond to 85% load (pre-peak), 95% load (post-peak) and a load that yields CMOD near ultimate failure respectively. The load-CMOD responses thus obtained, are used later in this section to quantify the fracture responses of these mortars.

Figure 11 shows the maximum principal stress contours (for the mortar containing 10% iron powder) at three different stages of load-CMOD response for the XFEM model incorporating CDP. These stages correspond to three points in Figure 10 (b) where the 85% load is denoted by point P1 (pre-peak), 95% by P2 (post peak) and the point P3 stands for a load that yields a CMOD near ultimate failure. The figure corresponding to point P1 does not show any crack formation since the maximum principal stress failure criterion is not met. On the other hand, the figure corresponding to point P2 show cracks that have grown with a stress concentration at the tip of the crack. The figures corresponding to P3 depict that the cracks have propagated almost completely leading to failure.

Figure 5.11 Max principal stress contours for mortar beams with 10% iron (a) P1 (b) P2 (c) P3
To calculate the Mode I critical stress intensity factor $K_{IC}$ (fracture toughness), the crack-extension values, obtained from XFEM as well as DIC (for comparison) at 95% of the peak load in the post-peak regime are used. These can be calculated using the two-parameter fracture model (TPFM) using Equations 13 and 14 [210,297].

$$K_{IC} = \frac{PL}{bd^{\frac{1}{2}}} F\left[\frac{a_{eff}}{d}\right]$$  \[5-13\]

$$F\left[\frac{a_{eff}}{d}\right] = [2.9\left(\frac{a_{eff}}{d}\right)^{\frac{1}{2}} - 4.6\left(\frac{a_{eff}}{d}\right)^{\frac{3}{2}} + 21.8\left(\frac{a_{eff}}{d}\right)^{\frac{5}{2}} - 37.6\left(\frac{a_{eff}}{d}\right)^{\frac{7}{2}} + 38.7\left(\frac{a_{eff}}{d}\right)^{\frac{9}{2}}]$$  \[5-14\]

Where the effective crack length $a_{eff} = a_0 + \Delta a$. The CTODc or the critical crack tip opening displacement is another fracture parameter from TPFM model that is computed at 95% peak load using XFEM simulation results as well as from DIC as shown in Table 3.

<table>
<thead>
<tr>
<th>Fracture Toughness ($K_{IC}$) [MPa.mm$^{0.5}$]</th>
<th>Crack tip opening displacement, CTODc (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron %</td>
<td>0</td>
</tr>
<tr>
<td>XFEM</td>
<td>20.36</td>
</tr>
<tr>
<td>Experimental (DIC)</td>
<td>19.50</td>
</tr>
</tbody>
</table>

The fracture parameters ($K_{IC}$ and CTODc) extracted from the XFEM-based simulation are found to be in very good agreement with those predicted from direct measurements of crack extensions, obtained from DIC for AAS mortar as well as mortars with varying iron powder content. The XFEM-based simulation framework involving maximum principal stress-based crack-initiation criteria along with a crack propagation criteria that implements bilinear traction-separation law in conjunction with the concrete damage plasticity (CDP) model, can be used as an efficient alternative to direct experimental techniques such as Digital Image Correlation (DIC) in these particulate-reinforced AAS mortars. The sensitivity of the CDP model parameters of concrete to the predicted performance of mortars is not very high, as noticed from the predictions.
4. CONCLUSIONS

This study shows that elongated metallic iron particulates, generated as a waste product from manufacturing applications can be used as particulate-reinforcement in alkali activated slag mortars with comparable strength and enhanced fracture properties. The elongated iron particles act as micro-reinforcement and improve the crack resistance of the alkali activated slag mortars. The fracture response was characterized through crack growth resistance curves (R-curves) obtained from a compliance-based approach using cyclic crack mouth opening displacement-controlled three-point bending tests on notched mortar beams. The crack growth resistances increased significantly with increasing iron powder content, thereby confirming the beneficial effects of iron powder on the fracture response of alkali activated slag mortars. A direct quantification of the fracture process zone parameters (width, length and area of FPZ) was accomplished using Digital Image Correlation (DIC). The significant increase in FPZ area correlated well with the significant increase in crack growth resistances achieved with particulate reinforcement, as increased area of FPZ dissipates significant amount of energy and thus provides improvement in fracture response.

The fracture response of notched beams under three-point bending were simulated using XFEM. The maximum principal stress criteria was adopted in this study for damage initiation. The total fracture energy obtained from a bilinear traction-separation response was used in conjunction with the concrete damage plasticity (CDP) model in ABAQUS™ to simulate crack propagation. The fracture parameters (K_{IC} and CTOD_C) extracted from the XFEM-based simulation were found to be in good agreement with those obtained from DIC for AAS mortar as well as mortars with varying iron powder content. The XFEM-based simulation framework provides for direct measurements of crack extensions (\(\Delta a\)) and fracture responses (K_{IC} and CTOD_C) in particulate-reinforced quasi-brittle materials as an efficient alternative to direct experimental techniques such as Digital Image Correlation (DIC).
Chapter 6

Strain sensing and damage detection ability of nanoengineered cementitious composites

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A microstructure-guided numerical approach to evaluate strain sensing and damage detection ability of random heterogeneous self-sensing structural materials

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ABSTRACT

Heterogeneous self-sensing materials that respond electrically to mechanical strains enable real time health monitoring of structures. To facilitate design and applicability of such smart materials with piezo-resistivity, a finite element-based numerical framework is being proposed in this paper for evaluation of electro-mechanical response and strain-sensing ability. Intrinsic heterogeneous nature of such composites warrants the need for microstructure-based study to have an insight into the effect of microstructural configuration on the macro-scale response. The microstructure-guided simulation framework, presented in this paper, implements interfacial debonding at the matrix-inclusion interface using a coupled interface damage-cohesive zone model and incorporates an isotropic damage model in the matrix under applied strain in the post-peak regime to obtain the deformed/damaged microstructure which is subjected to an electrical potential to simulate change in resistance due to applied strain. The applicability of the simulation framework is confirmed through its successful implementation on a smart structural material containing nano-engineered conductive coating at the inclusion-matrix interfaces. The predicted electro-mechanical responses correspond very well with the experimental observations and thus, the model has the potential to help develop design strategies to tailor the microstructure in these self-sensing materials for efficient performance.

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1. INTRODUCTION

Structural Health monitoring (SHM) provides valuable information on the reliability and safety of the structures and it can help develop strategies to save the structures before critical damage threatens the structural integrity [50,51]. Strain- and damage-sensing are integral aspects of SHM. Most of the load-bearing structures are very sensitive to damage and it can cause catastrophic failures leading to immense loss of life and property [50,52]. Therefore costly routine inspections have been used for maintenance of these structures. Traditionally, various non-destructive testing (NDT) techniques such as ultrasound testing, radiographic tests (X-ray) etc. have been used, although they are impractical and expensive for large structures. Thus, there has been a need for a real-time mixed global/local damage-sensing approach. For real-scale industrial structures, use of smart composites is gaining popularity in recent times for strain-sensing in structures [53–55]. In particular, such smart composites achieve damage-sensing capability by utilizing piezoresistivity which is an electromechanical phenomenon that enables certain electrically conductive composites to respond electrically under the influence of strain [56–63]. Electrical resistance methods in these composites have been shown to be sensitive to minor and microscopic changes that include defects or damage [59,63–65].

Design of such smart materials requires a reliable numerical method that can predict electro-mechanical response at different length scales. This paper presents a comprehensive microstructure-guided electro-mechanical response prediction framework for a large class of smart heterogeneous materials using finite element modelling. In particular, the numerical framework is applied towards prediction of strain-sensing efficiencies in smart cementitious composites for infrastructure applications. In cement-based materials self-sensing capability has been achieved using carbon fibers, steel fibers and carbon nanotubes [56,58,63,298]. Although a variety of experimental studies [57–64,299] report on electro-mechanical response of these systems under tension and compression, limited studies exist on prediction of strain-sensing and damage-detection efficiency in such self-sensing cementitious materials which is the primary goal of this research paper. The numerical simulation framework, presented in this paper, is developed for the first time in order to incorporate an applied strain range that encompasses both the elastic and the post-peak constitutive behavior thereby achieving both strain and damage sensing by electrical measurements in these cementitious matrices. The modelling scheme involves: (1) generation of representative microstructure of the heterogeneous composite using a stochastic packing algorithm; (2) application of periodic boundary conditions [110,236,300–302] in the representative unit cell to simulate a strain-controlled mechanical test scenario; (3) incorporation of interface damage to simulate
interfacial debonding at the inclusion-matrix interface; (4) incorporation of an isotropic damage theory for damage in the matrix in the post-peak regime; (5) determination of effective constitutive behavior of the heterogeneous material; (6) re-meshing the deformed/damaged geometry corresponding to any specific applied strain and (7) determination of electrical response of the damaged/deformed microstructure. Steps 6 and 7 are performed for strains both in the elastic and the post-peak regime to obtain change in electrical responses for all the applied strains. The versatility of this approach is verified on a smart self-sensing cementitious material enabled by nano-engineered matrix-inclusion interface [303]. This smart material uses thin multi walled carbon nanotube (MWCNT)-based polymeric films at the matrix-inclusion interface [64,65,303]. Thus, this paper intends to demonstrate a numerical framework to evaluate the strain- and damage-sensing efficiency of several heterogeneous materials facilitating microstructure-guided material design.

2. NUMERICAL SIMULATION FRAMEWORK FOR ELECTROMECHANICAL RESPONSE EVALUATION AND DAMAGE DETECTION

This section describes the framework which executes numerical simulation to evaluate electro-mechanical response of self-sensing materials using finite element analysis (FEA). Influence of damage and damage-sensing capability of the material is efficiently integrated into the simulation framework. Figure 1 summarizes the numerical simulation framework using a flowchart representation.

![Figure 6.1 Flowchart of numerical simulation framework](image-url)
The framework involves generation of a representative unit cell and evaluation of electromechanical responses implementing mechanical and electrical modules. The analysis framework is implemented here using a python script for ABAQUS™ solver. The mechanical module simulates a mechanical response of the unit cell under externally applied uniaxial strain and it accounts for interface damage at the matrix-inclusion interface. In addition, the mechanical module implements constitutive behavior of heterogeneous composites beyond the cracking strain (post-peak response) by implementing an isotropic damage model [96,97,130] in the matrix through a user-defined subroutine in ABAQUS™ [127,128,304]. An intermediate remeshing module imports the deformed configuration of the unit cell, obtained from the mechanical module and improves the quality of mesh before exporting the re-meshed unit cell to the electrical module as a starting geometry for the electrical analysis in order to achieve electro-mechanical response of the unit cell under applied strain. The electrical module obtains the deformed configuration of the unit cell from the remeshing module and obtains current distribution in the deformed unit cell under imposed electrical potential. Post processing of the relevant electrical responses in MATLAB© yields a homogenized change in electrical resistivity under different applied strains. Different components of the framework are detailed in the forthcoming sub-sections.

2.1 Generation of Representative Unit Cells

The unit cells are generated here using the Lubachhevsky-Stillinger algorithm [101,103,104]. This algorithm employs a hard contact model and hence particle overlaps are not allowed. First, the desired inclusions are randomly distributed inside the periodic bounding box with random initial velocities of the particles. The radius of each particle is first initialized as zero. The radius of \( i^{th} \) particle \( (r_i) \) in the next event is a function of the growth rate \( (g_i) \), which is tailored to attain the desired particle size distribution shown in Equation 1.

\[
\frac{dr_i}{dt} = g_i \tag{6-1}
\]

Here \( i = 1, 2, \ldots \) is the number of particles. The growth rate between time \( t^n \) and \( t^{n+1} \) is computed using a finite difference scheme as follows.

\[
g_i = \frac{(r_i^{n+1} - r_i^n)}{\Delta t} \tag{6-2}
\]

Where \( r_i^{n+1} \) and \( r_i^n \) are radius at time \( t^n \) and \( t^{n+1} \) respectively and \( \Delta t = (t^{n+1} - t^n) \). The particle radii are then updated as follows for time \( t^{n+1} \) by employing the growth rate and time increment \( (\Delta t) \) as follows.

\[
r_i^{n+1} = r_i^n + g_i \Delta t \tag{6-3}
\]
In addition, the position of particle ‘i’ at time $t^{n+1}$ i.e. $x_i^{n+1}$ is updated considering a constant velocity ($v_i^n$) between the time nodes.

$$x_i^{n+1} = x_i^n + v_i^n \Delta t$$  \hspace{1cm} [6-4]

The vector that connects the centers of particles ‘i’ and ‘j’ is obtained by subtracting the position vectors of the two particles.

$$\mathbf{I}_{ij}^{n+1} = x_j^{n+1} - x_i^{n+1}$$  \hspace{1cm} [6-5]

The particles ‘i’ and ‘j’ are expected to be in contact if the sum of their radii is equal to the length of the connection vector. The time step size can be calculated as

$$\Delta t = \min \left[ \frac{-v \pm \sqrt{v^2 - uw}}{u} \right]$$  \hspace{1cm} [6-6]

where $\Delta t > 0$ and $v$, $u$ and $w$ are given as.

$$v = \mathbf{I}_{ij}^n \cdot \left[ v_j^n - v_i^n \right] - \left[ r_i^n + r_j^n \right] \left[ g_i + g_j \right]$$  \hspace{1cm} [6-7a]

$$u = \left[ v_j^n - v_i^n \right]^2 - \left[ g_i + g_j \right]^2$$  \hspace{1cm} [6-7b]

$$w = \mathbf{I}_{ij}^n \cdot \left[ r_i^n + r_j^n \right]^2$$  \hspace{1cm} [6-7c]

Here, $v_i^n$ and $v_j^n$ are the velocities of particles ‘i’ and ‘j’ at time $t^n$. $r_i^n$ and $r_j^n$ are the radius of particles ‘i’ and ‘j’ at time $t^n$. $g_i$ and $g_j$ are growth rates for particle ‘i’ and ‘j’ respectively. The vector connecting the position of the two particles at time $t^n$ is given as $\mathbf{I}_{ij}^n = x_j^n - x_i^n$. The time step calculation (Equation 6) is performed for each particle pair that are being able to collide and thus minimum time step for all the possible collisions is adopted to move forward for the next event. All the particle positions $x_i^{n+1}$ are updated using the forward Euler scheme (Equation 4) and new search for the next collision(s) is started. The post-contact velocities are computed as follows.

$$v_{n_i}^{n+1^+} = \min \{ v_{n_i}^{n+1^-}, v_{n_j}^{n+1^-} \} - g_i ; v_{n_j}^{n+1^+} = \max \{ v_{n_i}^{n+1^-}, v_{n_j}^{n+1^-} \} + g_i$$  \hspace{1cm} [6-8]

Where $v_{n_i}^{n+1^+}$ is the velocity after the contact and $v_{n_i}^{n+1^-}$ is the velocity before the contact. Thus, all the above-mentioned steps are repeated and in the process of iterations the particles change position in the bounding box, collide and grow in order to obtain desired volume fraction. Finally, the obtained microstructural information is implemented via a python language script to enable it to be imported to a commercial finite element software. The formulations are found in [102].

2.2 Mechanical module

The mechanical module implements periodic boundary conditions [108,109], meshes the unit cell, implements interfacial damage at the inclusion-matrix interface and incorporates isotropic damage in the matrix in the post-peak regime as described in the following sub-sections.
2.2.1 Boundary condition

Once the unit cell is generated, it is imported to the mechanical module. The mechanical module is summarized in Figure 2. The unit cell is first meshed using the python script and Periodic boundary conditions (PBC) [110,236,300] are applied. PBCs have been applied successfully towards FE analysis of random heterogeneous materials [106]. Periodic boundary conditions are shown to be computationally efficient even with smaller size of unit cells facilitating faster convergence [101]. PBC ensures displacement and traction continuity across the boundaries of neighboring unit cells. In 2D, periodic microstructure the displacement field is given as follows.

\[ v_i(x_1, x_2) = \varepsilon^0_{ij} x_j + v^s_i(x_1, x_2) \]  \[[6-9]\]

Here, \( \varepsilon^0_{ij} \) is the applied strain tensor, and \( v^s_i \) is a periodic function representing the modification of linear displacement field due to the heterogeneous microstructure. On a pair of parallel opposite boundary edges the displacements are given as follows.

\[ v^{s+}_i = \varepsilon^0_{ij} x_j^{s+} + v^s_i \]  \[[6-10a]\]

\[ v^{s-}_i = \varepsilon^0_{ij} x_j^{s-} + v^s_i \]  \[[6-10b]\]

Here, \( s^+ \) and \( s^- \) are \( s^{th} \) pair of two opposite parallel boundary surfaces of the unit cell. The periodic function \( v^s \) is the same at both the parallel opposite edges due to periodicity. Subtracting 10b from 10a the difference in displacements on two parallel edges are obtained as follows.

\[ v^{s+}_i - v^{s-}_i = \varepsilon^0_{ij} (x_j^{s+} - x_j^{s-}) = \varepsilon^0_{ij} \Delta x_j^s \]  \[[6-11]\]

\( \Delta x_j^s \) is constant for an applied \( \varepsilon^0_{ij} \). The strain is applied on the unit cell using the system of equations through a reference point. The general form of system equations can be written as follows.

\[ v^{s+}_i - v^{s-}_i + v^{s\text{dummy}}_i = 0 \]  \[[6-12]\]

Such linear equations are implemented for all parallel face pairs in 3D unit cells. Strain is applied on the unit cell through the constraint equations to simulate a strain-controlled test scenario. More details on the PBC can be found in [100,102].

