

**ANALYSIS OF THE MECHANICAL BEHAVIOR OF
RECYCLED AGGREGATE CONCRETE USING 3D
MESOSCALE MODELLING**

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A Thesis Presented to the
COLLEGE OF GRADUATE AND INTERDISCIPLINARY STUDIES
KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

**In
CIVIL ENGINEERING**

DECEMBER 2024

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

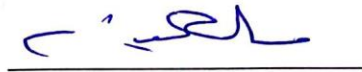
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To my parents, Alhaji Lawan Ahmad Muhammad and Hajiya Farida Lawan Muhammad, who have been the anchors of my life, teaching me the values of perseverance and humility. Your sacrifices and unwavering belief in me have been my greatest inspiration.

To my siblings, Dr. Sakina Lawan Muhammad and Abdullahi Lawan Muhammad, whose laughter and love have been my sanctuary through challenging times.

To the mentors who saw potential in me when I doubted myself, and to friends who walked beside me with patience and encouragement—this achievement is as much yours as it is mine.

And above all, to Allah S.W.T, whose endless blessings and guidance illuminated every step of this journey.

|

ACKNOWLEDGMENTS

First and foremost, I express my profound gratitude to Allah (S.W.T) for granting me the strength, wisdom, and perseverance to complete this work.

I am deeply indebted to my supervisor, Dr. Saheed Kolawole Adekunle, whose guidance, insightful feedback, and unwavering support were invaluable throughout this journey. Your expertise and encouragement have greatly enriched my research and personal growth.

I would also like to extend my appreciation to Dr. Faisal Mukhtar and Dr. Hammad Raza Khalid, whose critical input and advice were instrumental in shaping this work. Thank you for all the mentorship and career guidance. I also want to extend my appreciation to Dr. Asad Hanif, for all the academic mentorship, support, and assistance you have given me, not only in academic matters but also in personal matters.

To my KFUPM colleagues and friends, thank you for your companionship, discussions, and moral support, which made this journey more enjoyable and less daunting.

A special note of gratitude goes to my family—my parents, Alhaji Lawan Ahmad Muhammad and Hajiya Farida Lawan Muhammad, for their unconditional love, prayers, and sacrifices, and my siblings, Dr. Sakina Lawan Muhammad and Abdullahi Lawan Muhammad, for their constant encouragement.

Finally, I acknowledge the financial and material support provided by the KFUPM Graduate Scholarship and the Civil and Environmental Engineering Department, which made this master's program possible.

To everyone who contributed to this achievement, directly or indirectly, I am sincerely grateful.

TABLE OF CONTENTS

ACKNOWLEDGMENTS	VI
TABLE OF CONTENTS.....	VII
LIST OF TABLES.....	XI
LIST OF FIGURES.....	XII
LIST OF ABBREVIATIONS.....	XV
ABSTRACT.....	XVI
ملخص الرسالة	XVII
CHAPTER 1 INTRODUCTION.....	1
CHAPTER 2 LITERATURE REVIEW	5
2.1 Mechanical Properties of Recycled Concrete Aggregate	5
2.2 Modeling Methods for Recycled Concrete Aggregate	6
2.3 Mesoscale Geometrical Models.....	6
2.4 Aggregate Size Distribution.	8
2.5 Generation of Various Aggregate Shapes in 2D	10
2.5.1 Irregular Polygons.....	10
2.5.2 Circular and Elliptical Aggregates	11
2.6 Generation of Various Aggregate Shapes in 3D	12
2.6.1 Spherical aggregate	13
2.6.2 Ellipsoidal aggregate	13
2.6.3 Polyhedral aggregate.....	14
2.6.4 Polygon-based framework.....	15
2.6.5 Crushed aggregates	17

2.7 Aggregates with Rough Surface Texture	18
2.7.1 Aggregates with rough surface texture	18
2.7.2 Surface subdivision	19
2.7.3 Displacement mapping and Laplace smoothing	20
2.8 Various Techniques for the Generation of Mesoscale Model	23
2.8.1 Take and place method	23
2.8.2 Place and squeeze method	25
2.8.3 Random walking algorithm	27
2.8.4 Random fractal method	30
2.8.5 Motion simulation and heuristic packing algorithm	30
2.9 Methods of Overlap Detection	31
2.9.1 2D mesoscale model	31
2.9.2 3D mesoscale model	34
2.10 Numerical Analysis Techniques and Constitutive Material Models	37
2.11 Comparison of the Different Mesoscale Model Generation Algorithm	39
 CHAPTER 3 METHODOLOGY	 41
3.1 Local Background Grid Method	41
3.1.1 Initiation of the global background mesh	41
3.1.2 Material attribute identification using local grids	42
3.2 Generating A Mesoscopic Structure With pyMesoscale	44
3.3 Material Properties	46
3.4 Discretization of the Geometric Domain	47
3.4.1 Element type	47
3.4.2 Mesh size	48
3.5 Boundary Conditions	48
3.6 Finite Element Solver	49
3.7 Constitutive Material Model	49
3.8 Simulation Matrix	52
 CHAPTER 4 RESULTS	 53
4.1 Mechanical Mesoscale Modeling of Randomly Attached Mortar on Recycled Concrete Aggregate .	53
4.1.1 Uniaxial compression test	53
4.1.2 Uniaxial tension test	57

4.2 Mechanical Mesoscale Modeling of Fully Enclosed Attached Mortar on RCA.	60
4.2.1 Uniaxial compression strength test	60
4.2.2 Uniaxial tensile strength test.....	62
4.2.3 Comparison of fully enclosed and randomly attached recycled concrete aggregate	63
4.3 Mechanical Mesoscale Modeling of Combinations of Natural And Recycled Concrete Aggregates... ..	65
4.3.1 Uniaxial compression strength test	65
4.3.1 Uniaxial tensile strength test.....	65
CHAPTER 5 DISCUSSION	66
5.1 Comparison of the Effect of Aggregate Volume Fraction and Randomly Attached Mortar on the Mechanical Properties of Recycled Aggregate Concrete	66
5.2 Comparison between the Simulated Uniaxial Compression Strength Tests with Experimental Results from Literature	67
5.3 Comparison between the Simulated Uniaxial Tension Test with Experimental Results	70
5.4 Comparison between the Randomly Attached Mortar and Fully Enclosed Mortar of Simulated Specimens	72
5.5 Combination of Natural and Recycled Aggregate Concrete	73
5.6 Comparison of the Efficiency of pyMesoscale with Existing Approaches	75
CHAPTER 6 CONCLUSION AND RECOMMENDATIONS.....	77
6.1 Conclusions	77
6.2 Recommendations	79
REFERENCES.....	80
PUBLICATIONS	96
VITAE	97

LIST OF TABLES

Table 1: Characteristics of the mortar. [22]	5
Table 2: Adjusted quadrant angle $\delta i'$	32
Table 3: Calculation time (s) for concrete with polyhedral aggregate produced by various algorithms [40].	34
Table 4: Comparison of various mesoscale model generation techniques.	39
Table 5: Mechanical properties of RAC Mesoscopic phases [20].	46
Table 6. Conducted Simulation Program.....	52
Table 7: Compressive strength of concrete at various replacement rates of recycled aggregate [145]	74
Table 8: Comparison of computation time vs aggregate volume fraction of pyMesoscale with popular mesoscale generation methods from literature [112]	75

LIST OF FIGURES

Figure 1 Recycled concrete aggregates composition [3]	1
Figure 2. (a) Virgin aggregate (b) Recycled concrete aggregate (c) Typical RAC. [11] ...	2
Figure 3. The three different scales used in modeling concrete [6].....	3
Figure 4. Geometric model showing aggregate elements, ITZ elements, mortar elements and symmetrical slide of spherical, ellipsoidal and polyhedral shaped aggregates. [40].....	9
Figure 5. Examples of 2D circular, elliptical and polygonal aggregates [40].	9
Figure 6. Generation of 2D convex polygonal <i>aggregate</i> [14].....	11
Figure 7. Generation of 2D elliptical and polygonal aggregate [57].	11
Figure 8. Utilization of the sine function to make ellipsoidal aggregates to have a non- uniform surface [60].	12
Figure 9. Spherical and Ellipsoidal Aggregates [65].	14
Figure 10. Generation of Polyhedral aggregate (a) Irregular development of octahedral structures in an auxiliary sphere (b) Convex hull of 20 arbitrary points [55].....	15
Figure 11. Generation of a convex polygon aggregate [66].	16
Figure 12. New vertices generation for a convex polygon [67].	17
Figure 13 Polytopes shapes with varying numbers of random points [68].....	18
Figure 14. Illustration of the cell fracture algorithm and use of the algorithm in generating rough surface polygonal aggregates [70].....	19
Figure 15. non-smooth planar surface modeling [70].....	21
Figure 16. (Top) Creation of aggregates with a crushed stone look, (Bottom) Forming of aggregates with a gravel-like texture [70].	22
Figure 17. Rough and smooth surface texture of crushed stone-like aggregate [70].	23
Figure 18. Diagram showing the virtual sphere's location and intersection verification [68].....	25
Figure 19. (left) Place and Squeeze Method (a) Positioning the aggregates within an enlarged RVE box (b) Compacting the aggregate into a squeezed RVE Box. (right) Accelerating the packing and compression process though the use of the sub-algorithm [83].	27
Figure 20. 3D and 2D initial and target placing domain for RWA [57].....	28
Figure 21. Illustration of rotation and translation of random walking algorithm [57].	29
Figure 22. Computational cost comparison for both IRWA and RWA: (a) Circular (b) Elliptical (c) Polygonal shaped particles . [84].....	30
Figure 23. 2D Schematic Illustration of the resultant force as an effect of the overlap between the particles [80].	31
Figure 24. Real aggregate is fitted in a rectangular manner [95].....	35
Figure 25. The detection conditions for any two rectangles that overlap [95].	36
Figure 26. Packing procedure for aggregate #2 (a) calculating the practical minimum distance, $d_{eff, min}$, reduction of, $d_{eff, min}$, to d_{min} . [10].....	37

Figure 27. (Top left and right) Illustration of the Lattice Element Model, (Bottom left) Illustration of the discrete element model (DEM), (Bottom right) Depiction of the Rigid Body Spring model [11,100].	39
Figure 28. Depiction of the global background mesh. (a) arbitrary placement of aggregate in the local background grid. (b) conventional aggregate and ITZ identification method (c) aggregate element identification (d) ITZ element generation (e) new aggregate addition (f) intrusion detection [112].	42
Figure 29. Material attribute identification. [112].	43
Figure 30. Flowchart of the local background grid method.	43
Figure 31. Interconnectivity of the various programs used with pyMesoscale.	44
Figure 32. Packing of 3D polygonal aggregates within a representative volume element (RVE) using pyMesoscale and visualized with ParaView. from left, attached mortar, ITZ, aggregate, matrix, mesoscale model.	45
Figure 33. Depiction of attached mortar across various research papers confirming the fact that attached mortar isn't always evenly distributed across the surface of the stone fraction.	45
Figure 34. Array of some of the generated recycled concrete aggregates using pyMesoscale.	46
Figure 35. Array of some of the generated recycled concrete aggregates using pyMesoscale [115].	48
Figure 36. (Top) Depiction of Boundary Conditions [117] (Bottom) Coupling Interaction and application of load and displacement boundary condition on the upper and lower surfaces of our mesoscopic model in Abaqus CAE [114].	49
Figure 37. Uniaxial σ - ϵ as utilized within the Concrete Damage Plasticity Model (CDPM) [1]	50
Figure 38. σ - ϵ relationship of various mesoscopic phases at different aggregate packing densities.	54
Figure 39. σ - ϵ and force-displacement relationship of UCST for various aggregate packing density.	55
Figure 40. Compressive damage evolution across the RAC specimen, attached mortar, and ITZ at an increasing rate of 4 steps.	57
Figure 41. Compressive damage evolution across the Matrix, 3D RAC, and Cut section of 3D RAC at an increasing rate of 4 steps.	57
Figure 42. σ - ϵ relationship of various mesoscopic phases at different aggregate packing density.	58
Figure 43. σ - ϵ & force-displacement relationship of UTST for various aggregate packing densities.	58
Figure 44. Tensile damage evolution across the RAC specimen, attached mortar, and ITZ at an increasing rate of 4 steps.	59

Figure 45. Tensile damage evolution across the RAC specimen, attached mortar, and ITZ at an increasing rate of 4 steps.	59
Figure 46. DAMAGEC evolution through our mesoscale model with 60% aggregate volume fraction with randomly attached mortar on RCA varying with a step of four (4).	60
Figure 47. Translations and Rotations at 60% aggregate volume fraction for randomly attached mortar on recycled concrete aggregate varying with a step of four (4)..	60
Figure 48. Compressive (fully enclosed) σ - ϵ relationship of various mesoscopic phases at different aggregate packing density.	62
Figure 49. Compressive & Tensile (Fully Enclosed) σ - ϵ relationship at different aggregate packing density.	62
Figure 50. Tensile σ - ϵ relationship of various mesoscopic phases at different aggregate packing density.	63
Figure 51. Compressive and Tensile σ - ϵ relationship of randomly attached and fully enclosed recycled concrete aggregate at different aggregate packing density.	64
Figure 52. Compressive σ - ϵ relationship of UCST at different natural and recycled concrete aggregate blends.	65
Figure 53. Comparison with compressive σ - ϵ relations of mesoscopic phases compared with Ren et al. [1].	66
Figure 54. Comparison with tensile σ - ϵ relations of mesoscopic phases compared with Ren et al. [1].	67
Figure 55. Comparison of simulated, experimental, fib code compressive tensile σ - ϵ relations of recycled aggregate concrete [18,112,140,141]	68
Figure 56. Less damaged upper and lower portion of cubic recycled aggregate concrete specimen.	69
Figure 57. Angled cracks as demonstrated in simulation and experiments of Zhuo et al. [142].	69
Figure 58. Uniaxial compression strength test failure pattern of simulated cubic sample (below) and that of BS EN 12390-3:2019 [143]	70
Figure 59. Uniaxial tensile strength test as available in fib Model Code [139], Liu et al. [144], Ren et al. [1] and this study simulated cubic concrete specimen.	71
Figure 60. Randomly attached and fully enclosed simulation σ - ϵ relationship in compression and tension.	72
Figure 61. Randomly attached and fully enclosed simulation σ - ϵ relationship in compression and tension.	74
Figure 62. Computation time (s) vs Aggregate volume fraction (%) of pyMesoscale with different mesoscale generation techniques [112].	76

LIST OF ABBREVIATIONS

RAC: Recycled Aggregate Concrete

RCA: Recycled Concrete Aggregate

ITZ: Interfacial Transition Zone

NAC: Natural Aggregate Concrete

UCT: Uniaxial Compression Test

UTT: Uniaxial Tensile Test

AVF: Aggregate Volume Fraction

CDPM: Concrete Damage Plasticity Model

|

ABSTRACT

Full Name : Faisal Lawan Muhammad
Thesis Title : Analysis of the Mechanical Behavior of Recycled Aggregate Concrete Using 3D Mesoscale Modeling
Major Field : Civil Engineering
Date of Degree : December 2024

Mesoscale modeling is a part of multiscale modeling used to understand the fracture behavior and mechanics of concrete and its composites. The mesoscale level consists of the mortar, aggregates, and the interfacial transition zone, which provides the most insights into the mechanical behavior of fracture for concrete. Although several studies have been conducted on the mesoscale modeling of concrete, little attention has been given to the mesoscale modeling of concrete incorporating recycled concrete aggregate (RCA) as a partial replacement of virgin aggregates. This study implemented the local background grid method to create pyMesoscale, a python library that can generate polygonal aggregate for concrete mesoscale models of high aggregate volume fraction ($> 70\%$). With finite element meshing included in the model generation workflow, pyMesoscale is 5800% faster than the traditional random addition method. The mechanical properties of concrete with varying aggregate volume fractions and random and fully enclosed attached mortar (AM) were studied and compared to previous experimental results reported in the literature. The random AM approach was found to be more accurate than the approximation of fully enclosed attached mortar on RCA. The compressive behavior of concrete was more affected by the variations in packing density and attachment pattern of AM, where the model with a 40% aggregate volume fraction displayed the highest compressive strength. The tensile behavior of concrete was less affected by these variations. The study also investigated 30%, 50%, and 100% replacement of natural aggregates with randomly attached RCA. The concrete's mechanical property was observed to degrade with increasing recycled aggregates proportion, agreeing with existing literature.