2.2.2 Incorporation of Interfacial Debonding
The mechanical module incorporates interfacial debonding at the inclusion-matrix interface. The interfacial debonding is implemented here using a continuum damage model coupled with cohesive zone model (CZM) \cite{196,305,306}. Here, a continuity in displacement is ensured by implementation of zero-thickness interface elements. Such zero-thickness interface elements have been implemented successfully to model relative slip or separation on a predetermined surface in \cite{154,307}. The theoretical framework of CZM involves a phenomenological model of failure where the assumed fictitious micro-cracks in the cohesive zone can exhibit interactive stresses, thereby enabling application of traction-separation law \cite{197,308}. The separation in the traction-separation law is characterized here using an equivalent interface opening ($\lambda$). Here, $\lambda$ consists of positive normal displacement jump $\langle [u_n] \rangle$ and tangential displacement jump $[u_t]$ across the zero-thickness interfacial elements as shown in Equation 13.

$$\lambda = \sqrt{\langle [u_n] \rangle^2 + [u_t]^2} \quad [6-13]$$

The characteristic value of equivalent interface opening, $\lambda_0$ denotes the limit beyond which the traction at any interface element decreases with increasing $\lambda$. When $\lambda < \lambda_0$, the equivalent traction $\sigma_c$ is expressed using a penalty stiffness $K_p$ as follows.

$$\sigma_c = K_p \lambda \quad [6-14a]$$

when $\lambda \geq \lambda_0$, the following relationship is implemented \cite{154,309}.

$$\sigma_c = f_t \exp \left( \frac{-f_t (\lambda - \lambda_0)}{G_F} \right) \quad [6-14b]$$

Where $f_t$ is the tensile strength and $G_F$ is the total fracture energy. $\lambda_0 = \frac{2G_F}{f_t} = \frac{f_t}{K_p}$ Where initial fracture energy, $G_F = \frac{K_{IC}^2}{E}$, $K_{IC}$ is the mode-I fracture toughness and $E$ is the Young’s modulus.

The equivalent traction is integrated over the volume to obtain the potential $\phi$, the partial derivatives of which with respect to normal and tangential components of the displacement jump yield the normal traction $t_{cn}$ and tangential traction $t_{ct}$ respectively as shown in Equation 15.

$$t_c = \begin{pmatrix} t_{cn} \\ t_{ct} \end{pmatrix} = \begin{pmatrix} \frac{\partial \phi}{\partial [u_n]} \\ \frac{\partial \phi}{\partial [u_t]} \end{pmatrix} \quad [6-15]$$

The mechanical tangent material matrix $C_c^t$ can be expressed as partial derivatives of the resulting traction with respect to displacement jump as shown in Equation 16.

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It should be noted here that the above formulations are applied for tension, when the interface opening in the normal direction is positive. In case of compression the normal interface compressive pressure is given as follows.

\[ t_{cn} = K_p [u_n] \]  

[6-17]

Therefore, the mechanical tangent material matrix can be expressed as follows.

\[
C_c^u = \begin{bmatrix}
\frac{\partial t_{cn}}{\partial [u_n]} & \frac{\partial t_{cn}}{\partial [u_t]} \\
\frac{\partial t_{ct}}{\partial [u_n]} & \frac{\partial t_{ct}}{\partial [u_t]}
\end{bmatrix}
\]

[6-16]

The tangent material matrix \( C_c^u \) is transformed to the local co-ordinate system to obtain stiffness matrix of each cohesive element. While the penalty stiffness governs the traction-separation law with increase in \( \lambda \) when \( \lambda < \lambda_0 \), the mechanical stiffness matrix is modified at every iteration with increasing \( \lambda \) based on phenomenological damage model when \( \lambda \geq \lambda_0 \). Damaged mechanical stiffness matrix for interface elements obtained is used as the initial stiffness of the cohesive elements in the next step with increment in \( \lambda \). Here, progressive debonding has been characterized with increasing \( \lambda \) using a scalar interface damage parameter \( D_c \) which is defined as follows.

\[
D_c = \frac{\lambda}{\lambda_{cr}}
\]

[6-19]

Where \( \lambda_{cr} \) corresponds to equivalent interface opening at very low traction values in the post-peak regime of the traction-separation behavior, generally computed at 0.1 \( f_t \) in the post-peak regime [154]. The numerical simulation of the CZM extended damage model, as explained above, is implemented here using user-defined subroutine in ABAQUS\textsuperscript{TM} and it requires initial fracture energy \( (G_f) \), total fracture energy \( (G_F) \) and tensile strength of matrix \( (f_t) \) as input [214].

### 2.2.3 Damage in the matrix

In order to incorporate damage in the matrix in the post-peak regime, a damage module is incorporated inside the mechanical module. A continuum damage model is implemented here in the matrix once the applied strain exceeds the elastic limit \( (\varepsilon_{EL}) \). Assuming isotropic stiffness degradation, the damage variable, \( D \) is given as [95–97,130] follows.

\[
\sigma = (1 - D) C : \varepsilon
\]

[6-20]
Where the effective stress tensor is denoted by \( \sigma \), \( \mathbf{C} \) denotes fourth order tensor of elasticity and \( \varepsilon \) is the strain tensor. The value of damage, \( D \) ranges from 0 (undamaged) to 1 (completely damaged). The damage rate denoted by \( \dot{D} \) assumes only zero or positive values which can be explained by its proportionality with the damage energy release rate [96]. The overall damage \( D \) is a weighted sum of its tensile and compressive parts \( (D_t \text{ and } D_c) \) that addresses the difference in tensile and compressive behavior of heterogeneous materials as shown in Equation 21 [96,97].

\[
D = \alpha_t D_t + \alpha_c D_c
\]

[6-21]

For uniaxial tension value, of the parameter \( \alpha_t \) becomes 1 and the parameter \( \alpha_c \) becomes zero whereas the values of the parameters \( \alpha_t \) and \( \alpha_c \) are taken as zero and 1 respectively for uniaxial compression [96]. A non-local equivalent strain \( \bar{\varepsilon} \) is used to obtain the tensile and compressive damage, \( D_t \) and \( D_c \) respectively which is defined as [95,96] follows.

\[
\bar{\varepsilon} = \sqrt{\sum_i <\varepsilon_i>^2}
\]

[6-22]

Where \( <\varepsilon_i> \) is the positive part of the principal strain. The damage \( D_t \) and \( D_c \) evolve as a function of \( \bar{\varepsilon} \) as per the Equation 23-a and 23-b[95–98,130] follows.

\[
D_t(\bar{\varepsilon}) = 1 - \frac{\varepsilon_{D_b} (1 - A_t)}{\bar{\varepsilon}} - \frac{A_t}{\exp[B_t (\bar{\varepsilon} - \varepsilon_{D_b})]}
\]

[6-23-a]

\[
D_c(\bar{\varepsilon}) = 1 - \frac{\varepsilon_{D_b} (1 - A_c)}{\bar{\varepsilon}} - \frac{A_c}{\exp[B_c (\bar{\varepsilon} - \varepsilon_{D_b})]}
\]

[6-23-b]

Where \( \varepsilon_{D_b} \) is damage initiation threshold (the ratio of tensile strength to the Young’s modulus for quasi-brittle materials). The model can be fitted to experimentally obtained uniaxial tensile and compressive constitutive response of various matrices to obtain corresponding values for the parameters \( \varepsilon_{D_b} , A_t , B_t , A_c \text{ and } B_c \). The material continuum damage is implemented here using user defined subroutine in ABAQUS™ [304]. The mechanically deformed/damaged geometry thus obtained is exported to re-meshing module to improve the quality of mesh as explained in the forthcoming section.
2.3 Intermediate Re-meshing Module

The deformed or damaged geometry of the unit cell, obtained from mechanical module, is re-meshed using this intermediate module. This module implements remeshing using a MATLAB subroutine. The subroutine operates on the deformed geometry and performs re-meshing/ mesh-refinements wherever the aspect ratio of the elements exceeds 3. The remeshing module, thus improve the quality of mesh in the deformed/damaged unit cell. The re-meshed deformed or damaged unit cell is then exported to the electrical module for electrical analysis.

Figure 6-2 Schematic representation of the mechanical module
2.4 Electrical module

The electrical module imports the deformed and re-meshed unit cell and assigns electrical properties to the component phases. In order to characterize the electrical response of the damaged unit cell, the damaged elements in the matrix are modeled with an electrical conductivity that decreases proportionally with the mechanical damage variable D. The electrical conductivity of the damaged elements ($\sigma_i$) can be expressed in terms of the initial conductivity ($\sigma_{i-1}$) as follows.

\[
\sigma_i = (1 - D)\sigma_{i-1}
\]  

[6-24]

Similar relationships have been successfully implemented for thermal analyses coupled with mechanical damage elsewhere [154,310]. At every state of progressive damage, the conductivity is reduced proportional to the damage variable D. As the material damages fully, the simulation framework theoretically assumes an infinite resistance. In order to characterize the electrical behavior of the mechanical damage on the inclusion-matrix interface, the interface elements where the interface damage variable ($D_c$) reaches 1, are considered a perfect resistor with infinitely high electrical resistance.

After assignment of material properties, boundary conditions are incorporated. All other faces except the ones perpendicular to Y axis are insulated as can be seen in Figure 3. A unit potential is applied across the microstructure in the Y direction as shown in Figure 3. The electrical module computes current density ($\vec{J}$) from the input electrical conductivity($\sigma$) of component phases and the applied electric field ($\vec{E}$) using Ohm’s Law ($\vec{J} = \sigma\vec{E}$). The simulation yields the electric field and current density distribution in the unit cell which when volumetrically averaged by a post-processing module yields the average electrical conductivity as per Equation 25 [216,311].

\[
\sigma = \frac{\vec{I}}{\vec{E}}
\]  

[6-25]

For a comparative representation, the average electrical conductivities ($\sigma$) are expressed in terms of the fractional change in resistance (FCR) which is the ratio of the change in resistance ($\Delta R$) and the bulk resistance of mechanically undeformed microstructure ($R_0$) as shown in Equation 26 [216].

\[
FCR = \frac{\Delta R}{R_0} = \frac{\sigma_0}{\sigma} - 1
\]  

[6-26]

Where $\sigma_0$ is the conductivity response of the mechanically undeformed microstructure. In order to characterize the electrical response of the damaged microstructure, the damaged elements are
modeled as insulators as explained earlier. The additional resistivity thus imparted to the overall microstructure leads to a different trend in FCR plotted with strain beyond the elastic limit.

Figure 6.3 Schematic representation of the electrical module

The microstructure guided electro-mechanical simulation can be performed at different length scales so as to obtain macro-scale electro-mechanical response of heterogeneous smart materials. The numerical simulation framework, presented herein, can be used towards prediction of macroscopic electro-mechanical response of several random heterogeneous smart materials facilitating microstructure-guided material-design. In the forthcoming section, the numerical prediction scheme is applied to a smart cementitious material enabled by a nano-engineered matrix-inclusion interface to evaluate the effectiveness of the modelling framework.
3. APPLICATION OF THE MODEL TO A SMART STRUCTURAL MATERIAL CONTAINING NANO-ENGINEERED INCLUSION-MATRIX INTERFACES

This section describes the application of the aforementioned framework to a smart self-sensing cementitious material enabled through a nano-engineered cement-aggregate interface [65,303]. Such conductive coatings contain carbon nanotube (CNT) based thin latex films, the synthesis and application procedure of which is discussed in detail in [64,312]. These films are deposited on sand via airbrushing thus enabling a higher degree of dispersion in the composite matrix of the composite with a lesser carbon content than conventional CNT dispersion techniques [303,313]. Such conductive coatings are experimentally shown to be extremely effective in self-sensing applications [65,303]. The forthcoming sub-sections apply the electro-mechanical simulation framework to elucidate the influence of interfacial debonding, electrical conductivity and thickness of coating for a compressive understanding. In addition, this section also compares the numerical simulation results, obtained from the simulation framework for the smart self-sensing cementitious material with the experimental results reported in [65] with a view to validate the simulation framework.

3.1 Influence of conductive coating on the strain sensing and damage detection capability

As explained earlier, the mechanical module is first initiated which generates the unit cell using Lubachhevsky-Stillinger algorithm [103–105], meshes the unit cell, applies periodic boundary conditions and implements a displacement-controlled simulation to obtain the deformed unit cell. Here, the volume fraction of sand is 45% [65]. The generated unit cell is shown in Figure 4(a). Sand particles ($d_{50}$ is 600 µm [243]) are dispersed in the unit cell of edge length 3 mm. The edge length of unit cell is adopted here as five times the mean diameter of sand particles. Similar relative size of unit cell with respect to size of inclusion has been successfully applied to evaluate micromechanical responses of cementitious composites in [101,106]. An absolute thickness of 10 µm of the conductive coating is adopted in this study unless varied to evaluate the influence of coating thickness. A thickness of 10 µm has been shown to yield an electrically conducting composite in [64]. This study also considers interfacial transition zone (ITZ) around the sand particles. The thickness of ITZ is considered to be 20 µm [144–146]. In order to implement interfacial debonding zero-thickness interfacial elements are implemented at the conductive coating-ITZ interface (refer to section 2.2.2). The unit cell is finely meshed using CPE4R elements in ABAQUS™. A mesh-sensitivity study was performed and a mesh containing 362137 CPE4R elements (in ABAQUS™) yielded converged solution. The converged mesh is shown in Figure
Here 2D unit cells are considered instead of 3D as a tradeoff between computational efficiency and demand. Similar 2D unit cells are successfully adopted for cementitious materials in [101,243].

![Microstructure](image)

Figure 6-4 (a) generated microstructure with the coated sand particles dispersed in hardened cement paste (HCP) matrix and (b) meshed microstructure

The mechanically deformed configuration, obtained from mechanical module, is imported to the remeshing module where the deformed geometry is re-meshed ensuring a good quality (aspect ratio \(\leq 3\)) of elements. The re-meshed unit cell is imported to electrical module for electrical analysis. The electrical module implements insulation at the edges parallel to y axis and applies a unit potential difference to obtain electric current distribution (ECD) and electric field in the unit cell. The post processing module computes the fractional change in resistance as explained earlier. The input material properties, shown in Table 1, are adopted from [64,146,216,243,314–318].

<table>
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<th>E (GPa)</th>
<th>(\nu)</th>
<th>(\sigma) (S/m)</th>
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<td>[243,316,319]</td>
<td>[243,316,319]</td>
<td>[216,314,315,318,320,321]</td>
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### Coating

<p>| | | | |</p>
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<tr>
<td>ITZ</td>
<td>10</td>
<td>0.2</td>
<td>0.002</td>
</tr>
</tbody>
</table>

#### 3.1.1 Consideration of interfacial debonding

The mechanical module implements a continuum damage model coupled with cohesive zone model (CZM) at the zero-thickness interfacial elements in between the conductive coating and the ITZ, as explained earlier, to simulate debonding at the cement paste-coated aggregate interface under tensile strains. The traction-separation law is defined by tensile strength ($f_t$), total fracture energy ($G_F$) and initial fracture energy ($G_F$) as explained earlier in section 2.2.2. Values of these parameters, adopted in this simulation are 2.7 MPa, 25 N/m and 19 N/m respectively as reported in [246,322,323]. It should be noted that values of these parameters for the interface elements are considered same as the HCP matrix in this study due to lack of data. Debonding subroutine is implemented as explained in section 2.2.2 and values of scalar interface damage parameter ($D_c$) are obtained for the zero-thickness cohesive interface elements. The electrical module assigns insulation behavior at the interface elements where the value of $D_c$ reaches 1.

Figures 5(a-1), (a-2) and (a-3) plot the interface damage parameter, $D_c$ (Equation 19) in the zero-thickness interfacial elements under applied strain of 0%, 0.00075% and 0.0161% respectively whereas Figures 5(b-1), (b-2) and (b-3) show the corresponding electric current densities under applied unit electrical potential. The figures suggest that the debonding areas increase progressively with increase in strain. Consequently, the electric current densities at the conductive coating gets altered resulting in change in the characteristics of the electrical response in the unit cell. Figures 5(b-1), (b-2) and (b-3) show overall reduction in the current density with progressive debonding and deformation due to increase in applied strain. Enlarged views of a sand particle under these strains also reveal alteration of ECD in the conductive coating with progressive interfacial debonding resulting in change in resistance and thereby change in FCR.
Figure 6-5 Influence of interfacial debonding on the electro-mechanical response: (a-1) interface damage parameter in the unit cell without any externally applied strain; interface damage parameter corresponding to applied strain of (a-2) 0.0075% and (a-3) 0.0161%; (b-1) ECD along Y direction for applied unit electrical potential corresponding to: (b-1) undeformed unit cell, (b-2) unit cell under applied strain of 0.0075% and (b-3) unit cell under applied strain of 0.0161%

In order to evaluate the influence of debonding on the FCR, a dimensionless scalar parameter, fractional interface debonding is introduced which can be defined as the fraction of the total
perimeter of inclusions that has de-bonded completely ($D_C=1$). Figure 6 shows the fractional interface debonding and FCR with variation of applied strain. The fractional interface debonding increases progressively with increase in tensile strain. Consequently, the FCR also increases due to additional resistance in the unit cell imparted by the de-bonded interface which makes the associated fraction of conductive coating ineffective. With progressive interfacial debonding, the stress in the matrix increases due to lack of stress-transfer from the matrix to the stiffer inclusions. Finally, the stress in the matrix reaches its strength when the strain is increased beyond 0.0161% and the damage in the matrix is initiated. Beyond this point, fractional interface debonding remains almost constant and the progressive damage in the matrix becomes dominant. The influence of progressive matrix-damage on the FCR is elucidated in the forthcoming section with a view to evaluate the damage-sensing capability of this smart cementitious material.

![Figure 6 - Fractional interface damage and FCR with varying tensile strain](image)

**3.1.2 Influence of conductive coating on damage-sensing capability**

This section implements a continuum damage model, explained earlier (refer to section 2.2.3), in the HCP matrix of the mortar microstructure to evaluate the damage-sensing capability of the smart material in the post-peak regime. The model assumes isotropic stiffness degradation and it requires the parameters $\varepsilon_{D_b}, A_t, B_t, A_c$ and $B_c$ for HCP matrix as input (Equation 23). In the context of tensile damage, the values of the parameters $\varepsilon_{D_b}, A_t$ and $B_t$ for HCP matrix are 0.0001, 1 and 10000 respectively which are adopted from the literature [154]. The damage model parameters in ITZ are considered to be same as the HCP matrix due to lack of data. The continuum damage model is implemented using user defined subroutine in ABAQUS™ and the scalar damage variable, D (Equation 23) in the matrix is obtained.
To obtain the electrical responses, the damaged microstructure is re-meshed and imported to the electrical module where the electrical conductivity of damaged elements was modified proportional to the damage variable $D$ (Equation 24). Figures 7(a-1), (a-2) and (a-3) plot the values of the damage variable ($D$) under applied tensile strain of 161, 170 and 210 $\mu\varepsilon$ respectively. While Figure 7 (a-1) doesn’t show any damage in the matrix, Figures 7 (a-2), (a-3) show progressive damage in the matrix with increase in the applied strain in the post-peak regime. The extent of interfacial damage (debonding) remains almost same beyond applied strain of 161 $\mu\varepsilon$. Figures 7(b-1), (b-2) and (b-3) show the influence of progressive matrix-damage (under applied tensile strain of 161, 170 and 210 $\mu\varepsilon$ respectively) on the electrical response. The general trend in the electrical responses suggest a decrease in the ECD with progressive damage.

In order to shed more light on the relationship between damage and electrical response, Figure 8 plots the overall variation of FCR and stress with increasing tensile strain. It can be observed clearly from Figure 8 that, the FCR increases almost linearly with increase in strain initially up to a tensile strain of approximately 25-30 $\mu\varepsilon$ beyond which the relationship becomes non-linear due to onset of interfacial debonding. As the damage in matrix initiates (beyond the peak stress), the rate of increase in FCR with respect to increase in strain increases rapidly and the sudden jump

![Progressive damage in HCP matrix corresponding to applied strain of (a-1)161 $\mu\varepsilon$, (a-2) 170 $\mu\varepsilon$ and (a-3) 210 $\mu\varepsilon$; ECD (A/m$^2$) in Y direction in the unit cells corresponding to applied strain of: (b-1)161 $\mu\varepsilon$, (b-2) 170 $\mu\varepsilon$ and (b-3) 210 $\mu\varepsilon$]
represents the onset of damage in the matrix. Thus, the relationship, shown in Figure 8, substantiates the strain-sensing capability of the smart cementitious material in the pre-peak regime as well as damage sensing capability in the post-peak regime.

![Graph showing tensile stress and FCR](image)

Figure 6-8 Progressive damage and FCR with increasing tensile strain

### 3.1.3 Influence of thickness and electrical conductivity of the coating

While the previous section highlighted the strain/damage sensing capability of the smart material, this section elucidates the influence of the electrical conductivity and thickness of the coating on the overall sensing efficiency. Figure 9(a) shows the influence of thickness of coating on the FCR while considering a constant electrical conductivity of 1000 S/m for the coating [314,315]. The general trend suggests that the FCR increases with increase in coating thickness for all the applied strains although the rate of increase in FCR with respect to coating thickness decreases beyond a thickness of 12 microns, a phenomenon often observed in non-conductive matrices with conductive phases [298,324]. Almost insignificant amount of increase in FCR is observed when the thickness increased from 18 microns to 30 microns. From the simulations, it is clear that a thin conductive film of around 10-20 microns thickness is enough to obtain the efficiency required for strain-sensing in these materials. Figure 9(b) shows the influence of electrical conductivity of the coating of thickness 10 microns on the overall FCR of the smart material. Variation of CNT loading in the latex matrix leads to a change in overall conductivity of the MWCNT-latex film deposited on the sand. A wide range of values of conductivity have been reported in literature[314,324,325], the maximum being 1000 S/m[314,315]. An almost linearly increasing trend of FCR is observed with the increase in the coating conductivity which can be attributed to the increasing overall conductivity of the system due to increase in the volume fraction of conductive coating. Trends in both Figures 9(a) and (b) suggest a significant increase in FCR when the strain is increased from
27 με to 81 με. This is attributed to the onset of interfacial debonding beyond 27 με which results in additional resistance and thereby increase in FCR as explained earlier in this paper. The parametric variations indicate that the FCR is more sensitive to change in coating thickness as compared to change in conductivity of coating within bounds. FCR increased more than four-folds when the thickness of coating increased from 8 microns to 20 microns whereas a relatively smaller increase (about 60%) in FCR was observed when the conductivity increased from 200 to 1000 S/m. Its significance lies in the fact that the experimental limitations of achieving higher coating conductivity with CNT loading [315] can be offset with the variation of thickness of such coatings to obtain a more sensitive overall system.

![Graph](image)

Figure 6.9 (a) Variation of FCR with varying coating-thickness; (b) relationship between FCR and the conductivity of the coating for different applied strains.

### 3.2 Comparison of simulation results with experimental observations

This section applies the numerical simulation framework to predict strain-sensing behavior of the smart cementitious material containing nano-engineered cement-aggregate interface under compression and compares the numerical simulation results with the experimental results reported in [65]. The mortar consists of 45% coated sand and the binder contains 25% ground granulated blast furnace slag (GGBFS) by weight as cement-replacement. The thickness of the conductive coating is 10 microns [64]. The material properties of sand, conductive coating and ITZ are reported in Table 1 [64,146,216,243,314–318]. The conductivity of the matrix is reduced by 20% owing to the presence of 25% GGBFS by weight [326,327] whereas the values of Young’s modulus and Poisson’s ratio of the binder matrix are considered same as that of HCP [328]. Interfacial debonding is incorporated using traction-separation law defined by the parameters initial fracture energy ($G_f$), total fracture energy ($G_{fT}$) and tensile strength of matrix ($f_t$). Values of these parameters adopted in
this simulation are considered same as the HCP matrix as reported earlier in the section 3.1.1. Here in case of compression, the tangent material matrix, shown in Equation 18, is used and the scalar interface damage parameter, $D_c$ is obtained in the matrix as well as in the ITZ. Isotropic damage under compression is incorporated using the parameters $\varepsilon_{D_h}$, $A_c$ and $B_c$. The values of these parameters used in this simulation are 0.0001, 1 and 10000 respectively [154]. The deformed/damaged unit cell is re-meshed and imported to the electrical module which computes electrical responses for varying strains as explained earlier in this paper.

Figure 10 compares the FCR values obtained from the simulation framework to the ones reported in an experimental study [65]. Figure 10(a) plots the simulation results considering only interfacial debonding without considering damage in the matrix. The simulated FCR values correspond well with the experimental measurements when the applied compressive strain is lower than approximately 0.16% whereas the simulated values diverge from the experimental observations at higher compressive strains. This can be attributed to the damage in the matrix which is not captured by the model. Figure 10(b) shows the simulated FCR values when isotropic damage model in the matrix is incorporated in addition to interface damage. Upon implementation of continuum damage in the matrix, the high strain FCRs also match closely with the experimental measurements as can be seen in Figure 10(b). Incorporation of the isotropic damage enables significantly improved prediction of FCR in the post-peak regime thus verifying applicability of the current simulation framework towards prediction of strain-sensing and damage-sensing capabilities of smart cementitious materials.

![Figure 10](image_url)

Figure 10 The simulated and experimental FCR with varying compressive strain (a) The simulation does not consider damage in the matrix; (b) simulation incorporates isotropic damage in HCP matrix
4. CONCLUSIONS

This paper presents a comprehensive numerical approach towards prediction of electro-mechanical response and strain-sensing capability of smart random heterogeneous materials. The framework first generates representative unit cell using Lubachevsky–Stillinger algorithm and the generated unit cell is imported into the mechanical module. The mechanical module applies periodic boundary conditions, meshes the unit cell, implements interfacial damage at the inclusion-matrix interface and incorporates isotropic damage in the matrix in the post-peak regime to obtain the deformed/damaged microstructure for any applied tensile or compressive strain. The deformed/damaged microstructure, obtained from the mechanical module, is imported into a remeshing subroutine that meshes the deformed/damaged unit cell and improves the quality of mesh for a better solution. The re-meshed unit cell is imported into the electrical module to obtain the electrical responses for the applied strain.

The applicability of the simulation framework is confirmed here through its successful implementation on a smart cementitious material containing nano-engineered conductive coating at the cement-aggregate interface. Representative microstructures of the smart cementitious material were first generated and the electro-mechanical responses were simulated using combined use of a mechanical module, remeshing module and electrical module. In the pre-peak regime, progressive interfacial debonding with increasing tensile strain resulted in significant progressive increase in FCR, signifying efficient strain-sensing capability of the material. With progressive interfacial debonding, the stress in the matrix kept on increasing and damage in the matrix was initiated in the matrix when the stress in the matrix exceeded the tensile strength. The onset of damage in the matrix was reflected in the form of significant jump in FCR, substantiating damage-sensing capability of the smart mortar. Parametric study with variations in thickness and conductivity of the coating revealed that limitations of achieving higher coating conductivity with increased CNT loadings [324] can be offset with the variation of thickness of such coatings to obtain a more sensitive overall system. The validation of the simulation approach presented here provides confidence on its capability to be implemented for various smart heterogeneous composites and it can help develop design strategies to tailor the microstructure for efficient performance.
Chapter 7

Spatial damage sensing ability of self-sensing cementitious composites using electrical resistance tomography

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Spatial damage sensing ability of metallic particulate-reinforced cementitious composites: Insights from electrical resistance tomography

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HIGHLIGHTS

- Spatial damage sensing ability of metallic waste iron powder incorporated cementitious systems is evaluated
- Evaluation of spatial damage sensing ability is performed using electrical resistance tomography (ERT)
- Spatial damage sensing ability improves progressively with increase in iron powder content
- Iron powder content 30% or greater (Cement-replacement) shows sufficient spatial damage sensing ability

GRAPHICAL ABSTRACT

Waste iron powder in cement

Effective property prediction

Spatial damage sensing

Micro scale

Meso scale

ERT reconstruction

A B S T R A C T

The paper evaluates the spatial damage sensing ability of self-sensing mortars containing up to 40% waste metallic iron powder by volume as cement replacement. The spatial damage-sensing ability is evaluated using a framework that integrates the electrical resistance tomography (ERT)-based conductivity reconstruction algorithm with multiscale numerical homogenization with a view to enabling structure-guided design of such self-sensing composites. The ERT-based framework uses experimentally measured boundary electrode voltages as input, assigns the effective conductivity of the composite (obtained from numerical homogenization) as initial estimate of the conductivity distribution, and initiates the iterative process involving the well-posed forward model and the ill-posed inverse problem to obtain the conductivity map in the damaged configuration. The reconstructed damage maps thus obtained, confirm sufficient spatial damage-sensing ability of mortars containing 30% or greater amount of iron powder validating the applicability of such self-sensing composites towards spatial damage sensing for health monitoring of structures.

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1. INTRODUCTION

Spatial damage sensing imparts valuable information on the reliability and safety of the structures. It can save the structures from catastrophic failures and can prevent immense loss of life and property [50,52]. Various non-destructive testing (NDT) techniques such as ultrasound testing, radiographic tests (X-ray) etc. have been traditionally used towards costly routine inspections for maintenance of these structures. However, such frequent routine inspections are impractical and very expensive for large structures in the long-term. Hence, a real-time damage-sensing approach would be beneficial under such scenarios. For real-scale industrial structures, use of multifunctional composites is gaining popularity for strain-sensing applications [53–55]. Electrical responses of such conductive composites have been shown to be sensitive to strain [56–63] and defects or damage [59,63–65]. Bulk electrical response obtained from electrical impedance spectroscopy (EIS) has been used for detection of cracks [66,67], fiber distributions [68,69], fiber orientations [70], and corrosion rate of reinforcing bars [71–74] in conductive cementitious composites. While several conductive fibers such as steel fibers [28,29], carbon fibers [32,33], multi walled carbon nanotubes (MWNT) [76,136] have been used to obtain strain-sensing ability in cementitious matrices, this paper incorporates metallic waste iron powder in mortars towards spatial damage-sensing. This waste iron powder is an industrial byproduct and it is generated in large quantities in electric-arc furnace (EAF) steel production facilities and shot-blasting operations of structural steel sections [242]. Traditionally, this waste iron powder is landfilled since it is not economically feasible to recycle steel from the waste powder [265]. Several million tons of such waste product is being landfilled all over the world. Such waste iron powder-incorporated cementitious composites have been shown to exhibit significantly improved fracture resistance [242,329,330] and strain-sensing ability [216] thereby achieving a multi-functional status. While the strain-sensing ability of the waste iron powder-incorporated cementitious composites has been demonstrated using bulk-electrical response in [216], this study employs an electrical resistance tomography (ERT)-based reconstruction algorithm [75–78] to evaluate the applicability of such composites towards spatial damage sensing. In ERT, several electrode pairs, attached to the surface of the sample, measure potential differences in response to an injected current and a spatial conductivity distribution map is obtained by solving an ill-posed problem [78–80]. ERT has been applied in traditional cementitious composites towards evaluation of moisture transport [331,332] and crack detection [75,333]. ERT has also been applied in recent years towards surface damage detection [76,334,335] and strain-sensing [336] applications in self-sensing concretes [76] for structural health monitoring (SHM). ERT-based spatial damage sensing usually requires a pre-damaged (pristine condition) reference conductivity map. Electrical resistance tomography (ERT)
has been successfully employed for imaging of moisture flow in cement-based materials [337,338]. ERT has also been used to evaluate chloride ingress in cementitious systems [339]. Besides, ERT-based sensing skins have been shown to detect surface damage patterns reliably in concrete structural members [340]. ERT has also been used for assessment of cracks in concretes [341,342] and fly ash-modified cementitious systems [343]. In this paper, the ERT-based image reconstruction framework is integrated with a numerical module [136] that performs numerical homogenization at different length scales based on known microstructural features of the material. The effective conductivity, thus obtained from multiscale numerical simulation serves as baseline reference conductivity of the pre-damaged configuration (pristine condition) that can serve as an input in realistic SHM applications. The baseline conductivity, thus obtained, is subtracted from conductivity map of the damaged configuration, obtained from the ERT framework, to generate spatial damage maps which are employed to evaluate the influence of metallic waste powder incorporation on the spatial damage sensing ability of mortars. Thus, the spatial damage-sensing framework integrates the ERT-based conductivity reconstruction algorithm with multiscale numerical homogenization module with a view to offer robustness and flexibility so as to enable tailoring of the material microstructure at different length scales for efficient design of such self-sensing metallic particulate-reinforced cementitious composites.

2. EXPERIMENTAL PROGRAM

2.1 Materials and mixtures

The cement used for the experiments is commercially available Type I/II ordinary portland cement (OPC) conforming to ASTM 150 [344]. The chemical composition of the oxides of different elements in the OPC is detailed in [329]. Metallic waste iron powder, obtained from industrial shot-blasting facility, is used in this study to replace OPC partially in the mortars. The iron powder primarily contains 88% Iron (Fe) and 10% oxygen (due to atmospheric oxidation) [242,329]. Traces of Cu, Mn and Ca are also present in the iron powder [242,329]. The median size of the iron particles in the powder is 19 µm [265,329,345]. Five different mortar mixtures were prepared with constant sand (median particle size 600 µm) volume of 50%. While the control mortar does not contain any iron powder, the other four mixtures contain 10, 20, 30 and 40% iron powder by volume as OPC-replacement. A water-cement ratio of 0.5 (mass-based) was used to prepare all the mixtures. This study does not consider water-to-cement ratio lower than 0.5 since such mixtures with lower water content do not show desirable rheological properties especially for the mixtures containing higher dosage of iron powder. The particle size distributions for OPC, sand and iron
powder are shown in Figure 1. These particle size distributions are obtained from laser diffraction analysis.

![Figure 1: Particle size distribution of the OPC, sand, and iron powder](image)

**Figure 1** The particle size distribution of the OPC, sand, and iron powder

While mortar mixtures were used for spatial damage sensing (ERT), companion paste mixtures were used for characterization of bulk electrical response (electrical conductivity) evaluation as well as for microstructural observations. For spatial damage sensing, cylindrical discs of diameter 50 mm and thickness 10 mm were prepared using mortar mixtures. Circular holes of radii 1 cm are drilled in the mortar discs 1.8 cm away from the center of the specimen (center to center distance) to evaluate the ability of damage-sensing through the ERT. Two different sample configurations were used containing one and three holes respectively. 30 mm diameter x 60 mm long paste cylinders were used for electrical conductivity measurements. The molds for electrical impedance/conductivity measurement were fitted with 3 mm diameter steel rods (electrodes) placed at 15 mm from both ends. Similar setup was successfully implemented for cement pastes in [346]. Four replicate specimens for each of these five mixtures were cast and demolded after 24 hours. This was followed by exposing the specimens to a moist environment with RH>98% at a temperature of 23±2°C for 28 days. The cured samples for EIS measurements were not removed from the molds and were placed in a sealed container with the exposed surface covered with a moist towel to maintain saturated conditions. Companion paste samples were also cast for microstructural evaluations.

**2.2 Effective electrical conductivity measurements**

The electrical conductivity of paste samples was measured using a Solartron 1260™ gain phase analyzer. Electrical impedance spectroscopy (EIS) has been used to characterize electrical conductivity of cementitious materials [347,348]. The 30 mm diameter x 60 mm length cylindrical
paste specimens (see Section 2.1) fitted with steel electrodes are used for EIS experiments. Alligator plugs from the impedance analyzer were attached to the steel electrodes and a frequency sweep was performed. Thus, the Nyquist plots were obtained from the EIS measurements. From the Nyquist plot, the bulk resistance ($R_b$) can be obtained as the value of real impedance where the imaginary impedance value is minimum (meeting point of bulk arc and electrode arc) [347]. The effective conductivity ($\sigma_{eff}$) can be calculated from the bulk resistance ($R_b$) as shown in Equation 1 [346,347]:

$$\sigma_{eff} = \frac{L}{R_bA}$$  \[7-1\]

Where $L$ is the specimen length and $A$ is the cross sectional area. Since, the EIS experiments were performed on the cylindrical samples with steel electrodes, the effective spacing between the electrodes as well as the effective cross sectional area cannot be measured directly. Hence, the cell constant ($L/A$) was obtained using 30 mm diameter x 60 mm long cylindrical tube along with the steel electrodes fitted at the same spacing as the samples. The tube was filled with 4% NaCl solution and the bulk resistance of the solution was obtained using EIS measurements. Using the known conductivity of the 4% NaCl solution (4.4 S/m) [346], the cell constant ($L/A$) of 28.5 m$^{-1}$ was calculated from the bulk resistance of the solution using Equation 1. This value of cell constant ($L/A$) was used to obtain effective conductivity ($\sigma_{eff}$) from the bulk resistance of paste samples ($R_b$) with varying dosage of iron powder.