ملخص الرسالة

الاسم الكامل: فيصل لاوان محمد

عنوان الرسالة: تحليل السلوك الميكانيكي للخرسانة المعاد تدويرها باستخدام النمذجة المتوسطة الحجم ثلاثية الأبعاد

التخصص: الهندسة المدنية

تاريخ الدرجة العلمية: ديسمبر 2024

النمذجة المتوسطة الحجم هي جزء من النمذجة متعددة المقاييس التي تستخدم لفهم سلوك الكسر وميكانيكا (ITZ)، الخرسانة ومركباتها. يتكون مستوى المتوسط الحجم من الملاط والركام ومنطقة انتقال الواجهة والتي توفر أكبر قدر من الرؤى حول السلوك الميكانيكي للكسر للخرسانة. على الرغم من إجراء العديد من الدراسات البحثية على النمذجة المتوسطة الحجم للخرسانة، إلا أنه لم يتم إيلاء سوى القليل من الاهتمام للنمذجة المتوسطة الحجم للخرسانة المجمعة المعاد تدويرها. لقد طبقنا في هذه الدراسة طريقة الشبكة وهي مكتبة بايثون يمكنها إنشاء نماذج متوسطة الحجم للخرسانة، pyMesoscale، الخلفية المحلية لإنشاء المعاد تدويرها متعددة الأضلاع ذات نسبة حجم عالية للركام ($< 70\%$). مع تضمين شبكة العناصر المحدودة في سير عمل إنشاء النموذج، في أوقات أقل من أربع دقائق (4) والتي كانت أسرع بنسبة من طريقة الإضافة العشوائية التقليدية مع تضمين الشبكة. تمت دراسة الخصائص الميكانيكية 5800% ومقارنتها (AM) لزيادة كسر حجم الكتل المتغيرة مع ملاط مرفق مغلق عشوائي ومحاط بالكامل بالتجارب السابقة والنتائج التجريبية الواردة في الأدبيات. حيث وجد أن نهج الملاط المرفق العشوائي أكثر تأثير السلوك الانضغاطي للخرسانة. RAC دقة مقارنة بتقريب ملاط مرفق مغلق محاط بالكامل على حيث أظهر كسر حجم الكتل بنسبة AM بشكل أكبر بالاختلافات في كثافة التعبئة ونمط أسلوب التعلق لـ أعلى قوة ضغط. تأثير السلوك الشد للخرسانة بشكل أقل بهذه الاختلافات. لقد اختبرنا في الدراسة 40% المرفقة عشوائيًا حيث لوحظ انخفاض الخاصية RCA استبدال 30% و 50% و 100% من الكتل الطبيعية بـ الميكانيكية مع زيادة نسبة الكتل المعاد تدويرها، وهو ما يتفق مع الأدبيات الموجودة |

CHAPTER 1

INTRODUCTION

Sustainable growth in the current era necessitates excellent waste management and waste recovery. Prior to deploying waste recovery processes, garbage must be segregated [1]. Due to rapid urbanization, expanding economic activities, and the expansion of industries, in addition to the creation of waste from building and dismantling activities—commonly known as construction and demolition waste (CDW)—has significantly increased, presenting a mounting issue for developing countries worldwide [2]. Aggregates produced from remnants of CDW are typically referred to as repurposed/recycled/reclaimed concrete aggregate (RCA) or crushed concrete aggregate (CCA) usually containing little amounts of debris making them suitable for reuse. Figure 1 displays the makeup of RCA specified by the European Standard EN 933-11. As shown in Figure 1, more than 90% of the total is composed of components that may be utilized to make concrete, such as aggregates, mortar, and particles combined with binding material. These aggregates enable the reuse of resources that would otherwise be discarded, which is crucial for the manufacture of sustainable concrete [3].

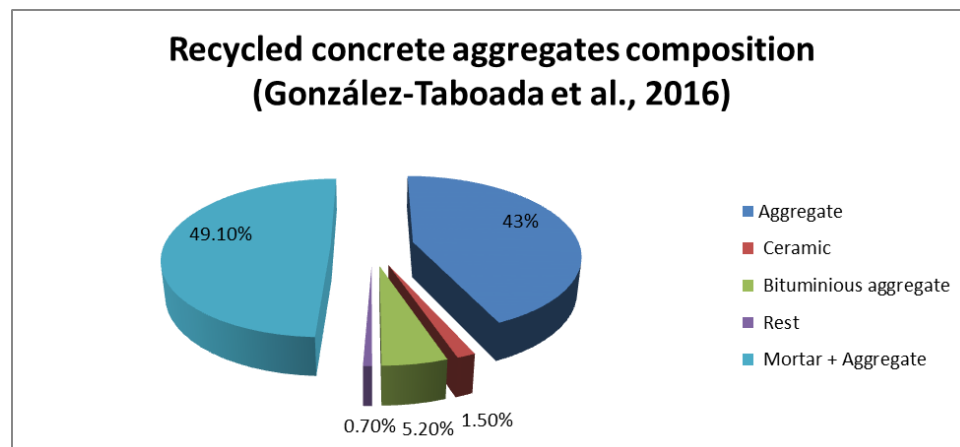


Figure 1 Recycled concrete aggregates composition [3]

Construction demolition waste removes the environmental risk associated with its disposal while also reducing project costs and conserving natural resources [4]. Given the worldwide depletion of natural resources and the increasing creation of debris from demolition, reclaimed concrete aggregate (RCA), derived from processing concrete debris from dismantled buildings—offers a potential alternative to natural aggregates. Its use can alleviate aggregate supply shortages while significantly reducing the volume of construction waste sent to landfills. [5]. Because RCA can be classified as fine or coarse, RCA and natural (virgin) aggregates (NA) are comparable, as illustrated in Figure 2. The structural and material characteristics of RCA and their influence on the behavior of RCA concrete or recycled aggregate concrete (RAC) under both its fresh and solidified forms have been extensively researched. As a result of increased porosity, reduced specific gravity, and lower bulk density of the attached mortar, RAC exhibits lower resistance to compression, impact, and wear resistance compared to natural aggregates. These properties are interrelated, with factors such as the amount of attached mortar, its density, and the original aggregate density affecting the overall RAC density. As the ratio of RCA in the volume of the concrete mixture rises, the RAC's mechanical properties generally decline, with the most significant strength reduction occurring at later ages [6]. The presence of porous cement mortar on the exterior and the increased water uptake of RCA contribute to a decline in the durability of RCA concrete as the proportion of RCA rises [7,8].



Figure 2. (a) Virgin aggregate (b) Recycled concrete aggregate (c) Typical RAC. [9]

The structural performance of concrete, including damage initiation, fracture characteristics, crack propagation, strain development, stress-path, stress-strain relationships, and other mechanical properties, can be analyzed at three distinct scales. On the macroscopic scale, concrete is considered as a homogenous material. On the mesoscale,

it is regarded as a multiphase structure made of the binder, larger particles, along with the interfacial transition zone (ITZ). On the microscale, the material is further detailed to include components like fine aggregates and binder the system, as depicted in Figure 3 [10–12]. The microscale level, although deep enough, is not often utilized as the meshing at the micropore levels is a computationally expensive endeavor [8]. With the apparent time and cost benefits offered working with the mesoscale [9], measuring crack initiation and fracture behavior across different phases of concrete are challenging in experimental settings due to the material's quasi-brittle nature and inherent nonlinearity, which introduces significant variability in the results [10]. As research in this field expands, mesoscale modeling is being extended to other types of concrete, including recycled RAC [11], asphalt concrete [12–14], fiber-reinforced concrete [15–18], polymer cement concrete [13,14], and concrete subjected to dynamic loads [15]. Research on the performance of concrete to transient loads, such as impact, blast, and penetration, have been widely conducted. These investigations have consistently shown that the dynamic behavior of concrete differs considerably from its static behavior [16,17].

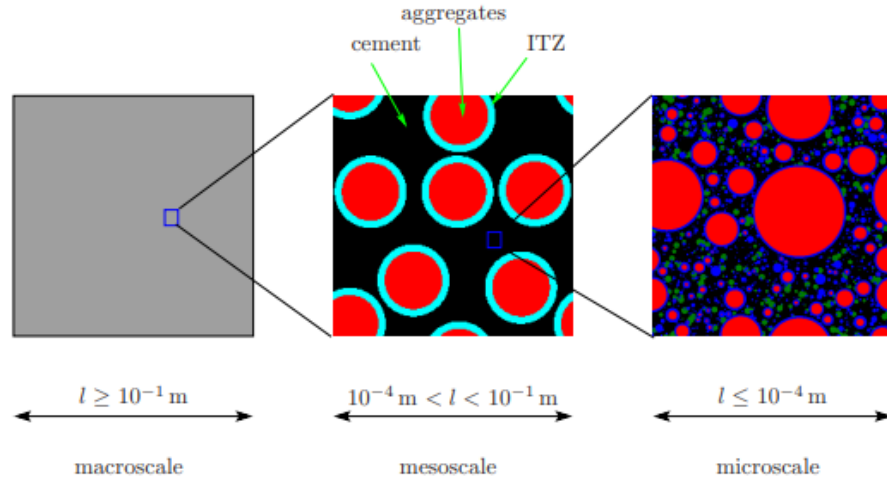


Figure 3. The three different scales used in modeling concrete [6]

There has been limited research on 3D mesoscale modeling of concrete that incorporates RCA, and the few available were published in 2024 [18]. Ren, et al [18] investigated the relationship between two-dimensional and three-dimensional mesoscale simulations with RCA, as well as the impact of adhered mortar on the structural properties and cracking propagation. They found that little to no simulation studies have been conducted on the

splitting tensile strength test (STST) of RAC even though experimental studies typically employ STST to evaluate the concrete's resistance to tension [19]. Limited benchmark data are available for direct comparison for STST and uniaxial tensile strength test (UTST) for RAC [18].

CHAPTER 2

LITERATURE REVIEW

2.1 Mechanical Properties of Recycled Concrete Aggregate

Concrete produced using reclaimed aggregates typically shows reduced mechanical properties than concrete produced with virgin aggregates (NAC) for several reasons. One factor is the weaker adhesion between the repurposed aggregates and the binding material. Moreover, recycled concrete aggregates (RCA) tend to have increased water permeability and uptake compared to lime-based sand, which could contribute to their reduced mechanical strength. Additionally, natural fine aggregates (NFA) possess a narrower interface transition zone (ITZ), which may positively affect the structural characteristics of concrete [20].

Table 1: Characteristics of the mortar. [20]

W/c	Replacement (%)	Flexural Strength (MPa)	Compressive Strength (MPa)
0.5	0	12.14	67.77
	10	13.06	66.63
	20	12.05	64.58
	30	10.861	57.23
	50	10.53	53.84
	100	8.54	42.09
0.65	0	10.63	55.98
	10	10.55	51.17
	20	10.21	49.32
	30	10	47.37
	50	9.16	46.92
	100	8	39.14

Except for a 25% replacement rate, Medina et al. [21] discovered that the fracture tensile strength dropped as the proportion of NA replaced with RCA. They added that it agreed

with earlier research findings from other scientists, concluding that RCA was appropriate for use in building homes.

2.2 Modeling Methods for Recycled Concrete Aggregate

Some of the methods that have been implemented in modeling concrete produced using recycled aggregates (RAC) involved the use of non-linear regression (NLR), model trees (MT), and Artificial Neural networks (ANN). Yu. Y et al. [22] conducted a similar study where ANN better predicted the 28-day compressive strength of concrete incorporating recycled aggregates than NLR and MT. Although these modeling methods can predict compressive strength or tensile strength, they have multiple drawbacks. Firstly, such methods are black boxes where the causality at which a prediction arrives at a particular value cannot be inferred or attributed. Secondly, these models require data collected from previous lab experiments, which are likely to be prone to experimental errors and will require more data to arrive at close to accurate results. Another major disadvantage of such methods is that they do not provide a visual depiction of cracking initiation and propagation and do not provide flexibility in specifying various material properties for novel material discovery.

2.3 Mesoscale Geometrical Models.

Internally, concrete is heterogenous which grants the mesoscopic level a unique way of examining the structural response and behavior of concrete such as beginning of microcracks as well as their coalescence to form major cracks [10]. Hence, mesoscopic models were developed to analyze the connection between the change in the model and the structural reaction to better predict its behavior and to minimize the cost and duration involved in conducting laboratory experiments [23]. The interface transition zone (ITZ) is considered the boundary linking the aggregate to the binding material, typically measuring between 10 and 50 μm , which is often too small to model realistically. This makes generating mesoscopic models computationally demanding. As a result, an ITZ thickness ranging within 0.1 to 0.4 mm (approximately 0.02 inches) is commonly adopted in modeling [10,24,25]. The small-sized aggregates of smaller than approximately 4.00 mm are usually considered to be part of the mortar, and their inclusion will require finer meshes for numerical studies leading to increased computational demand without causing a

significant change in the final mechanical response to be obtained [26]. However, aggregates that model fine aggregates tend to be more accurate modeling the development and propagation of cracks as micro-cracks are known to take place at the ITZ of fine aggregates [27,28].

The major steps involve in mesoscale modeling are the generation of aggregate shape, placement and packing of the aggregates, meshing and carrying out numerical simulations using common computational techniques like discrete element method [29,30], finite element method [27,31], lattice model [32,33]. Mesoscale modeling is not only used in observing the structural performance of concrete, even though this is the most mature usage of this method as observed from the available literature, but other applications also such as to study the chloride diffusion through concrete.

Mesoscale modeling is classified into two distinct types, the first of which is known as Continuum mesoscale modeling in which continuum finite element method for used for the numerical analysis and the second is known as Discrete mesoscale modeling where we use distinct elements such as trusses, grid-like beams and spherical shapes to represent the mesostructure model of concrete. This paper is on continuum mesoscale modeling.

The generation of these mesoscale simulation models have generally taken two forms such as the algorithmic approach and the use of Computed tomography (CT) scanners where the model is constructed using image processing techniques on the obtained volume image [14,34–37]. Various algorithms have been developed and utilized in generating and packing a set of aggregates within a limited volume where the larger the fraction of aggregates needed to be packed the higher the computation requirements to achieve it [14]. Some of these algorithms are the mesh – placement – identification – assignment (MPIA) [38], take and place method [39–42], take and place plus rotation [14], Delaunay Triangulation [43], Voronoi polygons [44], random fractal method (RFM) [45], random walking algorithm[46], convex extension method [47], Monte Carlo arbitrary sampling principle [48,49], aggregate random packing method [50,51], phase field method[52], random sequential addition (RSA) [53] Correlative Element Method (CEM) [54].

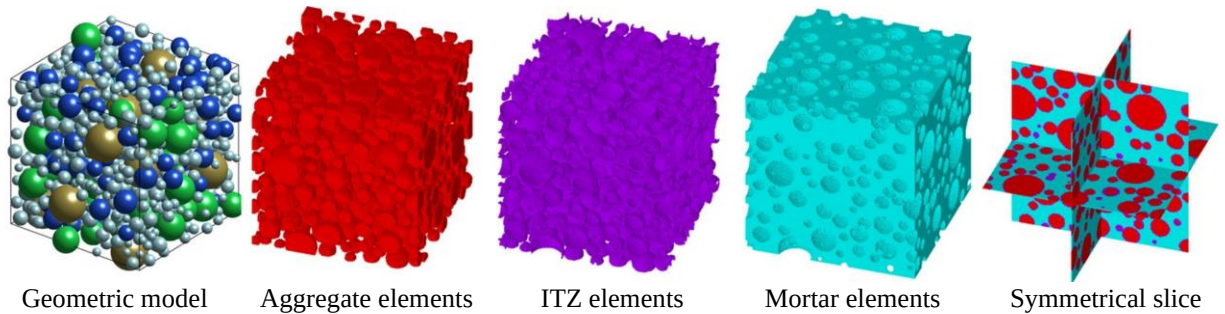
2.4 Aggregate Size Distribution.

The size distribution, or grading, of aggregates plays an tacit factor in establishing the quality of concrete. It impacts the packing density, which directly influences the material's properties. Typically, grading is expressed as the complete percent of particles that pass through a sequence of sieves with different sized openings [55]. One of the most widely used curves is the fuller curve developed by Fuller and Thompson with an equation.

$$P(d) = 100 \left(\frac{d}{d_{max}} \right)^n \quad (1.1)$$

Where P represents the total probability that an aggregate passes through a mesh opening of size d , d_{max} is the upper limit size of aggregate, and the exponent n is the distribution modulus, usually taken in the range of 0.3 to 0.5.

Various shapes, including spherical, ellipsoidal, and polyhedral, have been utilized to model aggregates in three-dimensional (3D) mesoscale simulations, as shown in Figure 4. In 2D models, aggregates are typically represented by polygons, ellipses, or circles, as illustrated in Figure 5. Spheres and ellipsoids are particularly suitable for modeling smooth-surfaced pea-gravel aggregates [11]. Real aggregates are angular in shape making it possible for local stress concentration to occur, eventually leading to the initiation of cracks [56]. Hence, representing natural aggregates particles with polyhedral can realistically reproduce the same behavior [57].



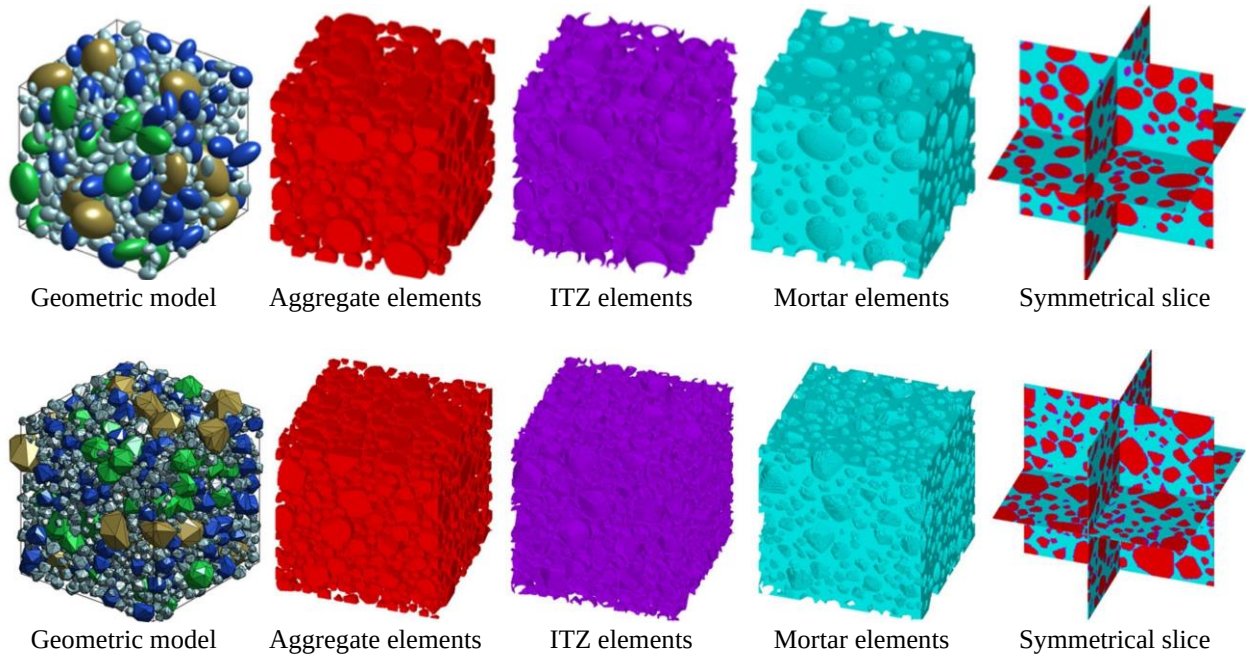


Figure 4. Geometric model showing aggregate elements, ITZ elements, mortar elements, and symmetrical slice of spherical, ellipsoidal, and polyhedral aggregates. [38]

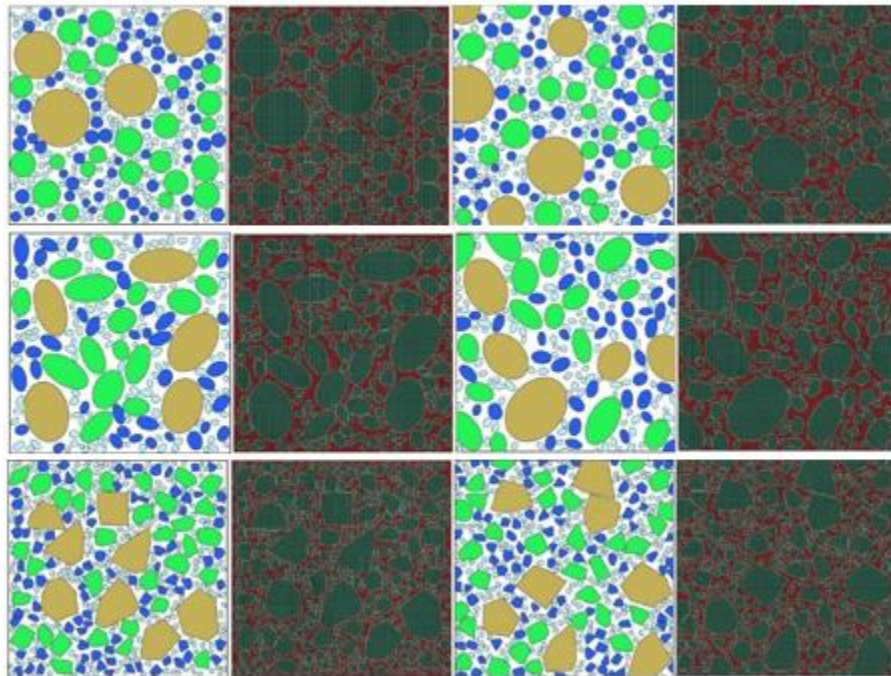


Figure 5. Examples of 2D circular, elliptical, and polygonal aggregates [38].

2.5 Generation of Various Aggregate Shapes in 2D

One of the first steps in generating mesoscale models is the generation of aggregate particles. In 2D, aggregate shapes are usually assumed to be either elliptical, circular, or polygonal. The choice of which to use often depends on the selected mesoscale model parametric algorithm and expected computational efficiency [10]. The generation of such aggregate shapes is quite straightforward. The next subsections offer a breakdown of the procedures.

2.5.1 Irregular Polygons

Generating an irregular polygon can be accomplished in two main steps:

1. Generate a regional reference frame featuring an origin and establish the first angle of rotation θ of the initial corner P_1 , given by

$$\theta = \frac{\eta}{n} 2\pi$$

where η represents a random value between 0 and 1, and n represents the number of sides of aggregate.

For all other i th corner, define the angular position φ_i and radial distance r_i for $i = 2, 3, \dots, n$.

$$\varphi_i = \frac{\left(\frac{2\pi}{n} + 2\pi\eta_i\right)}{\sum_i^n \left(\frac{2}{n} + \eta_i\right)}$$

$$r_i = \frac{d_{kL} + d_{kU}}{4} + (2\eta_i - 1) \left(\frac{d_{kU} - d_{kL}}{4}\right)$$

2. Connect the corner points to obtain a polygon with n edges, as depicted in Figure 6.

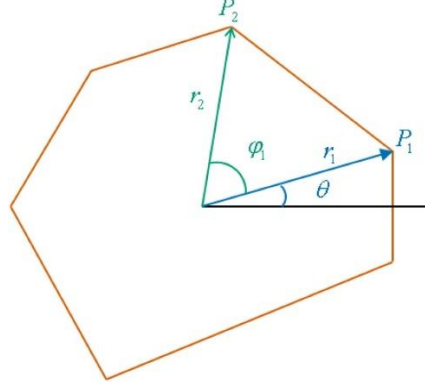


Figure 6. Generation of 2D convex polygonal aggregate [14].

2.5.2 Circular and Elliptical Aggregates

In 2D models, a circular aggregate is the most straightforward representation, created simply by specifying its diameter. For an elliptical aggregate, the longer axis (a) and shorter axis (b) must be defined, as shown in Equation 2 and depicted in Figure 7 [55]:

$$a = 1, \quad b = 0.3 + 0.5\eta_2 \quad (2.1)$$

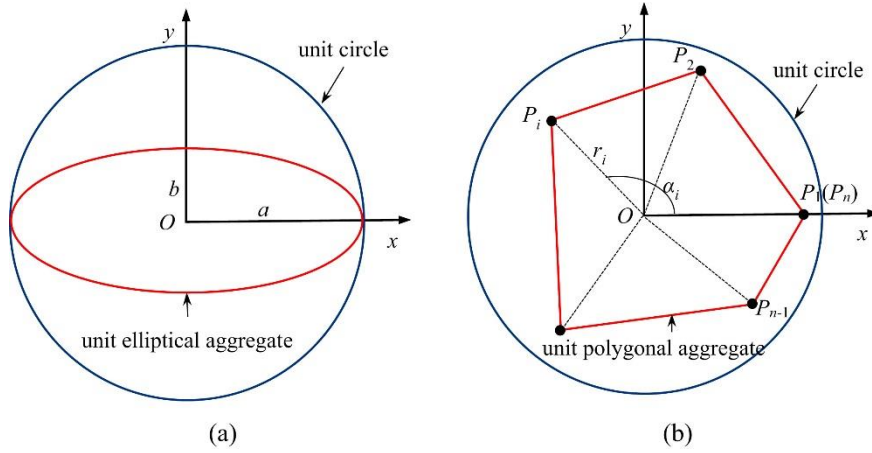


Figure 7. Generation of 2D elliptical and polygonal aggregate [55].

2.6 Generation of Various Aggregate Shapes in 3D

The distribution of local stress at the mesoscopic level is influenced by the nature of aggregates. The shape of the aggregate particles is crucial in determining how local stresses are distributed, which in turn impacts the commencement and progression of cracks [58]. In 3D mesoscale models, spherical, ellipsoidal, and polyhedral shapes are used while circles, ellipses, and polygons are used in 2D mesoscale models [46]. Spherical and ellipsoidal shapes offer low generation costs in terms of computational resources [49,59,60]. Spherical aggregates are created by specifying the particles' central positions and their radii, whereas ellipsoidal particles require nine parameters: three for the central points, three for the Eulerian angles, and three for the principal axes of the ellipsoid. [11] To solve this problem, Hafner et al. [58] gave a solution that involves using a sine function so that the final aggregate surface will not be smooth but rather full of non-uniform undulations, as illustrated in Figure 8. Qian [61] suggested the use of spherical harmonic functions to create non-uniformly shaped clusters. To precisely depict the mechanical behavior of aggregates, it is essential to select a shape that closely mimics the flaky, rough, and elongated surfaces of natural aggregates, as these characteristics play crucial roles in crack initiation, propagation, and local stress concentrations [39]. These made the polyhedral-shaped aggregates the desired mesoscale aggregate shape as they can realistically demonstrate this behavior [57].

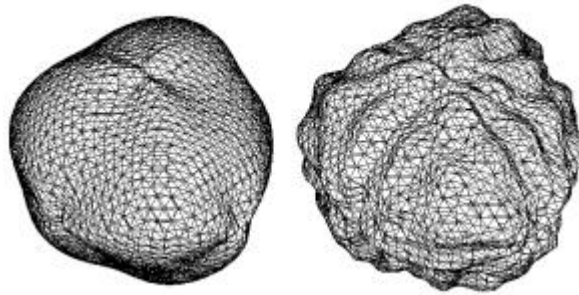


Figure 8. Utilization of the sine function to create ellipsoidal aggregates with non-uniform surface [58].

2.6.1 Spherical aggregate

The two variables that influence the shape and position of spherically shaped aggregates are the center coordinates $O(x_o, y_o, z_o)$ and radius r ranging in particle size from d_i to d_{i+1} , given by $r = \frac{d_i}{2} + \eta \times \frac{(d_{i+1}-d_i)}{2}$, where η is an arbitrary variable between $[0,1]$. To calculate the separation from a location $p_i(x_{pi}, y_{pi})$ and the center $O(x_o, y_o)$ to determine if that point is within the boundaries of the spherical aggregates, we use the equation $d_{pi} = \sqrt{((x_o - x_{pi})^2 + (y_o - y_{pi})^2 + (z_o - z_{pi})^2)}$. When $d_{pi} > r$, we consider the point to be outside the 3D sphere and when $d_{pi} < r$, we consider it to be inside the aggregate [38].