2.3 Electrical resistance tomography (ERT) for spatial damage detection

A diffusive imaging modality that enables estimation of the internal electrical conductivity distribution based on boundary current injections and voltage measurements is used here to validate the feasibility of ERT application in aforementioned mortars (see Section 2.1). Mortar discs of size 50 mm diameter and 10 mm thickness (with single and three-hole configurations) are used as mentioned in section 2.1. Thin copper film electrodes are cast into the samples (see Figure 2 (b)). Such thin copper film electrodes have been shown to provide sufficient electrical contact in the literature [76]. Here, a total of eight copper tape pairs are cast into each sample. The spatial resolution in ERT is greatly influenced by current injection patterns [79,349]. In this study, adjacent configuration of electrodes is adopted for current injection to obtain the boundary voltage measurement[79,349]. The electrode configuration and stimulation pattern as applied to the cylindrical samples are shown schematically in Figure 2(a). Here, the current is injected through a pair of electrodes and the voltages across other pairs of electrodes are measured. The custom data acquisition system (DAQ) system is built here using a 34980A multifunction switch fitted with a
built-in 6 ½ digit digital multimeter (DMM) from Keysight Technologies™. A Solartron 1260™ gain phase analyzer acts as a current source. The switch interfaces with a MATLAB code to enable simultaneous current injection across a pair of adjacent boundary electrodes while recording the voltages across the other pairs in adjacent configuration (Figure 2 (a)). The voltages, thus obtained, are used to obtain ERT reconstructed images as explained later in this paper. Figure 2(b) shows the experimental setup to obtain boundary voltages in a specimen with single-hole configuration for reference whereas the zoomed figure shows the electrical contact of the specimen with the embedded copper tape electrodes.

Figure7 - 2 (a) Current injection and boundary voltage measurements in adjacent configuration of electrodes (shown in green); (b) a single-hole disc sample configuration mounted on the ERT setup

2.4 Scanning Electron Microscopy

The companion paste samples with different dosage of iron powder were subjected to a microstructural evaluation. Small cube pieces (10 × 10 mm × 10 mm in size) were cut from the core of paste specimens using a diamond saw. Prior to polishing, the cut pieces were cleaned ultrasonically to remove the debris. Afterwards, the sample was impregnated in epoxy and vacuum-saturated followed by overnight curing. Several grinding/polishing steps were performed using SiC abrasives and finally the sample was polished using 0.04 µm colloidal silica suspension. The polished samples were imaged using a field emission environmental scanning electron microscope (FESEM) under backscattered mode for microstructural evaluations.
3. RESULTS AND DISCUSSIONS

This section presents the influence of iron particles on the spatial damage sensing ability of cementitious mortars. Figure 3 shows a schematic representation of the framework adopted in this study to achieve spatial damage sensing for heterogeneous composites. The framework performs numerical homogenization [329,350] at multiple length scales guided by the observed microstructure of such systems to obtain effective electrical conductivities which are validated against experimental EIS observations. The effective electrical conductivities, thus obtained, are used as input to the ERT-based reconstructed conductivity distribution algorithm module. In addition, the ERT module also requires experimentally obtained boundary voltages (section 2.3) of the target sample as input. The ERT module essentially solves an ill-posed inverse boundary problem by a forward model and an inverse problem to obtain reconstructed conductivity distribution map of the target sample facilitating spatial damage sensing.

![Flowchart](image)

Figure 3: A flowchart representing the sequence of computations and experiments to achieve spatial damage sensing.

The forthcoming sub-sections describe microstructural features of the iron powder distributed in the HCP matrix, evaluate the electrical conductivities of iron powder-incorporated HCP using EIS measurements and detail different components of the ERT-based conductivity reconstruction framework with a view to elucidate the influence of iron powder-incorporation on the spatial damage sensing ability of mortars. While microstructural evaluations serve as input to the microstructure generation algorithm [136,330,350] in the numerical homogenization module, the electrical conductivities of iron powder-incorporated HCP mixtures are used later to validate the numerical homogenization module.
3.1 Material Microstructure

Microstructural observations were performed to evaluate the size, shape and distribution of iron particles in the HCP matrix. Figure 4 shows representative micrographs for the mortar containing 30% iron powder as cement-replacement. Distribution of bright (owing to higher density) elongated iron particulates are clearly visible in the backdrop of the gray phases (indicating the reaction products) and the black areas (indicating pores in the BSE image). Some matrix cracks can be observed which are a result of sample preparation. An image analysis of several BSE images yielded an average aspect ratio of 12 for the elongated iron particles which is used later in this paper towards generation of representative unit cells for the microstructural analysis (See Section 3.3).

![Figure 4: BSE image of iron particles (bright areas) dispersed in HCP matrix where 30% volume of OPC is replaced by iron particles at (a) 35x (scale bar indicates 500 µm) and (b) 250x (scale bar indicates 100 µm) resolution.](image)

3.2 Experimental evaluation of the electrical response of pastes

This section describes the experimental electrical response of the iron powder-incorporated HCP with varying iron powder content. The Nyquist plots, shown in Figure 5(a), relate the resistance denoted by the real part of impedance ($Z'$) with the reactance denoted by the imaginary part ($Z''$) [347,348]. The Nyquist plot shifts to the left with increasing iron powder content signifying increased conductivity with iron powder-incorporation. Frequency-based AC impedance studies averts the polarization effects in cement based composites that would otherwise arise in DC measurements [351]. The high frequency arcs, as depicted in Figure 5(a), represent the bulk response of the composites enabling computation of bulk conductivity as described in Section 2.2. The computed bulk electrical responses are reported in Figure 5(b) showing significant increase in conductivity with increasing iron powder content. Such increase in conductivity is likely to influence the spatial damage sensing ability of cementitious systems which is explored in detail later in this paper.

![Figure 5: Nyquist plots relating the resistance and reactance of iron powder-incorporated HCP composites.](image)
Figure 5 (a) Nyquist plots showing the high frequency arcs and (b) computed bulk electrical conductivities for control as well as iron powder-incorporated HCP mixtures (error bars indicate standard deviation)

3.3 Multiscale numerical simulation

While the previous section elucidated experimental evaluation of the electrical response of iron powder incorporated HCP, this section performs numerical homogenization at different length scales so as to obtain homogenized electrical properties of the iron powder incorporated mortars that serve as input to macro-scale model for ERT module as explained later in this paper. Such an approach involves representation of the geometrical configuration of the different phases in the form of unit cells at different length scales. In this study, two interactive length scales at the paste level and mortar level are used for prediction of effective electrical responses. A schematic representation of the numerical simulation framework is shown in Figure 6. The forthcoming subsections elaborate the numerical simulation framework and its application towards prediction of effective electrical properties of iron powder incorporated mortars.
3.3.1 Numerical homogenization framework

3.3.1.1 Generation of unit cell
The unit cells are generated here using the Lubachhevsky-Stillinger algorithm [103,104]. This algorithm employs a hard contact model and hence particle overlaps are not allowed. Finally, the obtained microstructural information is implemented via a python language script to enable it to be imported to a commercial finite element software. The unit cell generation algorithm has been successfully implemented in [100,101,136] and adequately detailed in [103,104].

3.3.1.2 Boundary conditions
Once the unit cell is generated, it is meshed using the python script and periodic boundary conditions (PBC) [110,136] are applied. PBCs ensure a continuity of displacement and traction across boundaries of neighboring unit cells. PBCs have been applied successfully towards FE analysis of random heterogenous materials [106]. Periodic boundary conditions are shown to be computationally efficient even with smaller size of unit cells facilitating faster convergence [101]. More details on the PBC can be found in [100,102].

3.3.1.3 Homogenization of electrical properties
The numerical framework assigns intrinsic electrical properties to each phase of the periodically bounded unit cell. A unit potential is then applied across a face of the unit cell while the other edges

Figure 7.6 A numerical simulation framework computed at every length scale to obtain the effective electrical properties at that scale
are insulated. The electrical module computes current density ($\mathbf{j}$) from the input electrical conductivity ($\sigma_k$) of component phases ($k = 1,2,...n$) and the applied electric field ($\mathbf{E}$) using Ohm’s Law. The simulation yields the electric field and electric current density (ECD) distribution in the unit cell which when volumetrically averaged by a post-processing module yields the average electrical conductivity ($\sigma_{eff}$) as shown in Equation 2 [216,311].

$$\sigma_{eff} = \frac{\mathbf{j}}{E} \quad [7-2]$$

3.3.1.4 Post-processing and upscaling to macro-scale

The aforementioned analysis is implemented using ABAQUS™ solver and electric field/current density distribution in the unit cell are obtained. The post processing module employs a MATLAB® subroutine to obtain volume-averaged responses and effective electrical conductivity (using equation 2). The numerical homogenization process is explained schematically in Figure 6.

3.3.5 Application of numerical homogenization module towards effective electrical conductivity of iron powder-incorporated mortars

The numerical simulation for effective electrical conductivity prediction for iron powder-incorporated mortars involves two interactive length scales at the paste scale and the mortar scale as shown in Figure 7. These homogenizations are performed here at multiple steps in order to reduce the computational demand while maintaining computational efficiency [111]. Once the RVE is generated using the Python script, it is meshed and subjected to FE analysis under externally applied unit voltage gradient along x direction. The FE analyses are carried out in ABAQUS™ solver using DC2D4E quadrilateral elements. A MATLAB® script operates on the result files containing the volume of the elements and the responses to obtain the effective properties as explained in the previous section (Figure 6). At first, the iron particles are homogenized into the HCP matrix to obtain effective properties of iron powder-incorporated mortars which are used as matrix-properties in the mortar scale. The sand inclusions are homogenized into the effective iron powder-modified matrix in the mortar scale to obtain effective properties of the iron powder-modified mortars. Figure 7(a) shows the generated unit cell of iron powder-incorporated HCP for 20% iron powder incorporation as a representative case. The size and aspect ratio of iron particles are adopted based on microstructural observations. Figure 7(b) shows the representative unit cell for mortars where sand inclusions are embedded in the iron powder modified HCP matrix. The input electrical conductivities for HCP, iron particles and sand are 0.065 S/m, 100 S/m and $10^{-8}$ S/m respectively [216]. It needs to be noted here that the electrical conductivity value considered for HCP corresponds to moist condition[75,352] and thus, the influence of saturated condition is
incorporated in the numerical simulations. The volume fractions of the inclusions are mentioned earlier (section 2.1). The sizes of the unit cells, obtained from a size-sensitivity study, are shown in Figure 7 and any increase in size of unit cells beyond the ones shown in Figure 7 results in insignificant change in the obtained effective responses. Such relative size of unit cells with respect to size of inclusions has been successfully implemented towards prediction of effective properties in [100,101,136,329,350]. The effective electrical properties of iron powder-modified mortars, thus obtained, serve as input material property for the macro scale model involving spatial damage detection as explained later in this paper.

Figure 7 - (a) The paste microstructure with 20% iron particulates as cement-replacement; (b) mortar microstructure and (c) macro model

Figure 8 shows the electric current density (ECD) plots under applied voltage difference of 1 V across the edges along X axis for the cement paste scale with varying iron powder content. With increasing iron powder content, the ECD increases substantiating the increased electrical conductivity due to incorporation of conductive inclusions.
Figure 7-8 The ECD under applied voltage difference of 1V across the edges along X axis for the iron powder-incorporated HCP matrices containing (a) 10, (b) 20, (c) 30 and (d) 40% iron powder as cement-replacement.

Figure 9 shows the ECD plots for the mortar scale with varying iron powder content under applied voltage difference of 1V across the edges along X axis. Similar to paste scale, here also ECD increases with increasing iron powder content. Such increase in conductivity is likely to improve the spatial damage sensing ability of the mortars which is explored in detail later in this paper.

Figure 7-9 The ECD for the mortars containing (a) 10, (b) 20, (c) 30 and (d) 40% iron powder as cement-replacement under applied voltage difference of 1V across the edges along X axis.

The numerical homogenizations are performed for four different random microstructures at each scale for all the mixtures considered here. Table 1 lists the computed mean effective electrical conductivities of the pastes and mortars with varying iron powder content. The standard deviations were less than 1% of the mean in all the mixtures considered here. These values are further used in the spatial damage sensing framework towards validation of ERT application in such composites.
Table 7-1 Simulated effective electrical conductivities (S/m) for the composites at paste and mortar scales

<table>
<thead>
<tr>
<th>Iron powder %</th>
<th>Pastes</th>
<th>Mortars</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.065</td>
<td>0.039</td>
</tr>
<tr>
<td>10</td>
<td>0.083</td>
<td>0.05</td>
</tr>
<tr>
<td>20</td>
<td>0.104</td>
<td>0.063</td>
</tr>
<tr>
<td>30</td>
<td>0.136</td>
<td>0.083</td>
</tr>
<tr>
<td>40</td>
<td>0.194</td>
<td>0.118</td>
</tr>
</tbody>
</table>

3.3.6 Comparison of the predicted electrical conductivity with experimental observations

In order to elucidate the predictive ability of the numerical homogenization framework, explained before, this section compares the simulated electrical conductivities with the experimental observations (reported in section 3.2) for iron powder-modified HCP with varying iron powder content. The simulated conductivities and experimental observations are shown in Figure 10. A close correlation between the experimental and simulated conductivities is observed signifying efficacy of the numerical homogenization framework.

![Figure 10](image)

Figure 7-10 Comparison between simulated electrical conductivities and the experimental observations for iron powder-modified HCP

3.4 Spatial damage sensing in iron powder-incorporated mortars

This section aims to evaluate the applicability of ERT imaging technique to iron powder-incorporated mortars. The fundamental principle of ERT is governed by measured boundary voltages being characteristic of conductivity distribution in the specimen. However, an attempt to calculate the conductivity distribution from boundary voltage measurements leads to an ill-posed problem [75,80,353] implying that similar outcomes may be obtained from multiple inputs. Such problems are generally solved by an iterative approach. First, an initial conductivity distribution
(based on the homogenized conductivity from Section 3.3.5) is considered and the forward model calculates boundary voltages from the initial conductivity distribution. However, it is likely that the potential distribution thus obtained will have boundary voltage values different from the experimentally observed measurements owing to the presence of damaged regions. Thus, an iterative algorithm is followed to refine the estimated conductivity distribution. Towards that end, the inverse problem is initiated that imposes the experimentally obtained boundary voltages to obtain an improved conductivity distribution while minimizing the differences between the experimental and predicted boundary voltages, obtained from the forward model. The updated conductivity distribution thus obtained from inverse problem serves an input to the forward model. Thus, conductivity updating procedure starts iterating between the forward and inverse problem. The iterative procedure terminates when the error between the measured and predicted boundary voltages falls within a preset tolerance. The conductivity distribution in the damaged sample, thus obtained from ERT reconstruction, is compared against the homogeneous effective conductivity of pristine sample, obtained from multiscale numerical homogenization (section 3.3.5), to yield the spatial distribution of damage in the damaged sample. The algorithm is described using a flowchart in Figure 11.

![Flowchart representing the ERT algorithm](image)

**Figure 7.11 Flowchart representing the ERT algorithm**

### 3.4.1 The forward model

The forward model obtains boundary voltages of the target sample for a given spatial conductivity distribution. Figure 12 shows a schematic representation of the forward model. It assumes an initial conductivity distribution and obtains the corresponding boundary voltages using FE analysis. If the difference between the predicted and experimental boundary voltages exceed the threshold, the conductivity distribution is updated and the interactive process continues until the error is less than the tolerance.
Figure 7.12 Schematic representation of forward model for ERT

The Poisson equation that governs the forward model is given as [75,76,354,355]:

\[ \nabla \cdot \left( \sigma \nabla u(\vec{r}) \right) = 0; \quad \vec{r} \in \Omega \]  

[7-3]

Where \( \vec{r} \) is the spatial coordinate encompassing the conductivity \( \sigma(\vec{r}) \) and the electric potential \( u(\vec{r}) \) in the domain \( \Omega \). The current density \( \left( \sigma \frac{\partial u}{\partial \vec{n}} \right) \) along the outward unit normal \( \vec{n} \) through the boundary when integrated over the \( l \)th electrode yields the total current \( (l_t) \) through the electrode (electrode domain \( \tau_1 \)) as shown in Equation 4 [75,76] which serves as the first boundary condition.

\[ \int_{\tau_1} \left( \sigma \frac{\partial u}{\partial \vec{n}} \right) dS = l_t; \quad \vec{r} \in \tau_1 \]  

[7-4]

No current flows through the electrode-free boundary (domain \( \tau \)) (see Equation 5 [75,76]) and it serves as second boundary condition applied at the electrode-free boundary.

\[ \left( \sigma \frac{\partial u}{\partial \vec{n}} \right) = 0; \quad \vec{r} \in \tau \]  

[7-5]

The electric potential \( u \) under the \( l \)th electrode is conjugated with the potential drop due to imperfect contact between the electrode and the target sample. This imperfect contact is accounted for in the forward model in terms of contact impedance \( z_l \), resulting in a total electric potential \( U_l \) (Equation 6 [75,76]). This is applied for the electrode domain \( (\tau_1) \) as a boundary condition.

\[ u + z_l \sigma \frac{\partial u}{\partial \vec{n}} = U_l; \quad \vec{r} \in \tau_1 \]  

[7-6]

To maintain charge conservation, the net current flowing in all the electrodes is considered zero and the net potential is considered zero from the choice of potential ground.

\[ \sum_l l_t = 0 \]  

[7-7a]

\[ \sum_l U_l = 0 \]  

[7-7b]
The forward model in ERT is implemented using a finite element based procedure. The Poisson equation (Equation 3) can be multiplied by a sufficiently smooth arbitrary test function ($v$) and integrated over the entire domain ($\Omega$) thereby deriving the weak form, as shown in Equation 8 [76].

$$\int_{\Omega} v[\nabla \cdot (\sigma(\bar{r})) \nabla u(\bar{r})]] = 0$$ \hspace{1cm} [7-8]

A nodal voltage $u_i$ and shape function $\varphi_i$ (which can assume non-zero values at vertices) can approximate the electric potential $u^h$ in the realm of finite element theory as shown in Equation 9 [76].

$$u^h = \sum_{i=1}^{n} u_i \varphi_i \text{ (n=3 vertices for triangular elements)}$$ \hspace{1cm} [7-9]

Using Galerkin’s approximation and applying all the above-mentioned boundary conditions the following matrix equation is obtained [76,77,80].

$$\begin{bmatrix} A_M + A_Z & A_V \\ A_V^T & A_D \end{bmatrix} \begin{bmatrix} U \\ V_L \end{bmatrix} = \begin{bmatrix} 0 \\ I^d \end{bmatrix}$$ \hspace{1cm} [7-10]

Where the global conductivity matrix $A$ is formed by combinations of matrices $A_M, A_Z, A_V$ and $A_D$. The potential vector $B$ consists of the nodal values of potential $U$ and the potentials on the electrodes $V_L$. $I^d$ is the set of injected currents at the electrodes. The matrix entries for the global conductivity matrix are defined as follows:

$$A_M(i,j) = \int_{\Omega} \sigma^h \nabla \varphi_i \nabla \varphi_j dA$$ \hspace{1cm} [7-11a]

$$A_Z(i,j) = \sum_{l=1}^{L} \frac{1}{z_l} \int_{e_l} \varphi_i \varphi_j dA$$ \hspace{1cm} [7-11b]

$$A_V(i,l) = -\frac{1}{z_l} \int_{e_l} \varphi_i d\bar{r} \hspace{0.5cm} (i = 1:n, \text{ and } l = 1:L)$$ \hspace{1cm} [7-11c]

$$A_D(i,l) = \frac{1}{z_l} |e_l| \hspace{1cm} \text{for } i = l$$ \hspace{1cm} [7-11d]

$$A_D(i,l) = 0 \hspace{1.5cm} \text{for } i \neq l$$ \hspace{1cm} [7-11e]

The forward model is implemented in this paper using a MATLAB™ subroutine which provides voltage distribution from known conductivity distribution of the sample as per Equation 10.
### 3.4.2 The inverse problem

While the forward problem, explained in the previous section, is a well-posed problem, the inverse problem is an ill-posed problem. The inverse problem aims to reconstruct the internal conductivity distribution from boundary voltage measurements. Any small changes in boundary voltages results in large conductivity perturbations. An iterative technique described hereafter is used to solve the non-linear ill-posed problem. As mentioned earlier, an initial conductivity distribution is assumed at the onset of the iteration and the corresponding boundary voltages are obtained by the forward model. Thereafter, the inverse problem is invoked to yield an improved conductivity estimate from the imposition of experimental voltages. The updated conductivity distribution, obtained from inverse problem, are used again in the forward model to obtain corresponding updated boundary voltages. The iterative process terminates when the error falls within the threshold. To ensure a smooth and fast convergence, a regularization method is necessary while solving an ill-posed problem. A Tikhonov type regularization [76,78,80] is adopted in this study. The stable solution for conductivity is obtained by minimizing the residual error shown in Equation 12 [80].

\[
f(\sigma) = \| F(\sigma) - V \|^2_2 + \lambda \| L(\sigma - \sigma_k) \|^2_2
\]  

Where \( f(\sigma) \) is the residual error, \( F(\sigma) \) denotes the computed boundary voltages from the forward model corresponding to the updated conductivity distribution, obtained from the inverse problem in the previous iteration, \( V \) denotes experimentally obtained voltages, \( \lambda \) is the positive scalar regularization parameter, \( L \) is the regularization matrix imparting some prior information about \( \sigma_k \) (conductivity for \( k^{th} \) iteration). In the minimization process, the constrained problem is formed by incorporating \( 0 < \sigma < \sigma_b \) where \( \sigma_b \) refers to the background conductivity of the pristine sample obtained from numerical homogenization. The upper limit is fixed at \( \sigma_b \) since incorporation of damage reduces the overall conductivity of the sample. Minimization of Equation 12 yields the algebraic form of Tikhonov solution as shown in Equation 13a [80].

\[
h = (F'(\sigma_k)^T F'(\sigma_k) + \lambda L^T L)^{-1} (F'(\sigma_k)^T (V - F(\sigma_k)) + \lambda L^T L (\sigma_k)
\]  

where \( h \) is the increment in conductivity as shown in Equation 13(b).

\[
\sigma_{k+1} = \sigma_k + h
\]  

The updated conductivity distribution, thus obtained from inverse analysis, serves as input to the forward computations thereby improving the predictions. The iterative procedure terminates when
the error ratio \( \left( \frac{\|F(\sigma) - V\|_2^2}{\|V\|_2^2} \right) \) falls below 0.05\% [76]. The ERT reconstruction procedure, adopted in this study, is sufficiently detailed in [75, 80, 311, 355].

3.4.3 Reconstruction of conductivity maps for iron powder-incorporated mortars

A MATLAB™ script (EIDORS) [79, 80] implements the inverse computations and calls the forward model subroutine repeatedly in an iterative process to finally obtain spatial conductivity distribution for the mortars with varying content of iron powder. The value of the regularization parameter is considered 0.01 for comparative evaluation of damage sensing ability of waste iron powder incorporated cementitious systems. This choice enables reconstructed images of admissible quality. The background conductivity obtained from multiscale numerical homogenization (See Section 3.3.5) serves as baseline conductivity map (conductivity of pristine sample) for image reconstruction. The baseline conductivity maps are subtracted from the conductivity maps obtained from ERT algorithm to obtain spatial damage reconstruction. Figure 13 shows the original images of the samples (single-hole and three-hole configurations) along with corresponding reconstructed images for the mortars with varying iron powder content. General trend in these figures suggest that the damage sensing ability improves progressively with increase in iron powder content which can be attributed to the increase in composite conductivity with increasing dosage of iron powder. For a dosage of 30\% or greater iron powder, the reconstructed damage zones correlate very well with the actual location of damages in both single and three-hole configurations thereby validating the application of such imaging technique towards spatial damage
sensing in iron powder-incorporated cementitious composites.

Figure 7-13 Original images of the mortar disc samples showing (a) single hole configuration; (f) three-hole configuration, reconstructed damage maps for mortars containing (b) 10% (c) 20% (d) 30% and (e) 40% iron powder as cement-replacement for single-hole configuration; reconstructed damage maps for mortars containing (g) 10%, (h) 20%, (i) 30% and (j) 40% iron powder as cement-replacement for three-hole configuration

4. CONCLUSIONS

This study elucidates the influence of metallic waste iron powder-incorporation on the spatial damage-sensing ability of mortars. The spatial damage sensing is implemented using an ERT-based conductivity reconstruction framework. The ERT framework uses experimentally measured boundary electrode voltages as input to initiate the iterative process involving the well-posed forward model and the ill-posed inverse problem. While the forward model predicts the boundary voltage based on an assumed conductivity distribution, the ill-posed inverse problem reconstructs the conductivity distribution image by minimizing the residual error between the boundary voltages obtained from forward problem and the experimental boundary voltage readings. Moreover, the ERT-based framework adopted in this study integrates an efficient multiscale numerical homogenization module. The numerical homogenization module performs numerical homogenization at different length scales based on known microstructural features of the material and provides the reference conductivity of the undamaged configuration which is otherwise not readily available in realistic SHM applications. The effective conductivity obtained from multiscale numerical homogenization serves as baseline conductivity map for image reconstruction. The baseline conductivity maps are subtracted from the conductivity maps obtained from ERT algorithm to obtain reconstructed images that can spatially identify damaged patches. In addition,
the effective conductivity obtained from multiscale numerical homogenization is used as initial conductivity distribution (prior information) for the damaged configuration in the forward model thereby reducing the number of iterative processes and enhancing the efficiency of the ERT framework. The spatial damage sensing ability is found to be improving progressively with increase in iron powder content which can be attributed to the increase in conductivity with increasing dosage of iron powder. The mortars containing 30% or higher amount of iron powder as OPC-replacement show sufficient spatial damage detection ability thereby validating the application of ERT-based damage sensing approach towards spatial damage sensing in iron powder-incorporated cementitious composites.
Chapter 8

Strain sensing efficiency of hierarchical twill weave laminated composite

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Strain sensing efficiency of hierarchical nano-engineered smart twill-weave composites: Evaluations using multiscale numerical simulations

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Composite Structures

Abstract

This paper evaluates the strain-sensing ability of a nanoengineered hierarchical twill weave composite using multiscale numerical simulations. Piezoresistivity is incorporated in such composite by introducing carbon nanotubes (CNT) in the polystyrene (PSS) matrix so as to form a percolating microstructure. The glass fiber twill weave, which itself contains CNT-modified PSS matrix inside the yarns, is coated with thin film of such piezoresistive matrix to obtain the smart composite configuration. The methodology, presented in this paper, captures the hierarchical intricacies at multiple length scales and implements various mechanical damage mechanisms at subsequent interactive length scales as well as consequent electrical responses so as to yield macroscopic electromechanical response. The simulated responses show excellent correlation with experimental observations signifying the efficacy of the simulation methodology. Such a detailed multiscale approach can provide valuable insights towards tuning of structural hierarchies at multiple length scales for efficient design of smart woven laminated composites.

Keywords: Smart hierarchical composites; twill-weave composite; multiscale numerical simulations; micromechanics; Piezo-resistivity; Strain sensing
1. INTRODUCTION

Textile composites are widely used in aerospace, astronautics, marine, automotive and off-shore applications owing to their lightweight nature and exceptional mechanical performance [81,82]. Unlike traditional unidirectional laminated composites which are susceptible to inter-laminar damages, the woven fabrics offer enhanced through-thickness reinforcement thus significantly enhancing the damage tolerance. A long thriving knitting industry and the relative ease of fabrication has catapulted cost-effective plain/twill weaves among the most widely used composites in the modern era. However, with the ever-expanding domain of applications of such fiber reinforced composites, a variety of unforeseen circumstances have appeared including material defects, manufacturing errors, environmental-induced degradation, excessive loading, fatigue amongst others that can cause significant damages in forms of delamination, matrix-cracking, inter-laminar fracture, debonding and their combinations which can lead to catastrophic structural failure [83,84]. The intricacy of such damage mechanisms in a heterogenous structural material such as fiber-reinforced woven polymers pose a tremendous challenge in damage detection. The damages that initiate at micron scale between fibers and matrices or laminae are imperceptible to visual inspection and macroscale sensors like strain gauges, transducers and accelerometers. Emerging sensors like infrared thermometers [356], ultrasonic [357] and fiber optic sensors [358] can enable damage detection, albeit increasing complications. For instance, fiber optic sensors are susceptible to damage rendering vulnerable spots in polymer composites [359]. On the other hand, transducers and ultrasound sensors are susceptible to reduced sensitivity owing to electromagnetic interference resulting in low signal to noise ratios [86,360]. This paves the way for development of intrinsic sensors that can enable continuous monitoring while offering superior performance brought about via incorporation of nano-sensors like CNTs which are multifunctional in nature [85,86]. Toward that end, nano-engineered composites with CNT-incorporated thin films deposited on fiber weaves have been demonstrated in an experimental study [86] for strain sensing and damage detection. Such CNT-incorporated smart textile composites are reinforced by interlaced fibers thus offering superior mechanical performance owing to consistent through-thickness properties at reduced manufacturing cost. The assembly process in such fabrication processes [86,361] involves layer by layer technique (LbL) and surface modified fibers have been used in such composites to enhance CNT dispersion. Such design and manufacturing technique ensures piezo-resistivity of composites with reversible strain sensing and sufficient sensing-sensitivity. The mechanisms governing the strain sensitivity of such smart weave are the mechanically induced deformations that alter CNT positions or induce damage in matrix or interface thereby varying the overall current distribution in the microstructure. Strain sensing ability of such smart textile composites has been established
through experimental evaluation [86,87]. While the previous studies evaluated the performance of such composites experimentally, this study assimilates a finite element based framework that entails multiple hierarchical length scales toward obtaining macroscopic electro-mechanical response with a view to enable multiscale simulation-based design of such smart composites. There are various numerical studies available in the literature that account for uncoupled electrical or mechanical property prediction of nanocomposites with CNT modifications [362,363]. Simulation of strain sensing behavior of CNT-modified thin films has also been reported [87]. In the light of previous published literature, the uniqueness of the current study lies in its ability to incorporate the coupled electromechanical responses at various interactive length scales to account for the nano-engineered hierarchical composite while offering the flexibility of application in various weaves with different geometrical or strength characteristics. This is achieved by an integration of the various length scales to form a holistic framework capable of capturing piezo-resistive characteristics in a sequential multiphysics framework that can even be extended with thermomechanical characteristics [88], environmental degradation [89] or piezoelectric effects [90]. Such an approach offers robustness in its ability to incorporate nanoscale modifications that can significantly alter thin film characteristics thereby altering the sensing efficiency of the smart weave composites. Overall, the multiscale numerical simulations, presented in this paper, can potentially facilitate efficient material design of hierarchical nano engineered smart twill weave composites for a wide range of applications.

2. MULTISCALE ELECTRO-MECHANICAL RESPONSE OF SMART TWILL WEAVE COMPOSITES

Smart hierarchical textile composites with wavy yarns are inherently heterogenous in nature with a complex microstructure that necessitates computational homogenization at multiple length scales towards prediction of effective laminate properties ranging from stiffness to conductivity. Towards that end, microscopically heterogenous volumes are represented as unit cells at various scales. These unit cells are thereafter used to obtain homogenized properties by analytical and computational techniques. While analytical techniques [364,365] are quick and nimble on resources, those suffer from an oversimplification of heterogeneity often resulting in inadmissible predictions. Computational techniques [366,367], on the other hand, are accurate and can mimic the intricate microstructure involved in such heterogenous composites only being limited by computational expense. The multiscale computational homogenization essentially associates a heterogenous unit cell to every Gauss point of the virtual macro-homogenous structure at subsequent length scales. The robustness of the approach lies in its ability to capture both physical
and geometric evolution at each scale resulting in a homogenized constitutive relation at the macroscopic length scale. This is achieved by solving a boundary value problem on a unit cell with consistent boundary conditions obeying Hill-Mandel principle [368]. The discretized system of equations for a field $\psi$ (displacement for mechanical; electric field for electrical response) can be written in terms of the standard FE matrix $K$ (stiffness for mechanical; conductivity for electrical), vector of Lagrange multipliers $\lambda$ and vector of field values $\psi$ (vector of displacement values for mechanical; vector of electric field values for electrical) for any $\Omega \subset \mathbb{R}^3$ of the unit cell as follows [89]:

$$\begin{bmatrix}
K & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
\psi \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
0 \\
D \nabla \psi
\end{bmatrix}$$

[8-1]

Where $C = \int_{\Omega_B} H N^T N d\Omega$, $D = \int_{\Omega_B} H N^T X d\Omega$ with $N$ being matrix of shape functions, $X$ being matrix of spatial coordinates evaluated at Gauss points during numerical integration as guided by number of degrees of freedom and $H$ matrix reflects the boundary condition of the unit cell which assigns admissible distribution of traction forces on the boundary. For the periodic boundary conditions adopted in the mechanical study, the tractions are anti-periodic and $H$ matrix on opposite faces are $H^+ = -H^-$. Sample $H$ and $X$ matrices are available in [369,370]. Having solved the system of equations, the homogenized response $p$ (stress for mechanical; electric flux for electrical) of a unit cell with volume $V$ can be obtained by $(D^T \lambda)/V$. It is to be noted that the number of Lagrange multipliers $\lambda$ per node is equal to the number of degrees of freedom of the node. The aforementioned method enable computation of the homogenized response of the unit cell which under various conditions of field gradient can enable computation of the complete constitutive behavior at the subsequent scale. This is computed by $K \nabla \psi$ where $K = p$ subject to various field gradients. The computational homogenization approach described herewith enables computation of the electromechanical responses [371] of nano-engineered matrix incorporated textile composites at interactive length scales described hereafter, thus capturing the inherent heterogeneity in such composites. The interactive length scales are scale-separated (implying length scales are significantly separated) thereby enabling the application of first order computational homogenization described above.

The multiple length scales involved in a hierarchical smart twill weave composite is shown in Figure 1. The hierarchical smart composite, considered in this study for computational evaluation, contains CNT-incorporated PSS matrix and glass fiber weave. Thin film of CNT-PSS matrix surrounds the weave as coating which yields piezoresistive interactions in the composite. The LbL
assembly technique for fabrication of thin films, which is adequately described in the literature [85,361], proceeds with application of bilayers on the substrate. This study adopts a configuration containing 29 bilayers as reported in an experimental study [86]. In order to capture the various mechanical and electrical phenomena in the smart hierarchical textile composite, the scale-separated computational homogenization approach adopts three interactive lengths scales as shown in Figure 1.

Figure 8-1 Structural hierarchies in the smart textile weave composite

The macro-scale laminate is represented by a unit cell with a wavelength of the twill fabric. The yarns in the fabric are represented by a hexagonal unit cell representing the fiber arrangements in the tow. The matrix in the coated fabric is itself a composite with CNT-impregnated PSS. The representative unit cells of the weave and tow are benefited from the periodic characteristics of the weave architecture and the fiber distribution in the tows. On the other hand, the CNT-modified matrix is represented by a representative unit cell that implements periodicity during fiber generation. Such an intricate analysis necessitates accurate geometric parameters and fiber fractions at each scale as described hereafter. The forthcoming sub-section first evaluates electromechanical behavior of CNT-PSS nanocomposite matrix which serves as input for macroscopic electromechanical response prediction for smart twill laminate composite. The multi-physical approach towards prediction of electromechanical behavior follows a robust sequential strategy, as adopted in [136] whereby the mechanical deformations are captured in a deformed mesh which is
re-meshed and used as the starting geometry for electrical simulations. Thereafter, intrinsic electrical properties of the constituents are assigned and effective electrical response is obtained.

2.1 Electromechanical response of CNT-PSS nanocomposite matrix

2.1.1 Geometry generation and unit cell

In the CNT-PSS unit cell, a random 3D network of CNT fillers is generated, the distribution of which is obtained from [363], as shown in Figure 2 (a).