2.6.2 Ellipsoidal aggregate

The position and form of ellipsoidal aggregates are determined by the coordinates of their centroid $O(x_o, y_o, z_o)$, sa-major axis a , half-mean axis b half-minor axis c , rotation angles α , β and γ around the x , y and z axes, sequentially [11,38]. An ellipsoidal aggregate can fit through the opening of a sieve if its mean axis is less than the opening [62]. The three middle axes of an ellipsoidal aggregate can be calculated as:

$$b = \frac{d_i}{2} + \phi \times \frac{(d_{i+1} - d_i)}{2} \quad (3.1)$$

$$c = a \times [l_2 + \zeta \times (m_2 - l_2)] \quad (3.2)$$

Where, ϕ , η , and ζ are random variables in the interval $[0,1]$, m_2 and l_2 are taken as the maximum and the lowest values of the ratio calculated between the minor and major axis of the ellipsoid. While that of m_1 and l_1 represents the maximum and the minimum value between the average axis and the principal axis of the ellipsoid [38]. The three Eulerian angles α , β and γ are in the range $[0,360^\circ]$. A 3D depiction of both spherical and elliptical clusters is provided in Figure 9.

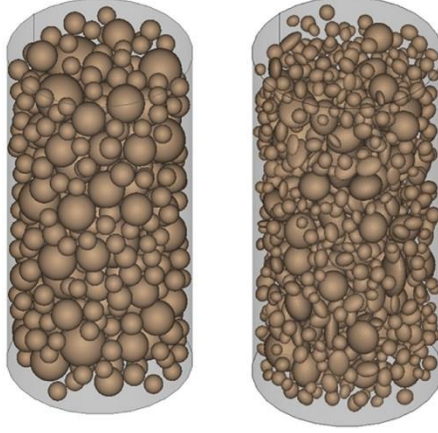


Figure 9. Spherical and Ellipsoidal Aggregates [63].

2.6.3 Polyhedral aggregate

Here we demonstrate how to generate random polyhedral aggregates using two methods. The first is the random growth algorithm. Firstly, we generate an octahedron aggregate with a base in an auxiliary sphere, afterwards, we extend the base from its longest edge. The center of the auxiliary sphere has an origin of O and the radius r is taken as $\frac{d}{2}$. We establish six vertices of the octahedron on the auxiliary sphere with a notation $A_i (i = 1, 2, \dots, 6)$. We can calculate the cartesian value of the six vertices using the angle of inclination θ and the azimuthal angle that is based on the spherical coordinates $x_i = r \sin \theta_i \cos \varphi_i$, $y_i = r \sin \theta_i \sin \varphi_i$, $z_i = r \cos \theta_i$. Controlling the form of the octahedral cluster and avoiding acute angles are crucial. This is done by adjusting the azimuth angle (φ) and the tilt angle (θ) of the six corners. The initial four corners are positioned along the horizontal circle of the supporting sphere, while the other two are positioned on the top and bottom hemispheres in sequence, as indicated in Equation 4.1 [53].

$$\varphi_i = \frac{(i-1)\pi}{2} + \frac{\eta_i \pi}{2} \quad (i = 1, 2, 3, 4) \quad (4.1)$$

$$\varphi_{i+1} - \varphi_i \geq \frac{\pi}{4} \quad 2\pi + \varphi_i - \varphi_4 \geq (i = 1, 2, 3) \quad (4.2)$$

Another approach to generating a polyhedral aggregate involves using Delaunay triangulation with the convex hull algorithm. By employing a set of random points in three

dimensions, a polyhedron can be created, with the vertex coordinates and associated topological relationships determined by the equation provided Equation 5.

$$r_i = \frac{d_k}{2} + \left(\frac{d_{k+1}}{2} - \frac{d_k}{2} \right) \eta_i \quad (5.1)$$

$$\theta_i = 2\pi\eta_i \quad (5.2)$$

$$z_i = 2\pi\eta_i \quad (5.3)$$

$$\theta_i = \frac{\pi}{2} \quad (i = 1,2,3,4) \quad (5.4)$$

$$\varphi_i = 2\pi\eta_i \quad (i = 5,6) \quad (5.5)$$

$$\theta_5 = \frac{\chi_5\pi}{4} \quad (5.6)$$

$$\theta_6 = \frac{3\pi}{4} + \frac{\chi_6\pi}{4} \quad (5.7)$$

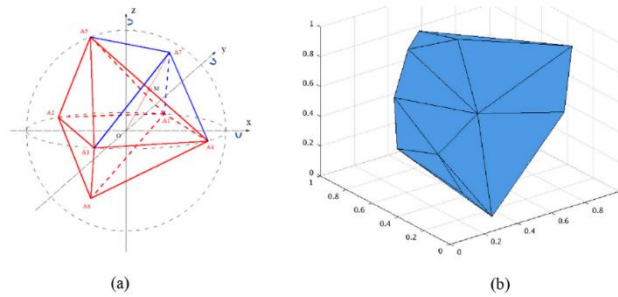


Figure 10. Generation of Polyhedral aggregate (a) Irregular development of octahedral structures in an auxiliary sphere (b) Convex hull of 20 arbitrary points [53].

2.6.4 Polygon-based framework

This process entails creating particles using a framework of randomly shaped polygons, which are then split into triangles, quadrilaterals, and pentagons dependent on the cluster size classification on the initial edge of the circular coarse aggregates as which is depicted in Figure 11. The following formula governs the polygon-based framework's neighboring vertices [64].

$$L_{min} = 2 R \cdot \sin\left(\frac{\pi}{2(n-1)}\right) \quad (6.1)$$

Where L_{min} is the smallest amount of space between base frame vertices, R is the aggregate's radius, n is the vertex count. The area of the freshly formed convex particle must fit the area of the original aggregate. Figure 11 illustrates the newly formed convex polygon particle.

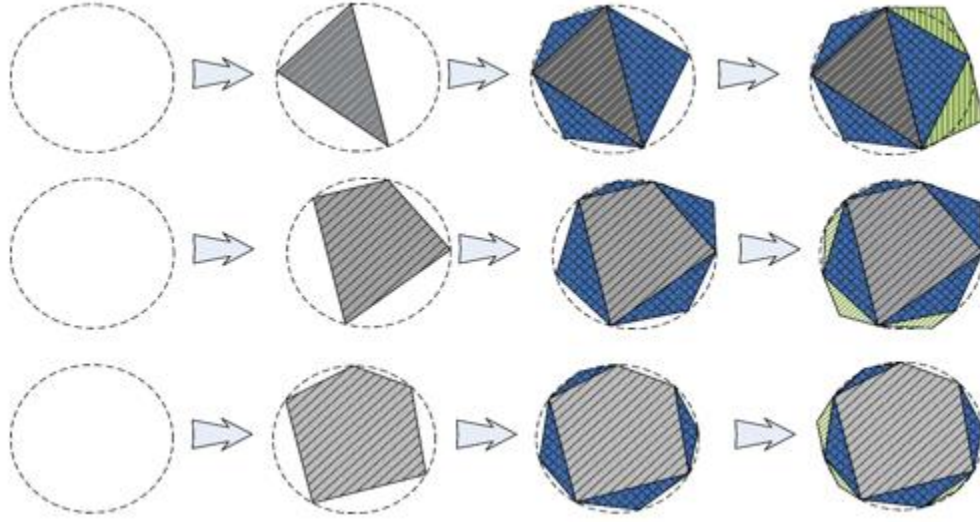


Figure 11. Generation of a convex polygon aggregate [64].

Polygon vertices can be denoted as $A_1, A_2, A_3, \dots, A_i, A_{i+1}, \dots, A_n$; respectively, the positions of the corners are represented as

$(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_i, y_i), (x_{i+1}, y_{i+1}), \dots, (x_n, y_n)$. We insert a new vertex on the outer semicircle in order for the diameter to be on the extended side of the polygon. To enhance the creation process speed, we first compute the angle β and the slope of the longer side as in Figure 12. We determine the location of the new point using Equation 7[65].

$$x_p = \frac{1}{2}(x_i + x_{i+1}) + \frac{1}{2} \sqrt{A_i + A_{i+1}} R_1 \cos(2\pi R_2), \quad (7.1)$$

$$y_p = \frac{1}{2}(y_i + y_{i+1}) + \frac{1}{2} \sqrt{A_i + A_{i+1}} R_1 \cos(2\pi R_2), \quad (7.2)$$

Where R_1 and R_2 are arbitrary numbers between 0 and 1. Therefore, the insertion point P cannot exceed the specimen domain. y_p ranges between 0 and h while x_p ranges between 0 and b which are the respective the specimen's breadth and length.

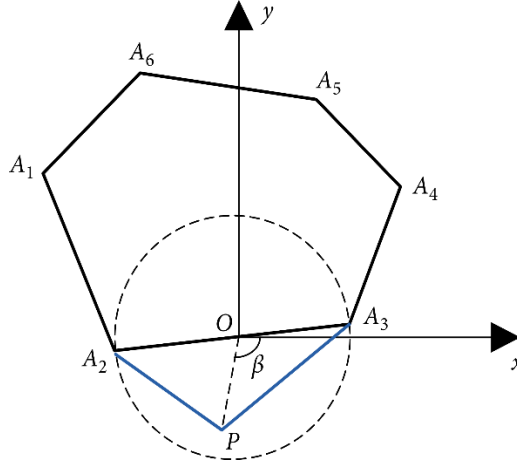


Figure 12. New vertices generation for a convex polygon [65].

The final size the size of the formed polygon must exceed the minimum S_{min} which is expressed as.

$$S_{min} = 0.3(S_A - S_B) \quad (8.1)$$

Where S_A and S_B are defined as the surface area of the polygon prior to and following the insertion of the new point.

2.6.5 Crushed aggregates

To create flaky and elongated aggregates, regular polytopes are altered through shrinking and stretching. A flaky shape is achieved by applying a random shrinking factor s ($s < 1$) to one dimension while proportionally expanding the others to preserve the aggregate's nominal volume. A polytope constructed with only 10 random points exhibits distinct edges and sharp angles, as illustrated in Figure 13. However, as the list of random points increases, the polyhedron's shape becomes progressively smoother [66]. The research considers the true overall shapes and ensures balanced processing time by adjusting the number of arbitrary points employed to generate the multi-faced geometric shapes, ranging

from 15 to 25. Subsequently, shrinking and stretching techniques are applied to produce stretched and flat particles.

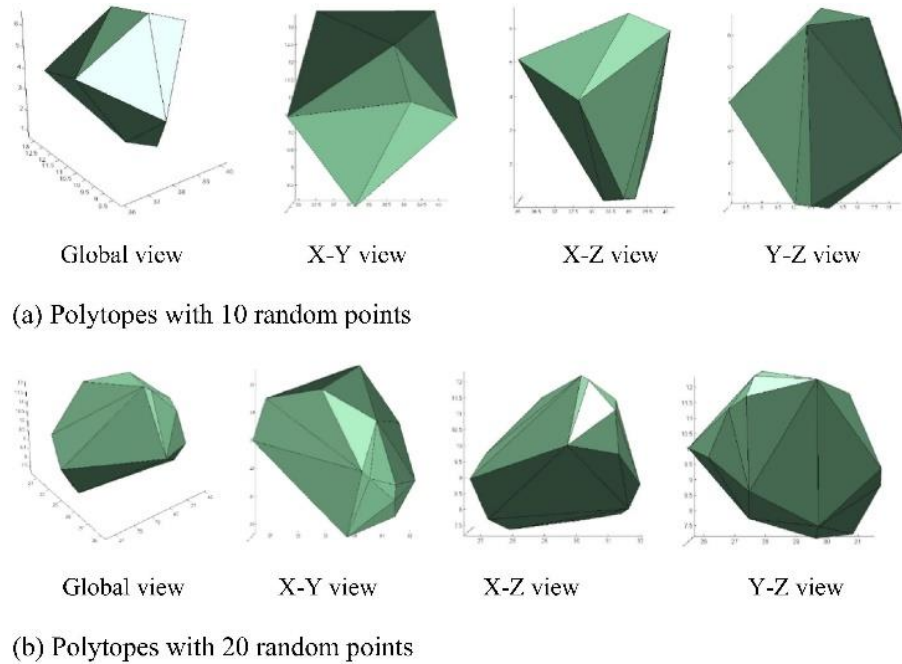


Figure 13 Polytopes shapes with varying numbers of random points [66].

2.7 Aggregates with Rough Surface Texture

Aggregate surfaces are known to have a rough surface texture. The generation of such types of aggregates comprises four primary algorithms: (a) Cell fracture, (b) Surface subdivision (Catmull-Clark subdivision algorithm [67]), (c) Displacement mapping, and (d) Laplace smoothing [68].

2.7.1 Aggregates with rough surface texture

The process begins by generating low-polygon aggregates through the cell fracture technique to replicate realistic aggregates with rough surface textures. This involves first utilizing the scatter method to produce random seed points or Voronoi patterns [69]. Subsequently, the Delaunay triangulation technique divides a territory into discrete triangular areas, separating the Voronoi diagrams [70]. Next, filling surface modeling is applied to fragments. In the final stage, each mesh within the Voronoi diagrams is

designated as a rigid body and allowed to expand during a real-time simulation. This approach, as demonstrated in Figure 14, enables the creation of low-polyhedral aggregates in a range of sizes [68].

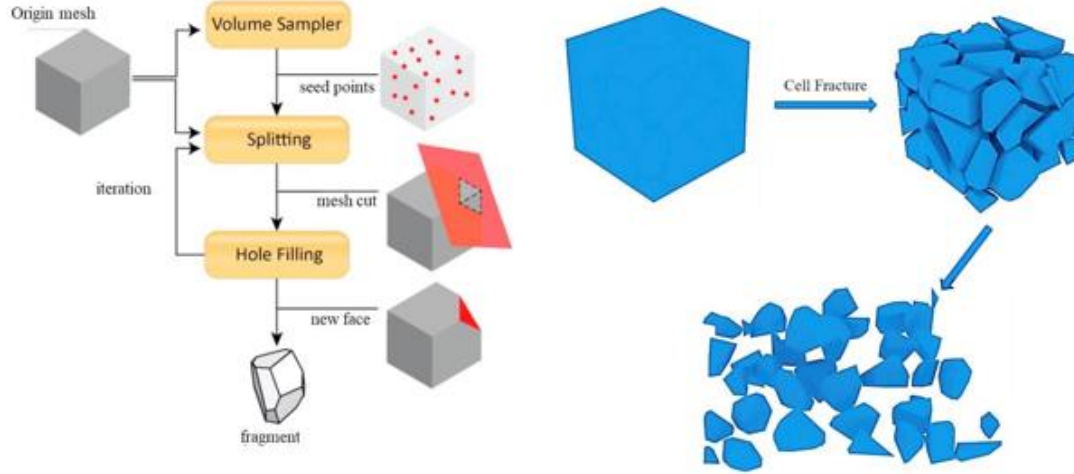


Figure 14. Illustration of the cell fracture algorithm and use of the algorithm in generating rough surface polygonal aggregates [68].

2.7.2 Surface subdivision

We must convert the shape of the convex shaped aggregates generated by the cell fracture algorithm to non-convex shaped by altering the coordinates of the aggregates using the function in Equation 9.1:

$$P'_i(x, y, z) = P_i(x, y, z) + [f_1(w_{ix}) \quad f_2(w_{iy}) \quad f_3(w_{iz})] P_i(x, y, z) \quad (9.1)$$

Where $P'_i(x, y, z)$ and $P_i(x, y, z)$ are the i th initial and altered coordinate of the aggregate, where $f_1 \ f_2 \ f_3$ are the weighing functions which can be defined as constant or random function. We construct the meshes of the aggregate using Delaunay Triangulation. We can further create complex aggregates by incorporating rotation, scaling and movement of the local meshes.

$$P''_i(x, y, z) = C_{rot} D_{move} E_{scale} P'_i(x, y, z) \quad (10.1)$$

Where C_{rot} , D_{move} , and E_{scale} symbolize the corresponding Localized rotation, translation, and resizing matrices respectively. $P''_i(x, y, z)$ shows the coordinates after transformation.