Figure 2 (a) Unit cell representing CNT-PSS and (b) meshed unit cell

CNTs are considered straight solid cylinders with a radius 2 nm. Their length follows a gaussian distribution with a mean value of 100 nm and a standard deviation of 20 nm. Size distribution of CNTs is adopted from the literature [363]. The generated RVEs have a size of 300nm edge length. Such size of RVEs have been shown to be representative in the literature [363]. A boundary wall conditioned approach, as demonstrated in [372], is adopted for this study that involves implementation of a cut-off boundary condition. Such cut-off boundary condition locally trims the fillers protruding the boundary of the unit cell followed by its translation into a respective position on the opposite face. This ensures material periodicity whereby the fillers exceeding the boundary of the unit cell are trimmed and the surplus is placed at the opposite boundary as if the unit cell is a part of a larger set of unit cells. The random microstructure with CNTs is generated by an iterative process whereby random inclusions are seeded and then subjected to a growth rate resulting in the desired particle size distribution. The positions of the inclusions are updated with a constant velocity for every time increment and thereafter checked for overlap. The time increment at every step is adopted to be minimum of those corresponding to every possible colliding inclusion pair.
The algorithm proceeds with assignment of updated positions resulting from collision and growth of inclusions in the bounding box at every step only to be terminated at the target volume fraction of 0.038. Such target volume fraction of CNTs has been shown to form percolating microstructure in [86]. The detailed formulations for unit cell generation are mentioned in [89,136]. The final step involves the implementation of boundary wall approach, as described earlier, to achieve periodicity. Thereafter, the RVE is meshed (Figure 2(b)) and periodic boundary conditions (PBC) are implemented by constraining nodes on parallel surfaces. Prescribed displacement (δ) is applied along x direction for tensile simulations. For shear loading, relative displacements (equaling δ/2) are imposed on faces normal to z. The formulations for PBC are adequately described in the authors’ previous publications [136,235,350]. Geometry generation, meshing and implementation of PBC are done using a python script and the analysis is performed using commercial ABAQUS™ software with cohesive elements for the interface and solid elements for matrix and fibers. The forthcoming sub-sections evaluate the effective mechanical and electromechanical behavior of CNT-PSS matrix.

2.1.2 Mechanical behavior of polymer nanocomposite

2.1.2.1 Matrix behavior

Constitutive equations for describing nonlinear material characteristics of damaged glassy polymers are adopted from [373]. Assuming an isotropic material, the uniaxial behavior of PSS matrix is defined using modified Bodner–Partom (BP) model [373,374]. The BP model [374] defines plastic flow as a correlation between the stress σ (its deviatoric component being denoted by σ′) and the effective plastic strain p as mentioned in Equation 2.

\[ \sigma = (Z_1 + Z_2) g(p) \]  

[8-2]

Where \( Z_1 \) and \( Z_2 \) are internal variables for hardening and softening respectively governed by the plastic work and \( g(p) \) is a rate dependent functional (rate being governed by parameter \( n \)) defined for glassy polymers as follows.

\[ g(p) = (8.660e3p)^{1/2n} \]  

[8-3]

In order to obtain the parameters \( Z_1 \), \( Z_2 \) and \( n \), the limiting values of the solution variables are determined from experimental stress-strain observations followed by suitable fitting methods as described in [373]. At the peak stress where the plastic strain \( p \) equals total strain, the value of \( Z_2 \) becomes zero (no softening) while the value of \( Z_1 \) is denoted as \( Z_{1o} \) (initial hardening value). In the
current scope of study, the rate dependence of the materials is limited to quasi-static loading which leads to a safe consideration of \( n \) being 9.2 [373] thus characterizing the hardening parameter \( Z_{10} \).

As observed from stress-viscoplastic strain relationships of glassy polymers, the work hardening rate exhibits a bilinear behavior with stress which can be described by two hardening parameters \( m_1 \) and \( m_2 \). This observation leads to the following relations between the hardening and softening variables \( Z_1 \) and \( Z_2 \) respectively with the plastic work \( W^p = \int_{t_0}^{t} \sigma \, dp \).

\[
Z_1 = (1 - \alpha) \, Z_{10} + \alpha \, Z_{10} \exp \left( \frac{m_1 \, W^p}{Z_{10}} \right) \tag{8-4}
\]

\[
Z_2 = Z_{2s} \left[ 1 - \exp(-m_2 \, W^p) \right] \tag{8-5}
\]

Where \( Z_{10} \) is the initial value of \( Z_1 \) (obtained from previous step at yield stress), \( Z_{2s} \) is the saturation value of the softening variable \( Z_2 \). A close observation of the bilinear work hardening rate and stress relationship for glassy polymers shows zero work hardening rate at a value of stress equaling plateau stress from which \( \alpha \) can be obtained around 0.2 for such materials. At the plateau stress, the plastic work is denoted by \( W^p \) which is used in Equation 4. The slopes of the bilinear relationships (bilinearly fitted between work-hardening rate and stress) are \( m_1 / Z_{10} \) and \( m_2 \). The saturation value of the softening variable is defined by Equation 6.

\[
Z_{2s} = \frac{1 + \gamma_1 / m_1 \, g(p)}{Z_{10} + m_2 / m_1 \, \exp \left( - \left( m_2 + \frac{m_1}{Z_{10}} \right) W^p \right)} \tag{8-6}
\]

Where \( \gamma_1 \) is the work hardening rate of the positive arm of the bilinear relationship at zero stress.

In order to characterize damage in glassy polymers, yields surfaces are defined in terms of normalized effective and hydrostatic stresses [375,376]. In the current scope of study, the PSS matrix is considered to be defect free. Once damage sets in such a material, the deviatoric inelastic strain \( \mathbf{p}' \) correlates with post damage stress \( \mathbf{\sigma}'_d \) (its deviatoric component being \( \mathbf{\sigma}'_d ) \) as per Equation 7 (Note that prior to damage initiation, \( \mathbf{\sigma}'_d = \mathbf{\sigma}' \)).

\[
\mathbf{p}' = (1 - f) \mathbf{\sigma}_e \mathbf{p} \left( \mathbf{\sigma}_d : \frac{\partial \phi_p}{\partial \mathbf{\sigma}_d} \right)^{-1} \mathbf{\sigma}'_d \tag{8-7}
\]

\[
\mathbf{p}^h = (1 - f) \mathbf{\sigma}_e \mathbf{p} \left( \mathbf{\sigma}_d : \frac{\partial \phi_p}{\partial \mathbf{\sigma}_d} \right)^{-1} q_1 q_2 f \mathbf{\sigma}_e \sinh \left( \frac{3}{2} q_2 \frac{\mathbf{\sigma}_d^2}{\mathbf{\sigma}_e} \right) \tag{8-8}
\]

Where \( q_1, q_2 \) are the internal variables characterizing the distortion phenomena, \( f \) is the void fraction, \( \mathbf{\sigma}_e \) is the equivalent stress (\( = \sqrt{3/2 \mathbf{\sigma}' : \mathbf{\sigma}' } \)) and \( \phi_p \) is the inelastic flow potential of the
material. Thus, the inelastic flow rule as quantified by the aforementioned parameters is defined as follows:

\[ p = \frac{2}{3} (1-f) \lambda \sigma_e^2 \left( \sigma_d' : \sigma_d' + q_1 q_2 \frac{f}{3} \sigma_e \sinh \left( \frac{3}{2} q_2 \frac{\sigma_h}{\sigma_e} \right) \sigma_d : I \right)^{-1} \left( \sigma_d' + q_1 q_2 \frac{f}{3} \sigma_e \sinh \left( \frac{3}{2} q_2 \frac{\sigma_h}{\sigma_e} \right) I \right) \]

[8-9]

Where while the parameter \( \lambda \) relates the inelastic strain and deviatoric stress prior to damage initiation as per Equation 10.

\[ \lambda = \frac{3 \ p}{2 \sigma_e} \]  

[8-10]

The damage in the material proceeds with void growth that result from void nucleation under loading conditions. A simplified model adopted from [373] captures the growth of voids resulting in damage propagation. The rate of void volume fraction growth denoted by \( \dot{f} \) is given by the following Equation.

\[ \dot{f} = 3 (1-f)p^h + \frac{f_N}{\sqrt{2 \pi}} \exp \left[ -\frac{1}{2} \left( \frac{p-e_N}{s} \right)^2 \right] p \]  

[8-11]

Where the constant \( f_N \) denotes the void volume fraction resulting from void nucleation, the normal distribution of which has a mean of \( e_N \) and a standard deviation of \( s \). In the current scope of study, the distortion phenomena governing the damage progress in polystyrene are adopted from calibrated models of such glassy polymers which are assumed to be defect-free initially, as mentioned in [373]. While the input Young’s modulus and Poisson’s ratio for PSS matrix are adopted as 2.4 GPa and 0.38 [377] respectively, the identified parameters, adopted from [373] for PSS matrix are tabulated in Table 1. For CNT, adopted Young’s modulus and Poisson’s ratio are 500 GPa and 0.3 respectively [378].

Table 8-1 List of parameters for the PSS matrix with corresponding units adopted from [373]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_0 )</td>
<td>( s^{-1} )</td>
<td>( 10^4 )</td>
</tr>
<tr>
<td>( n )</td>
<td>-</td>
<td>9.2</td>
</tr>
<tr>
<td>( Z_{10} )</td>
<td>MPa</td>
<td>34.9</td>
</tr>
<tr>
<td>( m_1 )</td>
<td>-</td>
<td>20</td>
</tr>
<tr>
<td>( m_2 )</td>
<td>MPa(^{-1} )</td>
<td>12.1</td>
</tr>
<tr>
<td>( Z_{2s} )</td>
<td>MPa</td>
<td>-12.8</td>
</tr>
</tbody>
</table>
2.1.2.2 Interface behavior

The interfacial failure of the CNT embedded in the polymer matrix is realized through cohesive finite element method using zero-thickness interface elements [154,235,306,379]. Such approach has been successfully implemented in the literature [136] for evaluation of electromechanical responses. Before onset of damage, the traction-separation cohesive surface behavior is defined as follows:

\[ \sigma = K\delta \]  \hspace{1cm} [8-12]

Where \( \sigma \) is the surface traction, \( K \) is the cohesive stiffness and \( \delta \) is the separation of contact surface. Since isotropic cohesive surfaces are implemented in this study, each of the orthogonal directions have equivalent stiffness, strength and fracture toughness. A bilinear traction-separation behavior with linear damage evolution is adopted here [380]. The damage initiation is governed by maximum stress criterion and is characterized by a damage variable that scales linearly from 0 to 1 from damage onset to complete damage, the corresponding respective separations being \( \delta^0 \) and \( \delta^f \). While \( \delta^0 \) is the separation at which the developed stress equals the strength of the interface, \( \delta^f \) denotes the separation at failure. The area enclosed by the bilinear traction-separation curve yields the fracture energy \( G_c \). In this study, the fracture toughness of 85 mJ/m\(^2\) [381] is adopted for the interface whereas the strength of 5 MPa [382] has been incorporated for CNT-PSS unit cell.

2.1.2.3 Effective mechanical response of polymer nanocomposite

The numerical analysis of a representative unit cell containing CNTs in PSS matrix helps to characterize the mechanical behavior of the matrix pockets in subsequent scales. Both tensile and shear loads are applied on the unit cell in a displacement-controlled setup. The development of
stresses in the virtual microstructure proceeds with concentration pockets around the fibers owing to the stiffness gradient between the inclusion and the glassy matrix. In the three-phase microstructure, the stiff inclusions are embedded in a weak matrix with weaker interfaces. Thus, with increasing strains, the interface damage initiates. The progressive debonding of the fibers with the surrounding matrix is demonstrated in Figures 3(a) and (b) at tensile strains of 0.0145 and 0.0175 respectively. As the debonding progresses at the fiber-matrix interface with increasing strain, the stress in the matrix keeps on increasing loading to onset of void growth in matrix, as captured in Equation 11. This enables quantification of local damage in the matrix. Figures 3(c) and (d) show the progressive damage at tensile strains of 0.02 and 0.03 respectively. A closer observation of the damage patterns reveals strands of local damaged patches, a characteristic of such glassy polymers.

![Figure 3](image_url)

**Figure 3** Progressive debonding and matrix damage at corresponding tensile strains of (a) 0.0145 (b) 0.0175 (c) 0.02 and (d) 0.03 respectively

The tensile behavior of the CNT-PSS nanocomposite is shown in Figure 4. The tensile strength of the matrix as required for subsequent simulation is found to be 24.8 MPa while the tensile modulus is 2.47 GPa. As observed from Figure 4, the initial modulus starts degrading once interfacial debonding sets in and it continues until the peak is reached. Beyond the peak, the stiffness degradation is significant implying onset of matrix damage. The plastic behavior of the matrix results in a curved peak.
The incorporation of CNTs in polymers leads to increase in the overall toughness of the composite which can be attributed to pull-out of CNTs besides de-bonding and crack bridging. The overall fracture toughness of the nanocomposite is given as [383,384]:

\[ G_c = G_m + \sum \Delta G_i \]  \[8-13\]

Where \( G_c \) is the fracture toughness of the overall nanocomposite, \( G_m \) corresponds to that of the matrix and \( \sum \Delta G_i \) denotes the additional fracture toughness brought about by the CNTs. The major contributors to the additional fracture toughness are attributed to the pull-out of CNTs (\( \Delta G_{pull-out} \)) and the interfacial debonding energy (\( \Delta G_{db} \)), as demonstrated successfully in [385]. The pull-out contribution of the CNTs is demonstrated in Equation 14.

\[ \Delta G_{pull-out} = \frac{\tau_i \psi_{po} l_e^2}{3r_f} \]  \[8-14\]

Where \( \tau_i \) is the interfacial shear stress, \( \psi_{po} \) is the volume fraction of pulled out fibers, \( l_e \) is the effective pulled out length and \( r_f \) is the radius of fiber. The contribution of the debonding to the fracture toughening can be captured by the following Equation [386].

\[ \Delta G_{db} = \frac{G_i l_f \psi_{db}}{\phi_f} \]  \[8-15\]

Where \( G_i \) is the interfacial fracture energy between CNT-PSS, \( \psi_{db} \) is the volume fraction of the debonded fibers, \( l_f \) and \( \phi_f \) are the lengths and diameters of fibers.

Figure 5 shows the progressive debonding of the fibers as simulated under tensile strains of 0.017 and shear strain of 0.006 respectively. Having ascertained the debonded volume fractions of the fibers, the enhancement of fracture energy can be computed as described earlier. While the input
matrix toughness is 0.49 kJ/m² [387], the effective fracture toughness of CNT-PSS nanocomposite, obtained from aforementioned simulation, is 0.6 kJ/m².

The input shear toughness for PSS matrix is obtained using a ratio of the shear to normal fracture toughness of 0.54, which has been successfully adopted for similar glassy matrices in [388]. From the shear simulations, a shear modulus of 1.2 GPa and strength of 6.2 MPa are obtained. The resulting shear toughness, obtained from simulation, for the polymer nanocomposite is 0.3 kJ/m². The homogenized responses, obtained here, are used as matrix properties for simulation of smart twill weave composites.

2.1.3 Effective electrical response of polymer nanocomposite

2.1.3.1 Modification of unit cell geometry to incorporate tunnels
As mentioned earlier, this study considers a target CNT volume fraction of 0.038 [86] so as to achieve percolation [363]. The interference of the tunneling effect zone is captured in this study by modeling the tunnel zones as domains surrounding the CNTs. Such a procedure of modeling CNTs without intersection while capturing the tunneling zone as domains has been successfully implemented towards percolation prediction in polymer nanocomposites [363]. Owing to deformations arising from loading conditions, the CNTs when separated by a distance less than 0.47nm [389] are considered to activate tunnels.

2.1.3.2 Establishing percolation
The percolation theory, introduced in [390], describes the transition from insulator to conductor based on the volume fraction of the conductors. In the current scope of study, the otherwise insulating matrix shows a sudden jump in its overall conductivity once the embedded conductors
(here, MWCNTs) form a conducting network. Beyond a certain threshold volume fraction, the conductive pathway is established among the clustering nanotubes which leads to a dramatic increase in the conductivity. The cut-off volume fraction that invokes the phase change from insulator to conductor is defined as the percolation threshold. The numerical simulation of the percolating microstructure involves generation of a periodic microstructure of a certain volume fraction of CNTs. Periodic unit cells are highly efficient in prediction of percolation onset as demonstrated in [372]. As mentioned earlier, two nanotubes are considered to be percolating when they are separated by a distance less than a cut-off distance (tunneling distance). Here in this study, the tunnel zones are considered to be of 2 nm thickness which is consistent with the value reported in the literature [363]. A cut off distance of 0.47nm [389] is considered. In a numerical framework, every tube is scanned along its projection in a plane to determine its connectivity with nearest neighbors while checking for percolation along the normal to the plane. The iteration for every nanotube terminates at the co-ordinate where the cut-off distance criterion is satisfied. The percolating path is traced out for each orthogonal direction towards ascertaining the percolation. Figure 6 shows percolation path for considered CNT volume fraction of 3.8%.

![Percolation unit cell showing the connected paths along X, Y and Z directions (grey: connected paths)](image)

2.1.3.3 Homogenized electrical response

In the current scope of study, the Joule heating effect is neglected. Similar strategy has been successfully considered in [363,389]. Once the percolating unit cell is obtained, the effective electrical conductivity is computed by the volume average of the electrical field, as mentioned in Equation 16 [363].

\[
\bar{\sigma} = \frac{1}{V} \int_{V} J dV \quad [8-16]
\]
Where $U$ is the potential difference across the faces of the unit cell, $J$ is the local electric current density and $V$ represents the volume. The input electrical conductivities, considered in this study, are $10^{-14} \, S/m$, $1.37 \times 10^6 \, S/m$ and $1.17 \times 10^{-4} \, S/m$ for the PSS matrix, CNT and tunnel respectively [363].

### 2.1.4 Effective electromechanical response of CNT-PSS nanocomposite

For effective electromechanical response of CNT-PSS nanocomposite, the iterative procedure initiates with a displacement-controlled mechanical loading which results in a deformed configuration and the solution dependent damage progresses in the RVE. A 3D spatial interpolation function is generated for every material domain in terms of the progressive damage variable. This study implements interpolated spatial distribution for defining solution dependent material properties at every domain [391]. A step operation applies proportional decrease in the elemental electrical conductivity depending on the state of damage. This is represented mathematically as follows [89,136]:

$$\sigma_i = (1 - D)\sigma_{i-1}$$  \[8-17\]

Where $\sigma_i$ is the current degraded conductivity, $D$ is the mechanical damage variable and $\sigma_{i-1}$ is the conductivity corresponding to previous configuration.

Thus, the effective electrical response of the RVE is obtained for several deformed configurations with varying strain. The electromechanical response of CNT-PSS nanocomposite is evaluated here using fractional change in resistivity (FCR) which is defined as follows [136]:

$$FCR = \frac{\Delta R}{R_0}$$  \[8-18\]

Where $\Delta R$ is the change in resistivity with varying strain and $R_0$ is the bulk resistivity of the material. The correlation of strain with FCR provides a deeper insight into the piezoresitive response of the CNT-PSS thin film which are later used to ascertain the electrical behavior of smart weave under mechanical loads. The current distributions in the RVE corresponding to different strain/damage states are shown in Figure 7. With increasing strain, as the damage progresses several non-conducting pockets start appearing which results in gradual decrease in the overall current flow.
Figure 0.7 Current density for (a) and (b) front slice and (c) and (d) end slice corresponding to strains of 0.0175 for (a) and (c) and 0.03 for (b) and (d) respectively.

Figure 8 shows the obtained FCR with varying tensile strain for CNT-PSS nanocomposite. While a linear correlation exists in the initial stages (strain up to 0.01), jumps are observed thereafter resulting in non-linear changes. While the linear changes can be attributed to the piezoresistive characteristics of percolated CNT network in the RVE, the non-linear responses at higher strains result from damages in the interface and matrix. Such mechanically induced phenomena change the current distribution in the RVE which results in increase the overall resistance of the composite (See Figure 4). The piezoresistive response of CNT-PSS nanocomposite, thus obtained, is used later as input matrix property in the analysis of smart weave as described hereafter.

Figure 8.8 Fractional change in resistivity with strain for CNT-PSS under tensile load

2.2. Multiscale electro-mechanical response of smart twill weave laminate:

This section utilizes the homogenized electro-mechanical responses of the CNT-PSS nanocomposite matrix and implements the progressive failure analysis of the hierarchical woven composite. The numerical framework incorporates the squeezing effects of the tows in contrast to often-considered unidirectional behavior. The smart twill weave is subjected to virtual tensile loads and its progressive failure is quantified. Towards that end, micromechanics-based failure criterion
is introduced in a multi-scale approach so as to predict the weave damage in the fiber and matrix level. This leads to a damage model that can effectively integrate complex damage mechanisms of the weaves. Having ascertained the deformed configuration, the electrical response is simulated in the discretized temporal domain corresponding to the mechanical states at such instants. This enables a piezoresistive behavior evaluation of the composite laminate in terms of the strain history correlated with the developed stress and fractional change in resistivity.

2.2.1 Geometries and boundary conditions:

The representative unit cell (160 μm x 160 μm x 270 μm) of the periodic fiber arrays within the tows of the weave is shown in Figure 9 (a).

![Figure 8](image)

Figure 8 9 Unit cell representing: (a) tow of the woven fabric with glass-fiber volume fraction of 52% (b) CNT-PSS matrix-coated twill weave fabric laminate.

Such representative unit cell was successfully adopted in [392]. The representative unit cell for CNT-PSS matrix-coated twill weave fabric laminate is shown in Figure 9(b). The periodic array for twill fabric are equal in length and width of 7.74 mm. The thickness of the coated laminate is adopted as 0.24 mm. The dimensions are representative of the 2x2 twill weave with the volume fraction of tow being 0.722 as adopted from [392]. The tows in the unit cell are balanced implying that the warp and weft tows have same waviness ratio and tow volume fraction while those are in full contact [393]. For the CNT-PSS coated woven laminate, the matrix is considered isotropic, with its input mechanical and strain dependent resistivity properties obtained from CNT-PSS simulations (see Section 2.1). The tow behavior is homogenized from the FE analysis of the fiber impregnated matrix unit cell (see Section 2.2.2). Having ascertained mechanical responses from the multiscale framework, the electromechanical responses are obtained by the interpolating strain maps that enable relevant resistivity assignment to the matrix as guided by progressive damage. The weave unit cell is generated in an open-source program TexGen [394] and subsequently solved in ABAQUS™. The representative unit cells at the tow and weave scales are periodically bounded
with individual face nodes being mapped to the opposite face, as enabled by a preprocessor coded in Python.

Adopting the repetitive nature of the unit cells at each scale, periodic boundary conditions are applied. The efficiency of such boundary conditions towards effective property prediction of inclusion embedded systems with various planes of symmetry are detailed in [395]. The relative displacement \( (u_i \text{ for } i = x, y, z) \) for each pair of nodes on the parallel boundary surfaces (represented by point A and point B lying on such faces) of the unit cell are given by the following Equation [392].

\[
    u_i^A - u_i^B = \epsilon_{avg}\Delta x_k
\]

Where \( \epsilon_{avg} \) is the average strain in the unit cell and \( \Delta x_k \) is the position vector connecting the points on the parallel boundaries. The boundary conditions are implemented by setting a constraint between each pair of nodes on the parallel boundary surfaces. The node pairs are correlated by a preprocessor to ensure the correspondence between such nodes on parallel surfaces. Such an implementation has been demonstrated in [396] to maintain traction and displacement continuity on the parallel surfaces.

2.2.2 Simulation methodology for mechanical response of smart twill weave laminate

The smart twill weave laminate comprises the fiber tows embedded in the resin with a tow-matrix interface. The overall framework followed in this study is elucidated in Figure 10. The laminate analysis commences with obtaining the homogenized properties of the fiber tow and the CNT-modified matrix. While the matrix properties are obtained from randomly generated unit cells (See Section 2.1.2), the homogenized fiber tow properties are obtained from the hexagonal unit cell (see Figure 9(a)). Having ascertained the constituent properties, the macro-scale laminate analysis is initiated. With increasing applied uniaxial tensile strains, the stress responses in the laminate elements are first obtained in each material domain (the tows and coated films with an interface). If the element represents the matrix, the homogenized constitutive response for CNT-PSS nanocomposite (explained earlier in Section 2.1.2.3) is adopted. The damage initiation and propagation in the matrix result in degraded overall stiffness. For the zero-thickness elements representing the tow-matrix interface, interfacial debonding initiation and propagation criteria is implemented as explained later in this paper. When the macro-scale laminate element represents fiber tow, constituent–level micromechanics of failure approach is invoked. Such an approach is adopted for fiber tow due to its orthotropic nature and respective failure criteria along different
directions. In this approach, at the integration points of the element, the micron-scale analysis involving matrix-glass fiber hexagonal representative unit cell is initiated and the failure status at the matrix and fibers is evaluated. This approach provides direct contribution towards stiffness-degradation of the macro-scale element if damage is initiated in the fibers or matrix within the tow. Thus, the aforementioned approach provides damage status at the matrix, fiber tow and matrix-tow interface which yields homogenized macroscopic tensile stress-strain responses for woven laminated composite. Figure 10 illustrates the framework for mechanical response prediction of woven unit cell. The input properties to the weave unit cell correspond to that of the homogenized tow (Section 2.2.2.1) and homogenized matrix (Section 2.1.2). The progressive debonding in the tow-matrix interface is detailed in Section 2.2.2.2. The tow analysis (Section 2.2.2.3) involves a micromechanical analysis that implements damage in matrix and fiber inside the tow. The thin film analysis involves damage initiation and progression in the matrix (Section 2.2.2.4). The stiffness degradation brought about by accumulated damages in the matrix and fiber are thereafter assimilated in the weave unit cell as a continuum damage tensor (Section 2.2.2.5).

Figure 10 Framework showing the mechanical response prediction of the smart weave unit cell

2.2.2.1 Homogenized tow properties: Input to weave unit cell

For fiber tow, the unit cell representing the tow (see Figure 9(a)) is bounded periodically and subjected to tensile and shear loadings (similar to Section 2.1.2) to obtain its effective properties. Table 2 lists the obtained homogenized tow properties which are used as input to the macro-scale laminated woven composite analysis.

<table>
<thead>
<tr>
<th>Table 2 Homogenized tow properties</th>
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<td>Parameters</td>
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176

<table>
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</tbody>
</table>

2.2.2.2 Response of Tow-matrix interface

This section elaborates the behavior of the tow-matrix interface implemented using zero-thickness cohesive elements. Progressive debonding of the tow-matrix interface helps to capture the stress gradients observed near geometric discontinuities in the weave composite. A bilinear traction-separation law is followed to characterize the cohesive elements at the interface of the yarns and the matrix. Before the damage onset, the linear traction separation law enforces an elastic behavior, as represented by Equation 20.

\[
\begin{pmatrix}
    t_n \\
    t_s \\
    t_t
\end{pmatrix} =
\begin{pmatrix}
    K_n & K_s & K_t \\
    K_s & K_s & K_t \\
    K_t & K_t & K_t
\end{pmatrix}
\begin{pmatrix}
    \delta_n \\
    \delta_s \\
    \delta_t
\end{pmatrix}
\]

Where \( t_i \) are the tractions, \( K_i \) are stiffnesses and \( \delta_i \) are separations of contact surfaces for \((i = n \text{ for normal and } s, t \text{ for shear})\). For numerical convergence, a large value of stiffness is adopted to represent perfect bonding at the interface elements without separation, as demonstrated in [397]. The damage initiation criteria is shown in Equation 21 [398].

\[
\left( \frac{t_n}{t_n^0} \right)^2 + \left( \frac{t_s}{t_s^0} \right)^2 + \left( \frac{t_t}{t_t^0} \right)^2 = 1
\]

Where \( \langle x \rangle \in R \) is defined as \( (x + |x|)/2 \).

After damage initiation, the progressive damage follows a BK criterion [392] towards softening behavior characterization as shown in Equation 22.

\[
G_C = G_{nc} + (G_{sc} - G_{nc}) \left( \frac{G_s + G_t}{G_s + G_t + G_n} \right) \eta
\]

Where \( G_C \) is mixed-mode fracture toughness, \( G_{nc} \) and \( G_{sc} \) are normal and shear critical toughness of the interface (See Table 3), \( \eta \) is a material constant (adopted as 1.45 [398]). The computation of
$G_i$ (for $i = n, s, t$) comprises the area under the corresponding traction-separation curve (for normal and shear loads).

The interface damage variable is similarly defined as follows.

$$D = \frac{\delta^f_m (\delta^m_{m} - \delta^0_m)}{\delta^m_{m} (\delta^m_{m} - \delta^0_m)}; \quad \delta^0_m \leq \delta^m_{m} \leq \delta^f_m$$

[8-23]

Where $\delta^m_{m}$ is the maximum value of $\delta_m$ (effective separation) throughout the loading history. The effective separation is given by $(\delta_m = \sqrt{\langle \delta_n \rangle^2 + \delta_s^2 + \delta_t^2})$. The effective separation at the onset of damage denoted by $\delta^0_m = \left(T_{int}/K\right)$ is given by the ratio of interfacial strength ($T_{int}$) and stiffness ($K$). The mixed-mode separation at failure denoted by $\delta^f_m$ is given by $2G_C/K\delta^0_m$ where $G_C$ is computed by B-K equation (see Equation 22). The tractions are continuously updated during the loading process as per the following Equation [398].

$$t = K\delta \quad \text{for elastic stage} \quad (\delta^m_{m} < \delta^f_m) \quad [8-24]$$

$$t = (1 - D)\bar{\tau} \quad \text{for softening stage} \quad (\delta^0_m < \delta^m_{m} < \delta^f_m). \quad [8-25]$$

Where $\bar{\tau}$ is the traction stress component calculated by linear-elastic traction separation behavior for the current separation displacement. The strength for tow-matrix interface is considered 1.5 times that of the transverse strength of the tow [399]. Thus, the strength is computed as 36 MPa from the yarn properties reported in [400]. The normal fracture toughness for coated glass systems is 0.280 J/mm², as determined in [401]. A similar value for normal toughness has been adopted in [398] which reports the shear fracture toughness as 1.45 J/mm² which has been adopted in the study.

The input interface properties are tabulated in Table 3.

### Table 8.3 Input properties for tow-matrix interface debonding

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Value</th>
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<td>strength</td>
<td>MPa</td>
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</tr>
<tr>
<td>$G_n$</td>
<td>J/mm²</td>
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<tr>
<td>$G_s$</td>
<td>J/mm²</td>
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</tr>
<tr>
<td>$G_t$</td>
<td>J/mm²</td>
<td>1.45</td>
</tr>
</tbody>
</table>

#### 2.2.2.3 Mechanical behavior of Tow

During the tow analysis, a micromechanics-based framework invokes a constituent level response prediction thus facilitating a multiscale analysis. This is brought about by computation of stresses
at the fiber and matrix material domains of the hexagonal unit cell representing the tow when macro-stress appears in the tow of the laminate. When the macrostructure is subjected to an external load, the micro-stress at the level of its constituents namely fiber and matrix are characterized in terms of amplification factors at salient points (refer to Figure 11) in a representative unit cell as follows [392,402,403]:

\[ \sigma = M \bar{\sigma} \]  \[8-26\]

Where \( M \) is the stress amplification factor, \( \bar{\sigma} \) is the macro scale stress and \( \sigma \) is the micro-scale stress. In order to determine the amplification factor, a periodic representative volume of the fiber and matrix (see Figure 11) is subjected to a FEA with unit traction boundary condition.

Under a single traction boundary (say \( \bar{\sigma}_i = 1 \)), the corresponding \( \sigma_i \) is obtained at representative distinct points in the matrix and the fiber (Figure 11). Since \( \bar{\sigma}_i = 1 \), the corresponding \( M_{ji} = \sigma_i \) which suggests that each component of the micro-scale stress at a point represents the amplification factor at that point. An array of judiciously chosen points (17 in fiber and 19 in matrix as shown in Figure 11), as adopted from [402] serve as the key points for efficient characterization of amplification factor of the fiber and matrix. Averaged amplification factors from the selected salient points are adopted for fiber and matrix separately. The methodology enables the computation of stresses at level of constituents (matrix and fiber) when the fiber tows are loaded in the laminate scale. Such a procedure has been successfully implemented towards multi-scale failure analysis of fiber-reinforced composite cylinder [403] and woven composite [392]. Figures 12 (a), (b) and (c) show a schematic representation of the macroscopic stress states while Figures 12 (d), (e) and (f) show the corresponding constituent level stresses (micro-stress distribution). Since the micromechanics framework enables computation of the stresses at the constituent level, the failure
Failure prediction of composites at the constituent level can be brought about by micromechanics of failure (MMF) theory. This translates to the tow behavior whereby almost the entire load is supported by the fibers for longitudinal loads. This justifies the characterization of fiber dominated damage initiation by a non-interacting maximum stress criterion. The fiber failure criterion is given by Equation 27.

\[
\frac{\sigma_f}{T_f} = 1; \frac{\sigma_f}{C_f} = 1
\]  

[8-27]

Where \( C_f \) and \( T_f \) are the compressive and tensile strengths of the fibers while \( \sigma_f \) is the fiber longitudinal stress at the micro scale. The matrix failure initiation criteria is adopted based on von Mises stress at micro level [392]:

\[
\sigma_{\text{matrix}} = 1
\]
\[ \frac{\sigma_{vm}^{m}}{T_{m}} = 1 \]  [8-28]

Where \( T_{m} \) is the matrix tensile strengths, \( \sigma_{vm}^{m} \) is the matrix von Mises stress at the micro level.

This study adopts damage evolution based on an energy equivalence between strain energy dissipated during failure and fracture energy at failure [392]. The following formulations culminating in a damaged stiffness matrix proceed with an iterative computation of the fracture energy of the stressed elements in the matrix and fibers. It is to be noted that the longitudinal and transverse directions in the orthotropic material are represented as \( l, t \) and \( z \) which are denoted by an index \( i \). The fracture toughness \( G_{i} \) over a characteristic element length \( l \), in purview of the crack band theory can be related to the dissipated energy rate per unit volume \( g_{i} \) as follows [404]:

\[ g_{i} = \frac{G_{i}}{l} \]  [8-29]

Where \( g_{i} \) is the area under the equivalent stress and equivalent displacement curve \( (= \frac{1}{2} \sigma_{	ext{eq}} \delta_{	ext{eq}}) \).

For every component, the equivalent stress and displacement per unit characteristic length are constructed as follows [392, 403]:

\[ \delta_{i,\text{eq}} = l \varepsilon_{i,11}; \quad \sigma_{i,\text{eq}} = \sigma_{i,11} \varepsilon_{i,11} / \delta_{i,\text{eq}} \] [for fiber]  [8-30]

\[ \delta_{i,\text{eq}} = l \sqrt{\varepsilon_{i,n}^2 + \gamma_{i,s}^2 + \gamma_{i,t}^2}; \quad \sigma_{i,\text{eq}} = \frac{\sigma_{i,n} \varepsilon_{i,n} + \tau_{i,s} \gamma_{i,s} + \tau_{i,t} \gamma_{i,t}}{\delta_{i,\text{eq}}} \] [for matrix]  [8-31]

Where \( \epsilon_{i,11} \) and \( \sigma_{i,11} \) are fiber longitudinal strains and stresses; while for matrix, \( \varepsilon_{i,n} \) and \( \sigma_{i,n} \) are longitudinal strains and stresses respectively; \( \gamma_{i,s}, \gamma_{i,t} \) and \( \tau_{i,s}, \tau_{i,t} \) are shear strains and stresses respectively along the transverse directions. For characterizing fiber failure, its longitudinal fracture toughness is considered. Meanwhile, a mixed-mode fracture energy B-K criterion [392] is adopted for matrix failure, as shown in Equation 32 [405].

\[ G_{TC} = G_{IC} + (G_{IIc} - G_{IC}) \left( \frac{G_{II}}{G_{I}+G_{II}} \right)^{\eta} \]  [8-32]

Where \( G_{I} = \frac{1}{2} (\sigma_{n} \varepsilon_{n}) l; \quad G_{II} = \frac{1}{2} (\tau_{s} \gamma_{s} + \tau_{t} \gamma_{t}) l; \quad G_{IC} \) and \( G_{IIc} \) are mode I and mode II fracture toughness of the matrix, \( \eta \) is a material constant. The damage variable based on effective displacement is defined as follows.

\[ d_{i} = \frac{\delta_{i,\text{eq}}^{f} (\delta_{i,\text{eq}} - \delta_{i,\text{eq}}^{0})}{\delta_{i,\text{eq}}^{f} (\delta_{i,\text{eq}} - \delta_{i,\text{eq}}^{0})}; \quad \delta_{i,\text{eq}}^{0} \leq \delta_{i,\text{eq}} \leq \delta_{i,\text{eq}}^{f} \]  [8-33]
Where $\delta_{i,eq}^0$ and $\delta_{i,eq}^f$ are equivalent displacements at damage initiation and complete failure states. For every component (matrix and fiber), the corresponding damage values $d_i$ in $l, t,$ and $z$ directions help to form the damage tensor $D$ for the components in the woven composite, as described in Section 2.2.2.5.