Iterations of the Catmull-Clark subdivision surface algorithm [67] are employed to refine the aggregate mesh. You can express the position of the face and edge as follows:

$$v_f = \sum_{i=1}^n \frac{1}{n} v_i, v_E = \frac{v + u + v_{F1} + v_{F2}}{4} \quad (11.1)$$

v_E , v_F , represents the number of points on edge E and face F . where v and u stand for the edge E 's terminus, and $F1$ and $F2$ for edge E 's neighboring faces. We can generate the new point using:

$$v' = \frac{1}{n} Q + \frac{2}{n} R + \frac{n-3}{n} v \quad (12.1)$$

Here, Q and R are the mean of the face points that are adjacent to point v , and R stands for the mean of the surface points that are next to the midpoint of point v . Another method of obtaining aggregates with a smooth surface is through Catmull-Clark subdivision. A subdivision is referred to as a basic Catmull-Clark subdivision if the subdivision surface is in-plane [68].

2.7.3 Displacement mapping and Laplace smoothing

Aggregates with a coarse surface texture are obtained by developing a mapping of local weight displacement. The algorithm for displacement mapping is represented by [67].

$$P'(u, v) = P(u, v) + d(u, v) \cdot n(u, v) \quad (13.1)$$

Where $P(u, v)$, $P'(u, v)$ are the inner and updated surface sets, and $n(u, v)$ stands for the surface normal field and $d(u, v)$ represent the displacement. However, when an intricate texture is applied directly, the surface exhibits a Gibbs phenomenon [71]. The displacement mapping algorithm allows for rewriting a localized weight-based displacement mapping in the subsequent way:

$$P'(u, v) = P(u, v) + [w(u, v)] \cdot d(u, v) \cdot n(u, v) \quad (14.1)$$

$[w(u, v)]$ is defined as the local weight vector. Figure 16 illustrates how to create a 2×2 mm plane (Fig. 15(a)) to incorporate rough surfaces and warped random texture (Fig.

15(b)). If the displacement mapping procedure is the only one used, the plane's surface exhibits sharp characteristics (Fig. 15(c) illustrates this; the displacement mapping factor is meant here). A realistic surface texture can be achieved by applying the displacement mapping method, the Catmull-Clark subdivision, and the Laplace smoothing technique. Figure 15(d)–(f) shows that on occasions where the count of iterations- n_{itr} of the Catmull–Clark subdivision equals 3, the plane surface is typically smooth. The hump displacement increases as the Laplace smoothing factor, λ , rises within the range of -0.1 to 0.1 (preventing a distorted mesh) (Fig. 15(d) and 15(e)) [68].

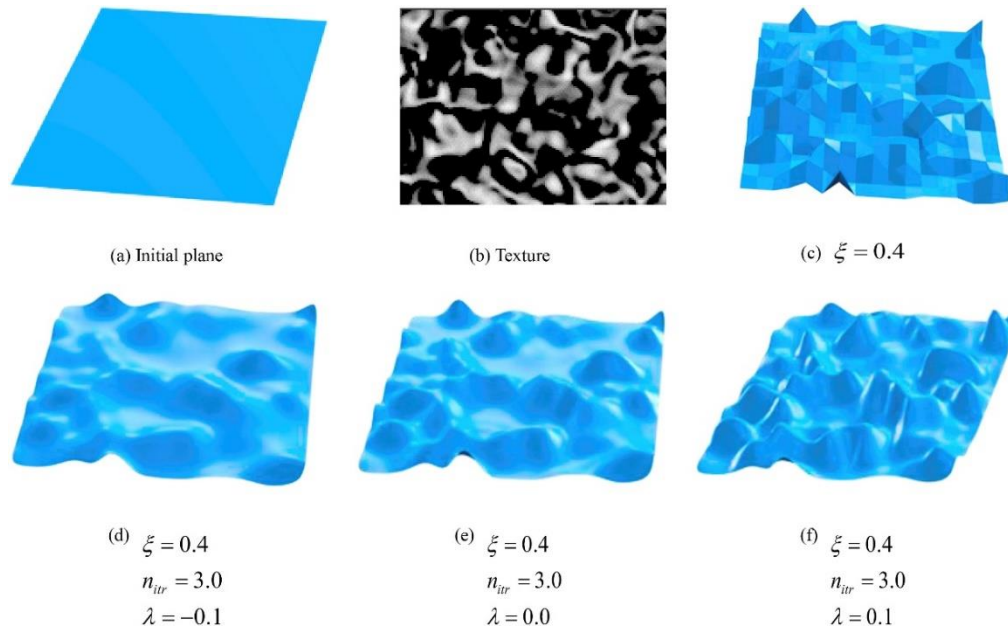


Figure 15. Non-smooth planar surface modeling [68].

Realistic aggregates can be built using the aforementioned techniques. The method of creating gravel- and crushed stone-like aggregate is depicted in Figures 16 (Top) and 16 (Bottom). There are the following four steps in it. Step 1 involved choosing an initial icosahedron with a cloud texture and an edge length of 1 mm. The actual circumstances ought to guide the texture selection. The following were put into practice: displacement mapping ($\xi = 0.2$), Laplace smoothing ($\lambda = 0.2$), and simple Catmull-Clark subdivision ($n_{itr} = 3.0$). As seen in Fig. 17, the aggregate's surface roughness is still unclear. Step 3 employed distorted noise texture to further alter the aggregate surface, bringing it closer to

reality. The accuracy of the created aggregates was then increased by using Laplace smoothing ($\lambda = 0.0$), Simple Catmull-Clark subdivision ($n_{sitr} = 3.0$), and displacement mapping ($\xi = 0.05$). In step 4, the original icosahedron's coordinate was changed at random. It should be noted that whereas gravel-like aggregates are expected to be created by Catmull-Clark subdivision, crushed stone-like aggregate is produced by simple Catmull-Clark subdivision. Figures 17 (Top) and 17 (Bottom) depict the stone-like and crushed gravel aggregates produced by the suggested model.

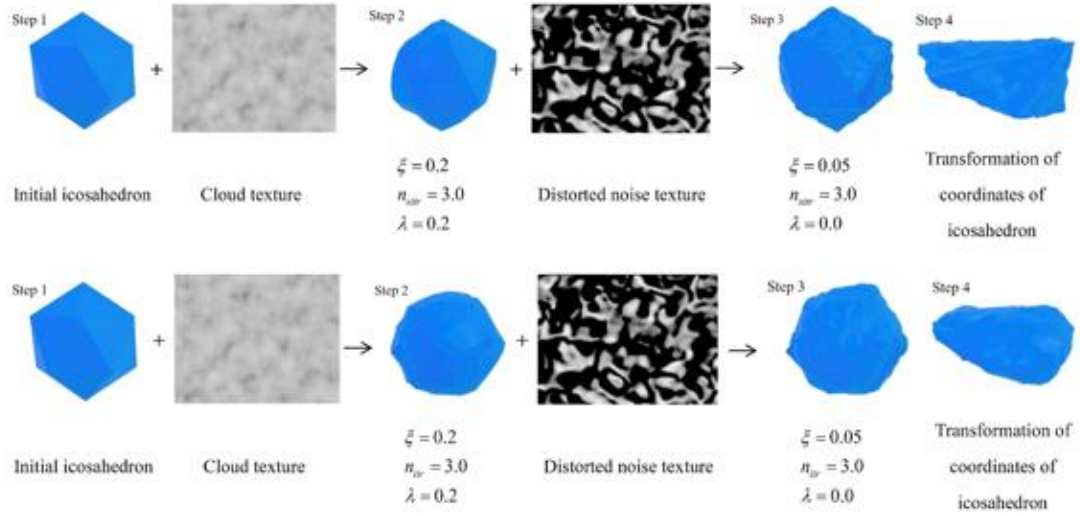


Figure 16. (Top) Creation of aggregates with a crushed stone look, (Bottom) Forming of aggregates with a gravel-like texture [68].

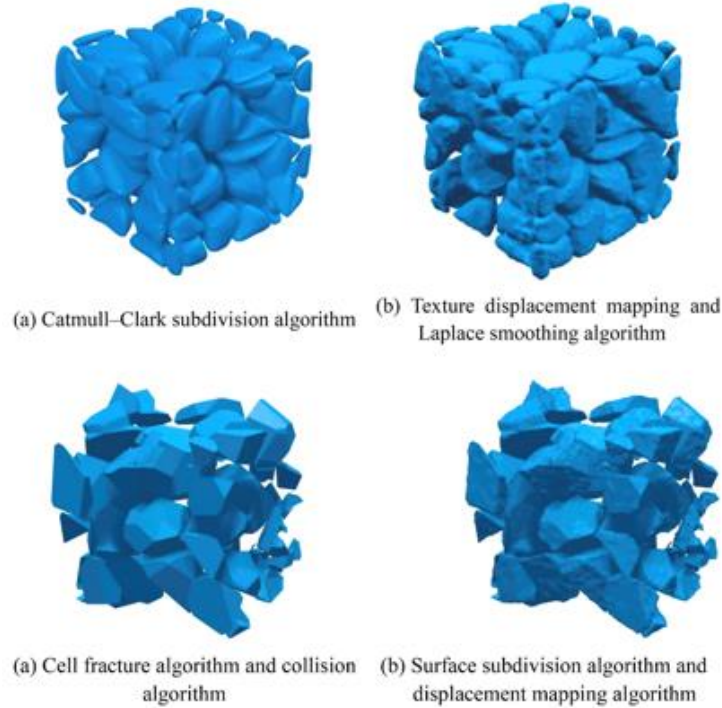


Figure 17. Rough and smooth surface texture of crushed stone-like aggregate [68].

2.8 Various Techniques for the Generation of Mesoscale Model

2.8.1 Take and place method

The take-and-place method is one of the oldest and most utilized generation techniques in mesoscale modeling as shown by its utilization in several research in this domain [12,14,72–75]. A major hurdle of this method is its inability to pack a large volume fraction of polyhedral aggregates with a limit of up to about 30% for polyhedral particles. These lead to the development of several techniques that improve the packing density such as the Creation of additional particles [76] and the introduction of the rotation technique [14]. For polyhedral aggregates, the aggregate shrinking method, which achieves a packing volume of 67%, is recommended [77]. Dongpeng Ma et al [14] utilized the take-and-place method and introduced a rotation procedure to replicate the actions of epoxy polymer concrete exposed to tension or bending forces. They conclude that a 75.6% aggregate volume fraction using the coarse aggregate void filling (CAVF) gradation and 73.9% using the fuller curve could be achieved at a 100% success rate. For spherical aggregates, the take-and-place technique is regarded as one of the most effective approaches for aggregate

packing because of its straightforwardness. The take-and-place technique can achieve reasonable volume fractions with modest computational resources.

As elaborated in the last paragraph, it has been shown that obtaining a high aggregate packing density with the standard take and place method is difficult. One of the major reasons is due to the lack of movement of placed aggregates [78]. An “occupation and removal” process was suggested and used to mark the areas occupied by aggregates using background grids. The algorithm notes that these marked areas are no longer used for the placement of new aggregates, leading to reduced computational cost [47]. Zhou et al. [66] introduced the supplementary aggregate algorithm to fill up the available aggregate areas and increase the aggregate volume fraction. Huang [79] developed a “place-and-squeeze” method, which simulates the settling process of natural soil particles. Similarly, Ma et al [80] introduced a settlement algorithm that replicates the vibration phenomena occurring during concrete placement.

2.8.1.1 Creation of supplementary secondary aggregates

As shown by Zhou et. Al [66], the low volume fraction for the packing of polyhedral aggregates employing the take-and-place technique. Enhancement techniques such as the creation of supplementary aggregates have been proposed and utilized to increase the packing density from the limits of 30-35% to 40-50%. Upon exhaustion of the take-and-place method, qualified neighborhood groups are selected to form the supplementary aggregates. The diameter of the neighborhood which is represented by a sphere should determine the size of the secondary aggregate to be created. The secondary aggregate will need to satisfy some criteria such as the non-overlap with already existing aggregate.

For each group of aggregates forming a neighborhood, the size of the virtual sphere's diameter should equal the upper limit of the size group d_2 and be utilized for the target space for the secondary aggregate. To illustrate this point, $d_2 = 7\text{mm}$ for the 5-7mm group. The process of generation of supplementary secondary aggregates can be divided into two major steps:

1. We randomly select the midpoint of the virtual sphere within the mortar enclosed by the neighborhood of surrounding groups of aggregates, as illustrated in Figure

18. At this point, all mortar components have already been meshed. A check is also carried out to ensure that the selected position causes no intersection with existing aggregates.

Figure 18. Diagram showing the virtual sphere’s location and intersection verification [66].

2.8.2 Place and squeeze method

For a collection of aggregate particles $A = \{a_1, a_2, \dots, a_n\}^T$ in a representative volume of element (RVE) of certain size V , the algorithm for the place-and-squeeze method is elaborated as follows:

1. Select the magnification factor $\lambda_0 = 1$ and the dimensions of the expanded $RVEV_0 = V$.
2. Position the aggregates within the initially selected RVE size V_0 according to the smallest bounding circles.
3. Check if we can position the aggregate in the enlarged RVE.
 - 3.1 . Goto step 4, Once all aggregates are positioned in RVE.
 - 3.2. We raise the magnification factor λ_i for any aggregate that cannot be inserted into the RVE.
 - 3.3. Reset the fresh geometrical dimension of the RVE as $V_i = V \times \lambda_i$.
 - 3.4.Re-confirm if all the aggregates can be inserted in the revised RVE size.
 - 3.5.Goto step 4, if all the aggregates can be inserted in the revised RVE.
 - 3.6.Goto to step 3.2, if any of the aggregate still can't be placed in the updated RVE.
4. Calculate the point between the bounding box and the aggregate and sort the aggregates with respect to their respective location to the bounding box.
5. Re-position the aggregates in correspondence to their location within the bounding box.
 - 5.1. Verify if the re-positioned particles intersect any aggregate.
 - 5.2. Keep re-positioning the particles until they can't be moved or repositioned along the subject's direction.
6. Calculate the squeezed RVE and compare it to the favorable RVE size.
 - 6.1. If the prescribed RVE size is larger than or matching the compressed RVE size, then the compression process is complete.
 - 6.2 Reset the magnification factor and repeat steps 2-6 if the compressed dimension is bigger than the recommended size.

An illustration of the place-and-squeeze method is illustrated in Figure 19.

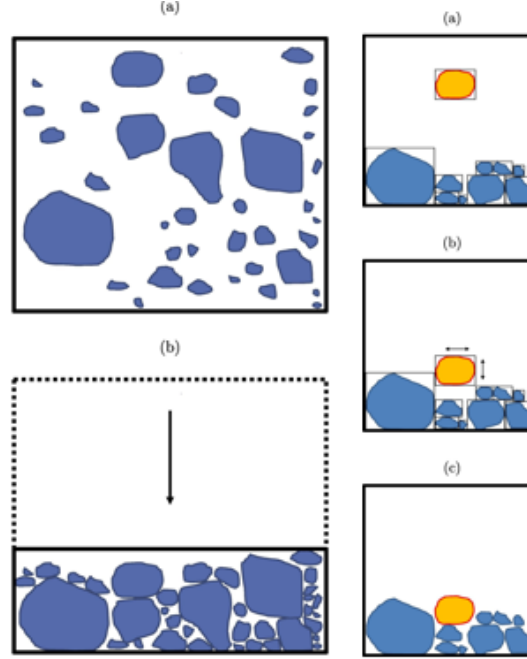


Figure 19. (left) Place and Squeeze Method (a) Positioning the aggregates within an enlarged RVE box (b) Compacting the aggregate into a squeezed RVE Box. (right) Accelerating the packing and compression process through the use of the sub-algorithm [81].

2.8.3 Random walking algorithm

Zhang Z et al [55] put forward the random walking algorithm (RWA) with the aim of improving computational efficiency while achieving a higher aggregate packing fraction. The approach emulated the movement of aggregates by proposing both rotational and translational action to the aggregates making the generated aggregate to be placed in the domain in a more spatially friendly manner. The RWA technique involves two main stages: the first is the initial positioning of aggregates, followed by random walking.

2.8.3.1 Initial placement of aggregates

At first, the aggregate is created in an initial placement area and subsequently relocated to a target placement area (i.e., the concrete block) using the random walking algorithm, as illustrated in Figure 20.

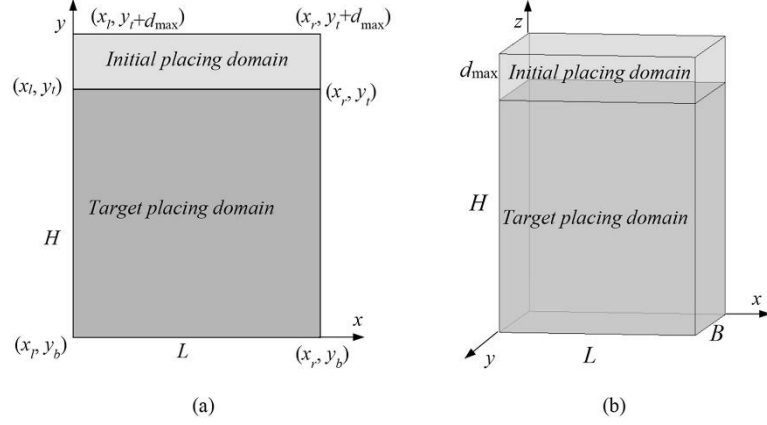


Figure 20. 3D and 2D initial and target placing domain for RWA [55].

A layer of aggregates is created and spread across the initial placement area, ensuring no collisions between them. The points of the central points of the aggregates in both 2D and 3D can be determined as follows:

$$x_i = \left(i - \frac{1}{2}\right) d_{s+1}, y_i = H + \frac{1}{2} d_{max}, (i = 1, \dots, n_x) \quad (15.1)$$

$$x_i = \left(i - \frac{1}{2}\right) d_{s+1}, y_i = \left(j - \frac{1}{2}\right) d_{s+1}, z_i = H + \frac{1}{2} d_{max}, (i = 1, \dots, n_x; j = 1, \dots, n_y)$$

Where n_x and n_y are the number generated aggregates throughout the x and y directions in the same order.

$$n_x = \text{int}\left(\frac{L}{d_{max}}\right), n_y = \text{int}\left(\frac{B}{d_{max}}\right) \quad (16.1)$$

We randomly specify the dimensions of each aggregate particle range, from d_s and d_{s+1} .

$$d = d_s + \eta_6(d_{s+1} - d_s) \quad (17.1)$$

2.8.3.2 Random Walking Algorithm

The movement of the layers of aggregates from the initial placing region to the target placing area simulates the pouring process. At this stage, the generated aggregates are not only restricted to translation but also rotation. With the assumption that aggregates can be repositioned in any direction horizontally but can only translate vertically under gravity

with the coordinates of the aggregate changing after a series of walks as shown in Figure 21.

$$x'_i = x_i + \eta'_1 l, y'_i = y_i - \eta_7 l; \quad (2D) \quad (18.1)$$

$$x'_i = x_i + \eta'_2 l, y'_i = y_i + \eta'_3 l, z_i = z_i - \eta_8 l, \quad (3D) \quad (18.2)$$

Where $\eta'_1, \eta'_2, \eta'_3$ are random numbers between the range of $[-1,1]$ and l is the length of walking [55].

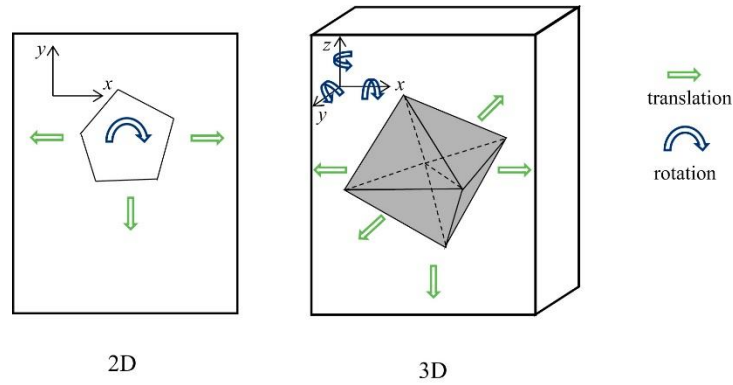


Figure 21. Illustration of rotation and translation of random walking algorithm [55].

2.8.3.4 Improved Random Walking Algorithm (IRWA)

An improvement was made to the random walking algorithm by Zhang Z et al. [82] in 2021 to prevent large-sized aggregates from intersecting with existing aggregates in the target placing domain during the pouring process, which leads to unsuccessful placement. The improvement made was to guarantee that the aggregates are positioned in the order of largest to smallest. A comparison of the two methods shows that for all aggregate shape types, IRWA can achieve a 50% packing density while RWA fails when polygonal and elliptical aggregates are involved [11]. The computational expense of IRWA is also smaller compared to that of RWA which is captured in Figure 22.

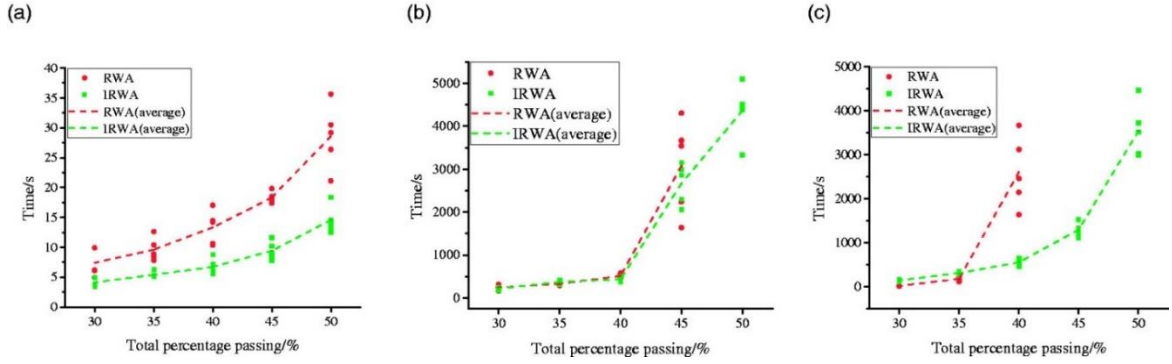


Figure 22. Computational cost comparison for both IRWA and RWA: (a) Circular (b) Elliptical (c) Polygonal shaped particles. [82]

2.8.4 Random fractal method

Generally, the method of generating mesoscale models for the purpose of modeling could be divided into three main types [83], the standard generation model (TGM) where the aggregates are first created and placed at random locations while avoiding overlap [84]. The second method involves algorithms that simultaneously generate and allocate at a single step [85]. In the third class, the aggregate placement location is determined, and the geometrical limits specified before the generation of the aggregate [86].

2.8.5 Motion simulation and heuristic packing algorithm

In this mesoscale geometry generation algorithm, particles are initially randomly positioned in a cylinder, and a dynamic motion simulation approach is used to separate the overlapping particles to abide by the three required conditions when placing aggregates [78]. There are numerous techniques for the separation of 2D geometries [87–90]. Most of these algorithms disregard the randomness of the particles and reorganize the particle arrangement using local search algorithms. The motion simulation technique allows the elimination of overlap without disregarding the spontaneity of the aggregate positioning. The particles with an unbalanced force are subject to motion in the cylinder as illustrated in Figure 23 until the overall elastic energy of the arrangement reduces to zero which signals the packing problem being solved [78].

Intuitively, the movement of the motion particles would range from intense to gentle with the reduction in the positioning energy which may be described as a cooling process. The

motion of particles does not always reduce the configuration's energy but contributes towards the formation of a uniform or stable arrangement.

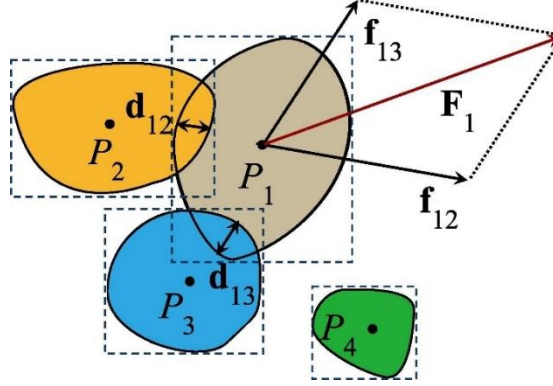


Figure 23. 2D Schematic Illustration of the resultant force as an effect of the overlap between the particles [78].

2.9 Methods of Overlap Detection

The most complex and computationally intensive task in the packing process of aggregates is collision detection during placing [78]. When packing the generated aggregates within a volume to create a mesoscale model, one of the placing requirements is that aggregates should not overlap and intersect other aggregates as well as the boundary of the volume [14]. These have led to the development of numerous algorithms that determine the relation between a point and a *particle* shape to prevent such overlap. A popular method is the area method, but a major disadvantage is the large amount of computation required when packing [38]. Several overlapping detection algorithms have been put forth, including the aggregate identification technique using a background grid [91,92], the fitting rectangle method [93], and the area discrimination method [94]. A few efficient methods will be discussed in the following subsections:

2.9.1 2D mesoscale model

2.9.1.1 Barycentric Coordinate Model

The corners of a simplex, such as a triad or pyramid are known as the barycentric coordinates. Assuming $(\lambda_1, \dots, \lambda_n)$ are the geometric center coordinates of the point P and $v_1, \dots, v_n$ are the points in the vector space V that make up a simplex. If Equation 19.1 When provided with a collection of aggregate is satisfied at point p in V , then

$$(\lambda_1 + \dots + \lambda_n)p = \lambda_1 v_1 + \dots + \lambda_n v_n \quad (19.1)$$

For every constant k that has a value other than zero, where $(k\lambda_1, \dots, k\lambda_n)$ belong to the geometric center coordinates of p . Regularized coordinates meet the requirements of $\lambda_1 + \dots + \lambda_n = 1$. One can divide a polygon with n sides into $n - 2$ triangles, and for each triangle, the geometric center coordinates of point p are determined. All the related barycentric coordinates are greater than 0 if point p lies within the triangle. Using Eq. (20.1), we can calculate for point p its barycentric coordinates.

$$[\lambda_1 \lambda_2 \lambda_3] \begin{bmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{bmatrix} = [1 x_p y_p] \quad (20.1)$$

2.9.1.2 Winding number method

This method's basic idea is to figure out how many turns the polygon that encircles point R has. The point is outside the polygon and the polygon does not encircle it only when the winding number is 0 [95].

$$qP_i = \begin{cases} 0 \\ 1 \\ 2 \\ 3 \end{cases} \text{ if } \arctan \frac{x P_i}{y P_i} \in \begin{cases} [0, \frac{\pi}{2}) \\ [\frac{\pi}{2}, \pi) \\ [\pi, \frac{3\pi}{2}) \\ [\frac{3\pi}{2}, 2\pi) \end{cases} \quad (21.1)$$

Each edge of the polygon's quadrant angle is specified as $\delta_i = qP_{i+1} - qP_i$. The quadrant angle that was modified is calculated using Table 2. Using all of the altered quadrant angles δ'_i , one may get the polygon's winding number that encircles the point R , as demonstrated by Eq [95].

$$\omega(P, R) = \frac{1}{4} \sum_{i=1}^0 \delta'_i \quad (22.1)$$

Table 2: Adjusted quadrant angle δ'_i

δ_i	0	1, -3	-1, 3	2ccw, -2ccw	2cw, -2cw
δ'_i	0	1	-1	2	-2

2.9.1.3 Broad Phase and Narrow Phase Detection

We first check for collision between points in the broad phase by checking for any overlap in a pair of particles AABB trees [96]. There won't be a collision between any two particles if their AABBs do not intersect. If not, narrow-phase detection ought to be carried out. The distance between two pairs of spheres with origin $O_i(r_i; x_i, y_i, z_i)$ and $O_2(r_2; x_2, y_2, z_2)$ is calculated using [78].

$$d(O_1, O_2) = \sqrt{((x_2 - x_1) + (y_2 - y_1) + (z_2 - z_1))} - r_1 - r_2. \quad (23.1)$$

However, the distance computation is rather difficult for general convex shapes. The definition of the separation between items A and B is:

$$d(A, B) = \|z_A - z_B\| = \min\{\|x - y\|: x \in A, y \in B\} \quad (24.1)$$

Where $z_a \in A$ and $z_b \in B$ are the respective pair points of the separation vector $z_A z_B$. It is expected that and have convex shapes in the distance question, or shapes that are curved inwards may be divided into a limited number of distinct convex shapes. The concave objects in the latter scenario are written as

$$A = \bigcup_{i=1}^{N_A} A_i, B = \bigcup_{j=1}^{N_B} B_j \quad (25.1)$$

2.9.1.4 Status Matrix Method

Based on the property that a polygon's centroid O is inside the polygon, The matrix representing the status approach is used to ascertain if a point is contained within the polygon [[51,97]. The edge L_i of the polygon is calculated using.

$$f L_i = a_i x + b_i y + c_i \quad (26.1)$$

Where a_i, b_i, c_i are known as the linear equation's coefficients of the corner $L_i, i = 1, 2 \dots \cdot n$, and n refers to the edges of the polygon.

The state matrix M_o records the spatial law between each edge and the coordinates of the polygon's centroid $O(x_o, y_o)$ by substitution into each side's respective linear equation.

When $f L_i(x_o, y_o) \geq 0$ recorded as 1 in M_o , shows that the centroid lies on or above the edge. When $f L_i(x_o, y_o) < 0$ then it shows that the centroid is beneath the corner as written down as 0 in M_o . Comparing the status matrix MR_i calculated using this procedure and M_o , when the two matrices are the same, we conclude that the point R_i is located within the polygon and vice versa.