### 2.2.2.4 Behavior of Matrix in laminated woven composite

The thin film/matrix analysis of the woven unit cell proceeds with inputs from the CNT-PSS nanocomposite homogenized response (Table 4). Damage initiation and propagation follow similar formulations as mentioned in Section 2.2.2.3 since the matrix remains the same inside or outside (film) of the tow. The damage values $d_i$ (similarly obtained as shown in Equation 33) characterize the stiffness degradation in the woven unit cell, as described in the forthcoming sub-section.

### 2.2.2.5 Damage in macro-scale weave unit cell

The constituent damages in the matrix and the fiber are assimilated for damage characterization in the representative unit cell of the macro-scale woven composite. Towards that end, the Murukami-Ohno damage model is adopted [392] as shown in Equation 34.

$$D = \sum D_i n_i \otimes n_i$$ \hspace{1cm} [8-34]

Where $D_i$ is the principal damage tensor and $n_i$ the principal unit vector (for longitudinal and transverse directions of the orthotropic material). It is to be noted that the ensuing damage in such composites is irreversible which leads to the damage tensor being the maximum damage encountered in the history. Thus, the damage of the fiber tows in the longitudinal direction is considered to be the maximum fiber damage value under longitudinal loading ($D_L = \max d_{fiber}$) while the damage for the transverse directions is considered to be the maximum in the matrix ($D_T = D_Z = \max d_{matrix}$). For the matrix, the tensor assumes an isotropic form with the maximum damage in the matrix corresponding to longitudinal loads. As per [392], the effective stress in damaged configuration is given by:

$$\sigma^* = \frac{1}{2} [(I - D)^{-1} \sigma + \sigma (I - D)^{-1}]$$ \hspace{1cm} [8-35]

Where $\sigma^*$ is the effective stress while $\sigma$ is the actual stress in the damaged configuration. The stiffness matrix in damaged configuration is defined as follows.
\[
\mathbf{C}(D) = \begin{bmatrix}
d_1^2C_{11} & d_1d_2C_{12} & d_1d_3C_{13} & 0 & 0 & 0 \\
d_2^2C_{22} & d_2d_3C_{23} & 0 & 0 & 0 \\
d_3^2C_{33} & 0 & 0 & 0 \\
d_4C_{44} & 0 & 0 & 0 \\
sym & d_5C_{55} & 0 \\
d_6C_{66} & & & & & 
\end{bmatrix}
\]

[8-36]

Where \(C_{ij}\) are the undamaged stiffness matrix coefficients, \(d_{1,2,3} = (1 - D_{L,T,Z})\), \(d_4 = \left(\frac{2d_4d_2}{d_4+d_2}\right)^2\), \(d_5 = \left(\frac{2d_5d_3}{d_5+d_3}\right)^2\) and \(d_6 = \left(\frac{2d_2d_3}{d_2+d_3}\right)^2\). For the user defined material subroutine, the tangent constitutive tensor in damaged configuration is given by.

\[
\mathbf{C}_T = \frac{\partial \sigma}{\partial \varepsilon} = \mathbf{C}(D) + \left(\sum \frac{\partial C(D)}{\partial D_L} \frac{\partial D_L}{\partial L} \frac{\partial L}{\partial \varepsilon}\right) : \varepsilon
\]

[8-37]

The matrix and fiber input properties are mentioned in Table 4. While the parameters for matrix used in the study are obtained from numerical homogenization of the CNT-PSS unit cell as explained earlier in this paper, the values for glass fiber are adopted from literature [406,407]. The formulations are implemented in a user defined subroutine and solved in ABAQUSTM.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Glass fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's Modulus</td>
<td>GPa</td>
<td>68</td>
<td>2.47</td>
</tr>
<tr>
<td>Shear Modulus</td>
<td>GPa</td>
<td>26.1</td>
<td>1.2</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td></td>
<td>0.22</td>
<td>0.3</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>MPa</td>
<td>1771</td>
<td>24.8</td>
</tr>
<tr>
<td>Shear strength</td>
<td>MPa</td>
<td>-</td>
<td>6.2</td>
</tr>
<tr>
<td>Normal toughness</td>
<td>kJ/m²</td>
<td>3.7</td>
<td>0.6</td>
</tr>
<tr>
<td>Shear toughness</td>
<td>kJ/m²</td>
<td>-</td>
<td>0.3</td>
</tr>
</tbody>
</table>

2.2.3 Macroscopic mechanical response of smart twill laminate

The implementation of the material behavior in the textile composite at interactive scales of the tow and the coated weave enables computation of the tensile response shown in Figure 13 on application of tensile load in the warp direction. The linear elastic behavior is observed up to a strain of 0.005 beyond which the matrix damage initiates. Another change of slope is observed at around a strain of 0.0095 which corresponds to the initiation of debonding of the tow. As the
debonding proceeds, the singular tows are stressed owing to localization of stresses due to lack of contact. This leads to damage propagation in the tow at a strain of around 0.015. Finally, this leads to fiber failure at a strain of around 0.018 following which there is almost an instantaneous drop in stress.

Figure 0-13 Macroscopic stress-strain response under tensile load applied parallel to weave

2.2.4 Electromechanical response of smart twill laminate

For electromechanical response, the conductivity of the glass fiber is considered 2.54e-11 S/m [408] and the electromechanical response of the coating matrix (CNT-PSS nanocomposite), as detailed in Section 2.1, is adopted to represent variation of electrical conductivity with varying state of strain. When damage initiates, a proportional decrease in the elemental electrical conductivity is considered, similar to the methodology detailed in Section 2.1.4. The piezoresistive nature of the nano-engineered composite as captured by the simulation enables the computation of the FCR. Figure 14 shows the electromechanical behavior of the coated weave. Figures 14 (a-d) show the tows at various states of strain while Figures 14 (e-f) show the damage response of the matrix. With increasing strain progressive damage in the yarns can be clearly observed in both weft and warp directions. The yarns in the direction of loading (Figure 14(d)) show higher damages than the transverse yarns (Figure 14(b)) as expected. Additionally, it can be observed that the damages in the yarns initiate at the crimp zones (see Figures 14 (a) and (c)) which can be attributed to the complexity in geometry resulting in concentrated stresses. Figures 14(e) and (f) show the progressive damage in the matrix. It is to be noted that the matrix damage initiates prior to that of the yarn. Thus, the state of damage in Figure 14(e) is higher than that of yarns in loading direction. This is evident from the macroscopic mechanical response whereby matrix damage initiates at 0.005. Figures 14(g) and (h) show the current distribution in the unit cell. It is observed that with
increasing strain, the overall current flow decreases resulting in an increase of resistivity. It is to be noted that the boundary conditions for the mechanical damage analysis (Figures 14(a-f)) are periodic while the electrical simulations (Figures 14(g-h)) are periodic in Y and Z directions with a potential gradient applied along X. Overall, the damaged and stressed areas correspond to the resistive zones thus increasing its overall resistivity with increasing strain.

![Figure 14](image)

Figure 14 Progressive damage in weft yarns (at strains of 0.13 (a) and 0.192 (b)) and warp yarns (at strains of 0.13 (c) and 0.192 (d)); Damage progression in CNT-PSS coating matrix corresponding to strains of 0.13 (e) and 0.192 (f); Corresponding electrical responses at a strain of 0.13 (g) and 0.192 (h)

Figure 15 shows the FCR with increasing strain for the coated textile weave for tensile loads. While the slight changes in FCR at around 0.005 strain can be attributed to the onset of matrix damage, significant change of slope at 0.085 results from tow debonding. Following the onset of damage in matrix and debonding of yarn, a non-linear response in FCR is observed which correlates with the damage propagation in both the matrix and tows. Beyond a strain of 0.02, the fibers fail as observed.
during mechanical simulations which is expected to result in another jump in FCR. However, the FCRs beyond the strain of 0.02 are insignificant in reality owing to the loss of structural integrity of such laminates.

![Fractional change in resistance with varying strain for CNT-PSS coated textile weave under tensile load](image1)

**Figure 15** Fractional change in resistance with varying strain for CNT-PSS coated textile weave under tensile load

### 2.3 Comparison of simulated responses with experimental observations:

Figures 16 shows a comparison between the experimental [86] and simulated gauge factors for the smart twill weave laminated composite. The gauge factor [62,216] is a measure of the sensing efficiency and it is expressed as a ratio of the FCR to the corresponding applied strain. Figure 16 shows excellent correlation between the experimental and simulated gauge factors and such good correlation suggests that the multiscale simulation methodology presented in this study can successfully predict the piezoresistive behavior of smart twill weave laminated composite.

![Correlation between experimental [355] and simulated gauge factors](image2)

**Figure 16** Correlation between experimental [355] and simulated gauge factors
3. CONCLUSIONS

This paper presents a comprehensive multiscale numerical approach towards prediction of electromechanical response of hierarchical smart twill weave laminated composite thin films. The approach, presented in this paper, is unique in its implementation of prediction of electromechanical behavior at the nano-engineered matrix which serves as the reference for the electromechanical simulation of the macro-scale textile in a micromechanics of failure based approach whereby the mechanical damage is computed at the scale of matrix and fiber thus taking into account the nano-scale sensory behavior of such composites. Moreover, the robustness of the approach lies in its ability to capture deformations and large strains at every length scale while taking into account the electrical behavior of the piezoresistive nano-engineered composite. To assess the prediction capability of the simulation methodology, simulated electro-mechanical responses with varying applied strain are compared with experimental responses available in the literature. Simulated responses show excellent correlation with experimental observations. Such good correlation between the experimental and simulated responses provides confidence on the ability of the simulation methodology to represent the complex hierarchical structures of the smart twill weave laminated composite thin film effectively at multiple length scales. Thus, the multiscale numerical simulations presented in this paper can help in developing strategies to tune the hierarchical structures at multiple length scales towards obtaining efficient material design for desired performance.

SUPPLEMENTARY SECTION

A. Mesh Generation

The procedure of meshing involves definition of free mesh for the matrix cube with the embedded inclusions (here, fibers). The periodic unit cell geometry comprises a cubic boundary with embedded inclusions. The meshing procedure culminates in a conformal tetrahedral mesh (with mappable nodes on opposite faces) in the periodic unit cell thus facilitating PBC application. A brief outline of the technique is mentioned herewith. The sequential process initiates with generation of a periodic surface mesh on each face of the cube. Thereafter, a surface mesh is generated on each inclusion followed by construction of a tetrahedral volume mesh inside the inclusion. Having generated the periodic surface mesh on the cube and the inclusion surface, a volume mesh is generated around every inclusion and the cube by inverting the orientation of the inclusion surface mesh triangles. The volume meshes thus generated (one inside the fiber and the
other between the inclusion and the cube) are united to form a conformal mesh. For the generation of cohesive elements at the interface of the inclusions and the matrix, the coordinates of the nodes on the surface of the inclusions are duplicated followed by a renumbering of nodes which are further connected to form elements with zero thickness. Needless to mention, the shape of the cohesive element is triangular (with a constant thickness initially zero) for ensuring compatibility with the tetrahedral mesh of the fibers and matrix surrounding it. The procedure for generation of surface meshes and subsequent volume meshes followed by the union is illustrated in a flowchart (See Figure A.1) and described hereafter.

Fig. 8- A.1. Meshing procedure adopted for inclusion-matrix periodic unit cells

The first step involving generation of surface meshes on each face of the periodic unit cell initiate with periodic distribution of nodes on the edges of each of the base-faces of the cube (one face per XY, XZ and YZ planes) which are appropriately translated to construct the opposite faces (along XY, YZ and XZ planes) of the cube. The second step of generating surface mesh on the inclusion surface is constructed by defining nodes on the lateral surface and the faces of the inclusions (for cylindrical fibers as adopted in the current study). The third step generates a volume tetrahedral mesh inside each inclusion with respect to the surface mesh. The fourth step involves renumbering of the nodes on the surface of the inclusion so as to invert the orientation of the triangles of the surface mesh on the inclusion with respect to the volume mesh inside the inclusion. With the reoriented inclusion surface mesh, a volume mesh is generated in the region between each inclusion and the cube. The final step ensures compatibility of the two sets of volume meshes (one set inside the inclusion and the other set in the region between the inclusion and the cube) at their shared boundary which is achieved by consecutive renumbering of nodes on the surface of the inclusion.
(which are shared by both sets of volume meshes) followed by the renumbering of nodes inside each inclusion; thus producing a conformal volume mesh with appropriate connectivity of nodes. The meshing procedure is summarized in a flowchart (See Figure A.1). Having obtained the conformal mesh, the PBC are applied on the unit cell. Towards that end, three sets of nodes are extracted. This is required to prevent over constraining of shared nodes (note that edge nodes are shared by adjacent faces while vertices are shared by orthogonal edges). The sets of nodes are as follows. First set: vertex nodes (8 in number for cubic cells), second set: edge nodes for each of the 8 edges on the cell and third set: nodes on each of the 6 faces. The second and third sets are further categorized as per their orientations (parallel to x, y and z directions). In a manner similar to the first step of mesh generation, the base-faces (along XY, XZ and YZ planes) are constrained to the opposite faces for a trivial application of PBC. The constraint equations can be found in [409,410]. It is to be noted that definition of reference points (distinct from the geometry) facilitates the application of the PBC whereby the displacements can be applied on the reference points. A similar methodology of conformal mesh generation is adopted for the 2x2 textile weave unit cell that generates tetrahedral solid elements in the yarns and the surrounding matrix with a similar PBC implementation.

**B. Mesh Convergence**

The mesh convergence studies for each scale: CNT-PSS scale, GF-epoxy unit cell and 2x2 tow-matrix unit cell are shown in Figures B.1(a), (b) and (c) respectively.

For the CNT-PSS unit cell, Figure B.1(a) shows the effect of element size on the homogenized stress-strain behavior. The sizes of the elements are chosen with respect to the mean fiber diameter. In order to capture the geometry of the fiber, the size of the elements are chosen below 0.8R_f (where R_f is the radius of the fiber). From Figure B.1(a), it can be observed that choosing an element size below 0.2R_f causes insignificant change in results. The corresponding number of elements are 1642270.

For the glass fiber-PSS matrix unit cell, Figure B.1(b) shows the variation of computed effective properties with the number of elements. An element size is chosen to adequately represent the geometry (upper limit being 0.8R_f). From Figure B.1(b), it can be observed that the optimum number of elements lies beyond 3x10^5. Thus, the chosen element size is 0.25R_f that generates 331836 elements.
For the 2x2 weave unit cell, Figure B.1(c) shows the homogenized stress-strain behavior for the 2x2 weave unit cell with different number of elements (Nelem). The chosen element size for the mesh is governed by the thickness of the unit cell (note that each yarn is 0.12mm thick). The matrix pockets between adjacent tows and the regions of crossovers govern the minimum element size. The mesh convergence study (see Figure B.1(c)) shows the optimum element size as 0.022 mm that generates 2223642 elements. Further refinement increases computational burden without significantly affecting results.

Fig.8- B.1. Mesh convergence studies for (a) CNT-PSS unit cell [stress-strain response for different element sizes wrt Rf: mean radius of fiber] (b) Glass fiber-PSS unit cell [computed effective properties vs number of elements] and (c) 2x2 weave unit cell [stress-strain response for Nelem: number of elements]

C. RVE size study for CNTs dispersed in PSS matrix unit cell

In order to generate a representative unit cell for the CNTs randomly dispersed in PSS, a size study for the same is carried out. This ensures that the sizes are large enough for adequate representation of features. It is to be noted that the volume fraction of the fibers being pegged at 0.038, a larger RVE size accommodates a higher number of inclusions. Additionally, the volume fraction adopted in the study is as per the experimental procedure and is higher than the percolating volume threshold of 0.028. Towards establishing the adequate RVE size, ten RVEs are generated for every edge length. Thereafter, UT tests are carried out along each of the orthogonal directions to calculate the homogenized Young’s modulus for every combination. Figure C.1 shows the variation of the predicted properties with RVE size. It can be observed that the fluctuations are high for RVEs of smaller sizes which eventually die out with a sufficiently large RVE size. Additionally, the directional properties converge for RVE sizes >= 300nm. Thus, the chosen RVE size is 300nm for
adequately capturing the isotropic behavior of the CNT-PSS unit cell. The chosen size invokes a trade-off between computational expense and prediction efficiency.

![RVE size study](image)

**Fig. 8- C.1** RVE size study (random CNTs dispersed in PSS matrix) for predicted $E_{11}$, $E_{22}$ and $E_{33}$ along orthogonal directions.

**D. Software and Tools**

The FE solver ABAQUS™ is used to carry out the computations. Custom pre-processors are coded in Python to generate RVEs for CNT-PSS and GF-PSS unit cells. Python API with FreeCAD is used to generate the geometries in Parasolid format which can be imported to ABAQUS CAE. A python 2.7 script in ABAQUS imports the geometry, inserts boundary triangles, generates volume meshes for every part and implements cohesive interactions. Constraints enforcing PBC and ties are generated as well. The generated odb are analyzed by a post-processor coded in Python. For the 2x2 textile, TexGen© GUI (powered by Python 2.7) is used to generate a 2x2 weave unit cell which is exported as a volume mesh with periodic conditions. The element positions and orientations (also exported from TexGen) are used to define local material orientations (note that warp and weft yarns are orthogonal to each other while the fiber bundle has distinct axial, transverse and out-of-plane material properties). Constraints and suitable BCs are thereafter implemented. The simulations are run from ABAQUS Command and the generated odb are analyzed. The material models for ABAQUS are coded in FORTRAN as user defined subroutines. The interpolation maps for translating mechanical responses to strain-induced electrical property inputs are generated in MATLAB. This facilitates an uncoupled multi-physics based implementation of piezoresistive behavior.

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