2.9.2 3D mesoscale model

2.9.2.1 Barycentric coordinate method

In a similar vein, the 3-D problem can also be handled using the barycentric coordinate method described in the overlap detection for 2D mesoscale model above. It is possible to break down a polyhedron into several tetrahedrons. For every tetrahedron, the barycentric locations of the point p are computed independently. The associated centroidal coordinates for a point inside a tetrahedron are all greater than zero. We calculate the barycentric coordinate $(\lambda_1 \lambda_2 \lambda_3 \lambda_4)$ of the the point p associated with vertices i, j, k, m .

$$[\lambda_1 \lambda_2 \lambda_3 \lambda_4] \begin{bmatrix} 1 & x_i & y_i & z_i \\ 1 & x_j & y_j & z_j \\ 1 & x_k & y_k & z_k \\ 1 & x_m & y_m & z_m \end{bmatrix} = [1 x_p y_p z_p] \quad (27.1)$$

2.9.2.2 Status Matrix Method

The procedure of the status matrix is also applicable to 3D. should the linear equation be expanded to the planar equation.

$$f_i(x, y, z) = a_i x + b_i y + c_i z + d_i \quad (28.1)$$

A comparison of the computation time required to efficiently place polyhedral aggregates using the three methods was conducted and it was discovered that the technique of the status matrix was less resource consuming, with the centroidal method while the volume method reflects a huge amount of time spent, hence placing it at the bottom of the list in terms of efficiency [38].

Table 3: Calculation time (s) for concrete with polyhedral aggregate produced by various algorithms [38].

Method	Calculation Time (s)
Volume method	13,575
Barycentric coordinate method	1002
Status matrix method	208

2.9.2.3 Rectangle Fitting Method

The idea is that aggregates are generated using rectangles mapping the size of the aggregates using several rectangles of varying sizes. The actual overlap detection takes place between a set of fitted rectangles, not the actual aggregates themselves. Initially, a matrix of the background mesh is generated with a grid size ranging from 1/10 to 1/20, and the aggregate mapping section is positioned on the background mesh. Next, the grid is combined vertically and horizontally to form rectangles, and the adjacent rectangles of the same length in the opposite direction are combined as well. Ultimately, the fit rectangle containing the fewest rectangles is chosen and recorded within the aggregate database. This means that two components, ① and ②, are kept for each aggregate, as illustrated in Figure 24 [93].

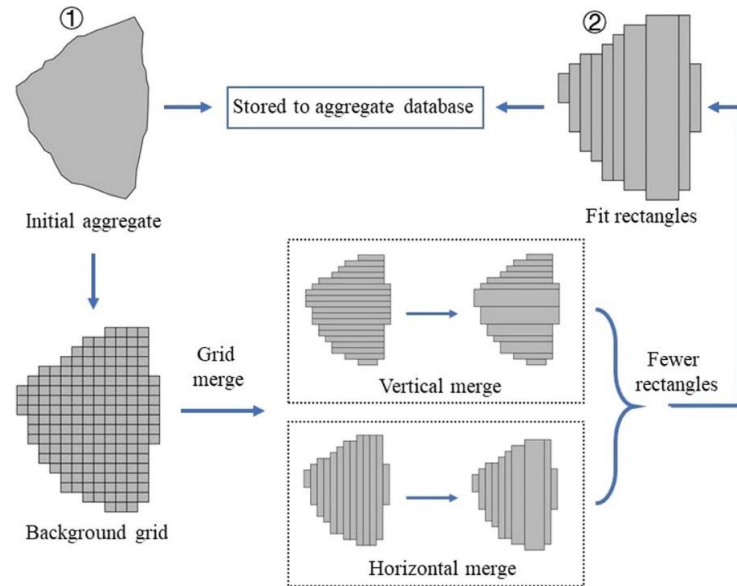


Figure 24. Real aggregate is fitted in a rectangular manner [93].

The condition for the detection of overlap of two rectangles is specified in Equation 29.1:

$$\begin{cases} dis|x_a, x_b| \leq (W_a + W_b)/2 \\ dis|y_a, y_b| \leq (H_a + H_b)/2 \end{cases} \quad (29.1)$$

Defining x_a, x_b, y_a, y_b as the centroid coordinates of both rectangles being checked for overlap while W_a, W_b, H_a, H_b represent The dimensions of the width and height of the rectangles respectively as depicted in Figure 25.

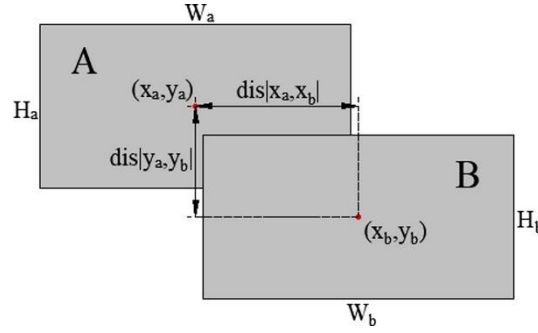


Figure 25. The detection conditions for any two rectangles that overlap [93].

2.9.2.4 Random Distribution Algorithm

This algorithm employs the radial distance method to effectively simulate the volume fraction of concrete samples using recycled concrete aggregates (RCAs), achieving a balance between computational efficiency and consistency with the stochastic methods. The approach involves calculating the radial distance between newly added aggregates and all previously included particles. By narrowing down the analysis to nearby aggregates and ignoring those farther away, the computational load gets reduced [10].

The radial distance method allows for any shaped inclusion, whether natural or recycled aggregate, to be encapsulated within a “virtual” sphere as illustrated in Fig. 31 (a), with a diameter equivalent to the nominal sieve diameter for its respective grading curve in the mix design. The required quantity of spheres to populate the sample aligns with the aggregate count, which is established based on the desired aggregate packing fraction in the design [10]. The packing procedure is shown schematically in Figure 26 (b). After identifying the minimum effective distance, $d_{eff,min}$, between the present aggregate and every other aggregate within the sample, this distance is adjusted to d_{min} , provided that this movement does not lead to overlap with existing particles [10].

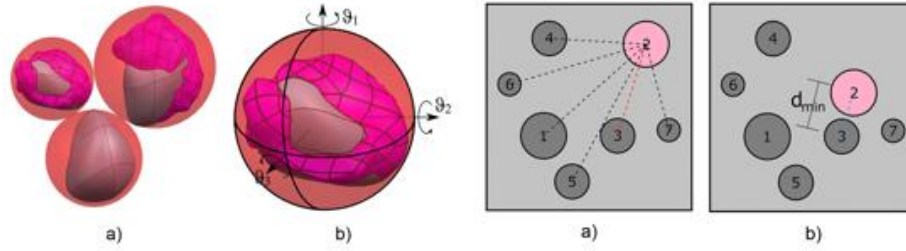


Figure 26. Packing procedure for aggregate #2 (a) calculating the practical minimum distance, $d_{eff,min}$, reduction of, $d_{eff,min}$ to d_{min} [10].

2.10 Numerical Analysis Techniques and Constitutive Material Models

After the geometric model of the concrete has been generated, the second stage of mesoscale modeling to be carried out is the numerical analysis. This typically entails using the finite element method to numerically analyze the generated model while having assigned suitable material properties to its phases[11]. Concrete is known to behave non-linearly with irreversible damage and plasticity. This non-linear behavior is to be captured by the distinct material constitutive properties of the individual phases.

In previous studies, traditional mathematical frameworks grounded in plasticity, models of elasticity, and viscoelastic behavior were used to characterize the non-linear behavior of concrete. By the 1970s, models such as continuum damage mechanics and nonlinear fracture mechanics were introduced for modeling crack growth and the deterioration of material rigidity in concrete. However, a major flaw of such techniques is the neglect of the heterogenous material behavior of concrete. They were unable to properly depict microcrack initiation, propagation, and coalescence in concrete [12].

The discrete element method (DEM) is a numerical approach used to replicate the behavior comprising aggregates, fine particles, and various part models the mesoscale as consisting of discrete particles engaging through friction forces, enabling the examination of particle-level behaviors. Each particle is defined by its velocity, location, weight, and various characteristics, as shown in Figure 28 (bottom left) [98,99]. The primary benefit of this model is its capacity to depict the complex dynamics among individual powder particles and their influence on the overall mesoscale behavior. However, its significant limitation

is the substantial computational power needed to accurately model the interactions between particles. Current solutions include the implementation of parallel computing methods and more advanced contact models. [100].

The lattice element method (LEM) is a continuum-oriented technique that enhances finite element methods (FEM) by incorporating the material's lattice structure, as illustrated in the top left and right sections of Figure 28. LEM is better suited to model materials like cellular solids, foams, and granular materials [101–103]. The advantages of this technique are its ability to capture local phenomena coupled with much better computational effectiveness in relation to continuum-based methods models such as DEM [104]. LEM also offers other advantages such as capturing stress concentration that are prevalent in materials exhibiting intricate internal structure. It enables the simulation of processes like collapse, buckling, and compaction at the microscopic level [100]. Additionally, this approach serves as a link between the small-scale and large-scale levels, enhancing the comprehension of the material's collective response. Within materials science, it contributes to understanding the structural characteristics of foams, porous materials, and blended materials featuring intricate microstructures [105]. Within biomechanics, the Lattice Element Method is utilized to analyze the behavior of implants and biological tissues with complex structures. [106].

The Rigid Body Spring Model treats the concrete sample as a collection of discretized polyhedra, where the faces of the polyhedra are linked by springs, as shown in Figure 27 (bottom right). The discretized components represent rigid bodies, and their deformation is modeled through the springs [107]. Unlike DEM, this approach avoids re-contact between adjacent powder particles, except for those where the spring connection is established at the start of the simulation. The rigidity matrix, which monitors unbalanced forces and applied loads, is not updated at each time step, resulting in higher computational speed [108].

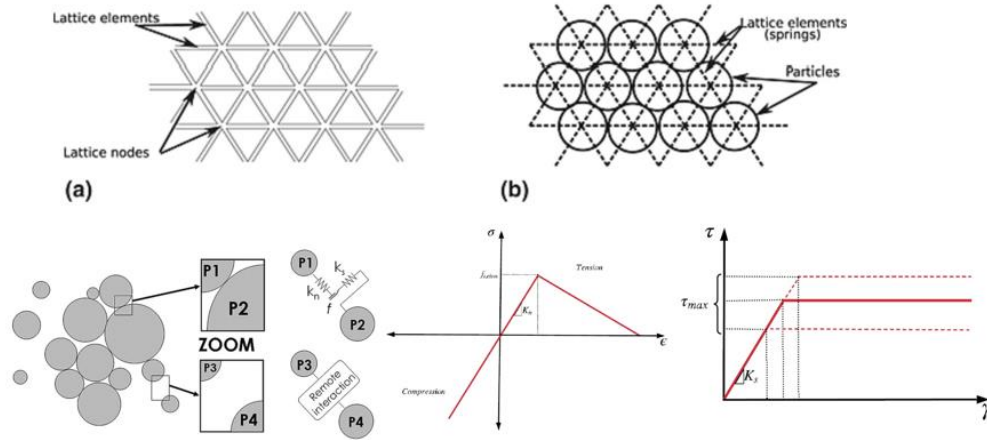


Figure 27. (Top left and right) Illustration of the Lattice Element Model, (Bottom left) Illustration of the discrete element model (DEM), (Bottom right) Depiction of the Rigid Body Spring model [11,100].

2.11 Comparison of the Different Mesoscale Model Generation Algorithm

Table 4: Comparison of various mesoscale model generation techniques.

References	Mesoscale Generation Algorithms	Remarks
[39–42]	Take and place	- Mostly used for the creation of a mesoscale model for low aggregate volume fraction $\sim 30\%$ for polyhedral aggregates [12,55,76]. - Hence, techniques such as aggregate shrinking are employed to reach fractions of up to 67% [77]. - For spherical and circular aggregates, the placement-and-take process can achieve a packing density of $40\%-50\%$ [82]
[14]	Take and place plus rotation	With the addition of a rotation procedure that simulates the packing of real-life aggregates, a packing density of up to 75.6% was achieved for epoxy polymer concrete using a coarse aggregate void filling (CAVF) grading [14]
[38]	Aggregate packing method	Aggregates are packed into the volume layer by layer. An advantage of this technique is the lack of necessity in checking for aggregate overlap which increases computational effectiveness. Nevertheless, it is challenging to prevent and correct the occurrence of gaps within the aggregate [97,109]

[45]	Motion Simulation method	The major advantage of this technique is the inherent elimination of particles overlap without disregard for the randomness of the particle structure [78]
[46]	Local Background Grid Method	This method is an efficient way of mesoscale model generation as the material attribute identification matrix does not allow the placement of newly generated aggregates in places already occupied by previously placed aggregates [110].

CHAPTER 3

METHODOLOGY

This chapter delves into the development and implementation of a **Local Background Grid Method** for generating 3D mesoscale models of recycled aggregate concrete (RAC), focusing on realism and computational efficiency. The approach leverages the Python library **pyMesoscale**, a tool designed to create highly representative mesoscopic structures of RAC that incorporate irregularly shaped polygonal aggregates, a departure from the traditional ellipsoidal aggregate models.

3.1 Local Background Grid Method

This method couples the arbitrary particle arrangement technique with the mapping method of the background grid. Aggregate placement and intrusion detection is a simple step in the local background mesh which increases the packing algorithm's efficiency by avoiding polyhedron disjoint calculations. A general overview of this procedure is illustrated in Figure 29 [110].

3.1.1 Initiation of the global background mesh

A 3D grid of size $L \times W \times H$ is divided into smaller elements or meshed along all dimensions with a size of e . It is advisable to select a reasonable size of element mesh in the spectrum of $\frac{1}{4} \sim \frac{1}{8}$ of the smallest dimension of aggregate, a larger size will not perfectly model the non-linear behavior of concrete while a smaller size will increase the computational cost during the numerical evaluation of the model, reducing efficiency [110].

The total number of elements along three dimensions can be calculated as $l = \frac{L}{e}, m = \frac{W}{e}, n = \frac{H}{e}$. making the actual dimension of the three-dimensional component to be $le \times me \times ne$, in cases where floating point values are obtained, they are rounded to the next whole number.

3.1.2 Material attribute identification using local grids

A three-dimensional array M_{ijk} ($0 \leq i \leq l-1, 0 \leq j \leq m-1, 0 \leq k \leq n-1$) is employed to store the material properties of the cells, with all cells initially assigned a value of 1, representing mortar. During placement, values of 3 and 2 are assigned to represent the aggregate and the interfacial transition zone (ITZ), respectively, as shown in Figure 29. Figure 28 illustrates the local background grid method, and a computational workflow of the algorithm is presented in Figure 30.

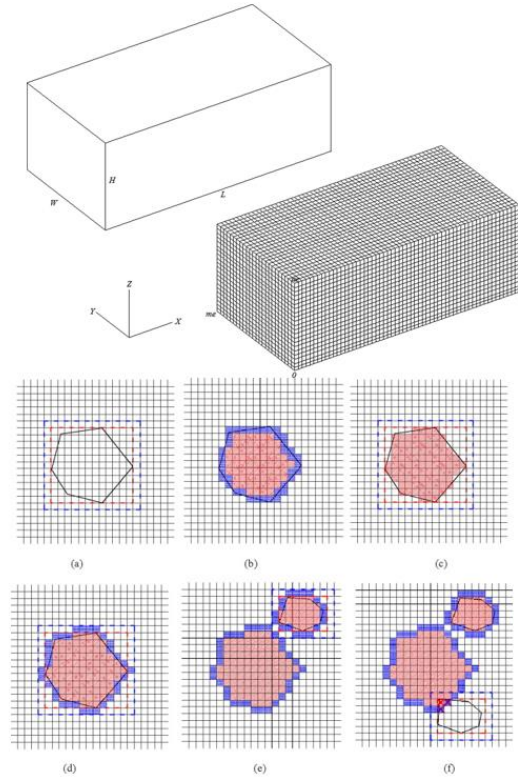


Figure 28. Depiction of the global background mesh. (a) arbitrary placement of aggregate in the local background grid. (b) conventional aggregate and ITZ identification method (c) aggregate element identification (d) ITZ element generation (e) new aggregate addition (f) intrusion detection [110].

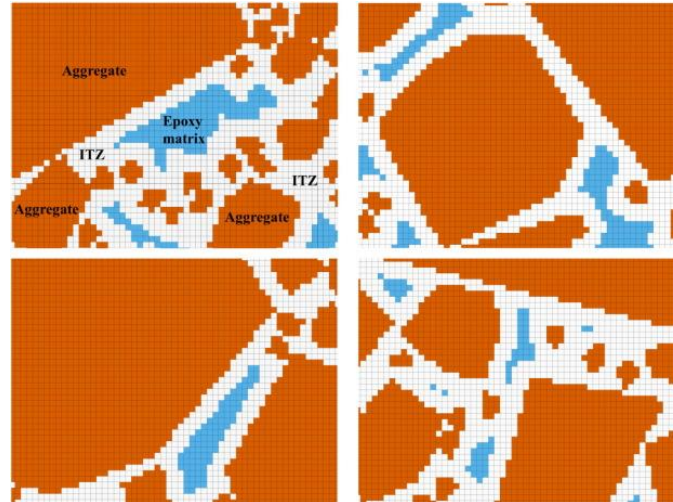


Figure 29. Material attribute identification. [110].

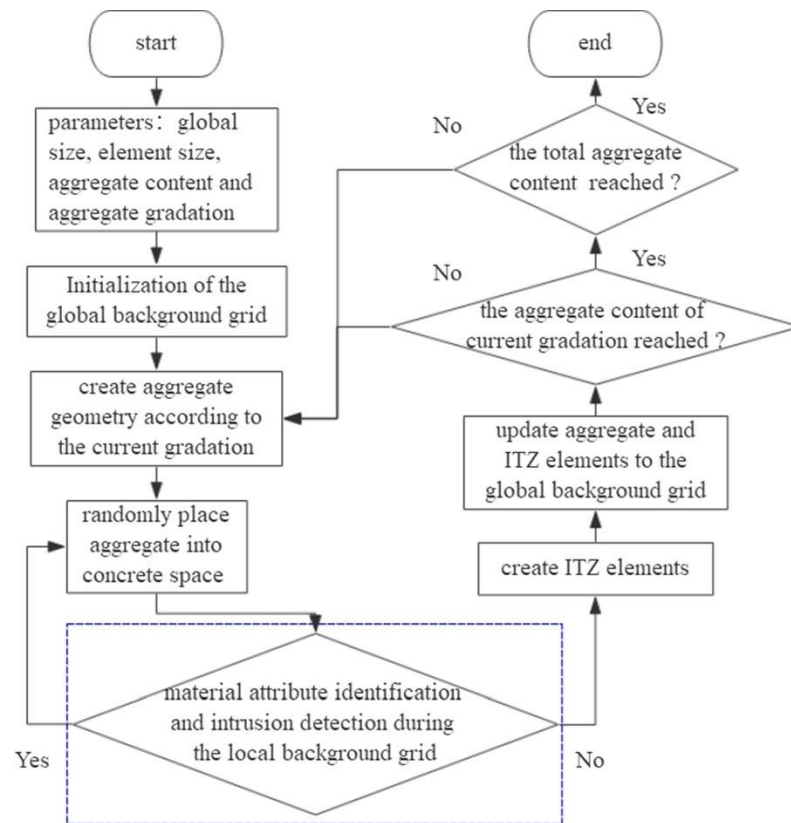


Figure 30. Flowchart of the local background grid method.

3.2 Generating A Mesoscopic Structure With pyMesoscale

As stated earlier, the local background mesh procedure was adopted in this study to generate 3D mesoscale models for recycled aggregate concrete, culminating in a user-friendly Python library, pyMesoscale. The model developed in this study stands out for its closeness to the real-life geometry and physical properties of recycled aggregate concretes. Most recent publications in this area [1,22,113] use ellipsoidal aggregates in the mesoscopic models and assume the attached mortar uniformly encloses the aggregate's surface. These approximations were intended to conserve computational resources as ellipsoidal aggregates are more computationally efficient than polygonal aggregates. However, polygonal aggregates are more representative of the real-life geometry of aggregates and capture their behavior better [11]. Figure 31 presents a flowchart depicting the interoperation of pyMesoscale with various components of related programs. A series of third-party libraries were linked within the Python environment to achieve low-level tensor manipulation for computational efficiency. pyMesoscale outputs two files, a *.vti file for visualization with Paraview and a *.inp file ready for importing into the Abaqus CAE simulation platform. Figure 32 shows the graphical representation of the polygonal aggregates using the Paraview Visualization software.

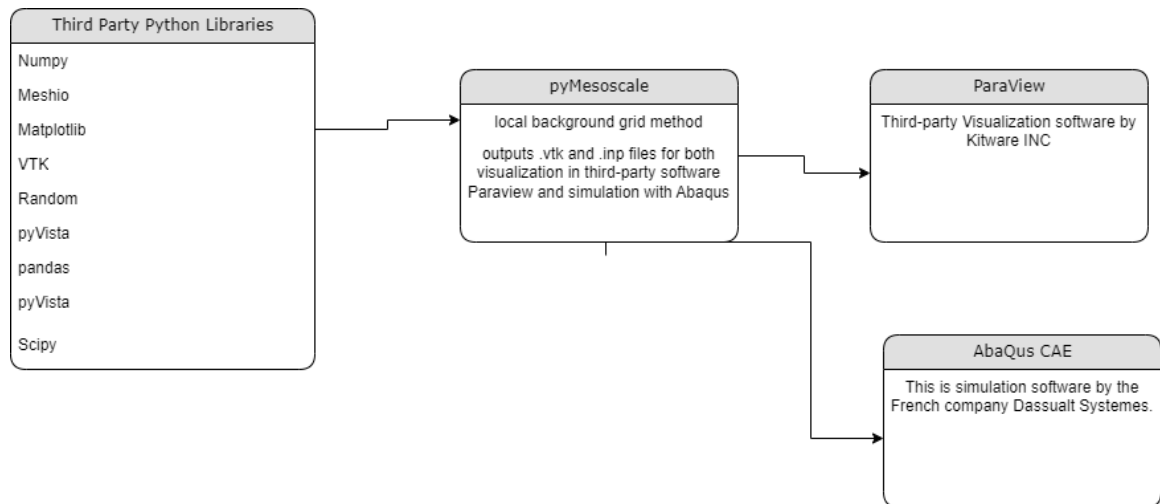


Figure 31. Interconnectivity of the various programs used with pyMesoscale.

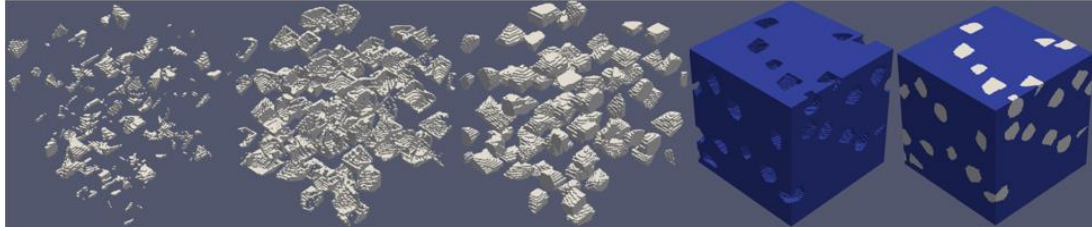


Figure 32. Packing of 3D polygonal aggregates within a representative volume element (RVE) using pyMesoscale and visualized with ParaView. From left to right: attached mortar, ITZ, aggregate, matrix, mesoscale model.

As illustrated in Figure 33, the attached mortar does not generally enclose the original aggregate's surface in a real-life RCA. Therefore, this study's approach veered away from the assumption, followed in most previous studies, that the attached mortar evenly encloses the base aggregate's surface. This may imply a high computational cost of model generation. However, empirical evidence has shown that using memory-efficient libraries like NumPy, written in low-level hardware-efficient code and accessible in Python environments, could lead to negligible computational cost differences. This results in a computationally cheap model that better predicts the fracture mechanics of recycled aggregate concrete.

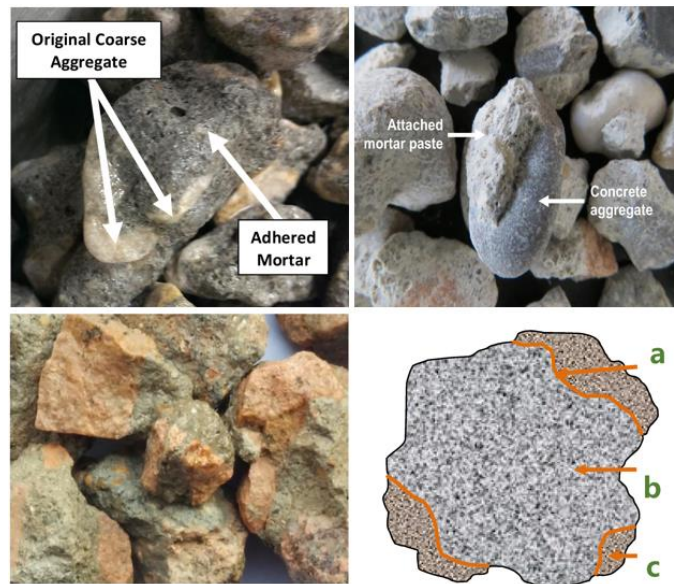


Figure 33. Depiction of attached mortar across various research papers confirming the fact that attached mortar isn't always evenly distributed across the surface of the stone fraction

The model developed utilizes a function that randomly extends the vertices of convex hull-generated polygonal aggregate by checking whether a randomly generated float between 0 and 1 is greater than a specified constant, e.g., 0.5 for a 50% chance of generating an attached mortar content. Figure 34 shows images of several generated recycled concrete aggregates.

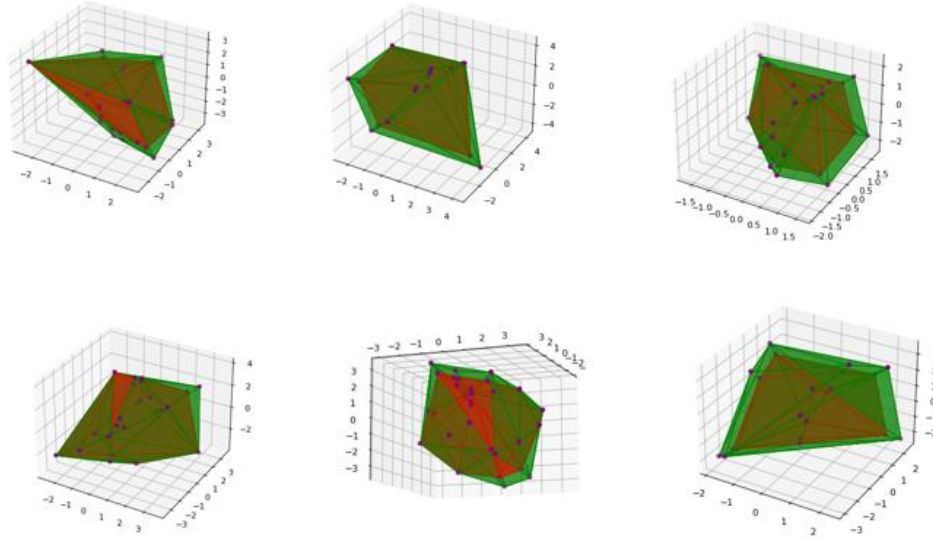


Figure 34. Array of some of the generated recycled concrete aggregates using pyMesoscale

3.3 Material Properties

In this study, the material and mix design follow the approach of Xiao et al. [112], who employed nanoindentation to assess the characteristics of the mesoscopic phase in RAC, along with their mechanical properties. In the adopted mix design, the old mortar was taken to be stronger than the virgin mortar, as this attuned with the findings of nanoindentation experiments. The material nuance of the various classes of RAC is explained in Table 5.

Table 5: Mechanical properties of RAC Mesoscopic phases [18].

Material phase	Modulus of elasticity (GPa)	Compressive strength (MPa)	Tensile Strength (MPa)	Calculation Time (s)
Stone fraction	80	-	-	0.16
Attached Mortar	25	45.0	3.00	0.22
New mortar	23	41.4	2.76	0.22
Old ITZ	20	36.0	2.40	0.20
NEW ITZ	18	33.1	2.21	0.20

Based on Table 5, natural aggregate (NA) remains intact during the failure of both conventional concrete and RAC mixtures. Consequently, its stress-strain (σ - ϵ) behavior is considered non-linear, with no damaged portion. Conversely, the mechanical behavior of the mesoscopic phases, such as ITZs, new mortar, and old mortar, is modeled using the concrete damage plasticity model (CDPM). This choice is justified for two reasons: (1) CDPM parameters are physically meaningful and can be calibrated through experimental data, and (2) the model effectively represents stiffness degradation.

The CDPM was first introduced by Lubliner et al. [113] and later refined by Lee and Fenves [113,114]. Figure 37 shows the stress-strain (σ - ϵ) response of concrete under uniaxial tensile (a) and compression stress (b). In compression, the material displays linear behavior until it reaches the yield stress, σ_{co} , after this point, plastic deformation (stress hardening) takes place until the material reaches its peak stress, σ_{cu} , is reached, followed by a softening phase. In tension, the material remains elastic up to the tensile strength, σ_{to} , beyond which strain softening occurs. The σ - ϵ responses for all mesoscopic phases, essential for deriving CDPM parameters, are determined according to the fib Model Code.

3.4 Discretization of the Geometric Domain

3.4.1 Element type

The C3D8 element is a three-dimensional hexahedral element featuring 8 nodes, each with three degrees of freedom (DOFs), well suited for capturing solid 3D structural elements and widely utilized in mesoscale modeling research [14,38]. Our mesoscopic model was generated using the custom-built pyMesoscale that utilizes the meshio open-source package in converting the generated *.vtk files to *.inp files, as stated earlier. The default element type in the generated *.inp file is C3D8RH, a reduced integration element type. There is a need to manually edit the element type to C3D8, the full-integration element version required for damage and fracture modeling in Abaqus, as shown in Figure 33.

```

878899, 7.200000000000000e+01, 1.000000000000000e+02, 1.000000000000000e+02
878900, 7.300000000000000e+01, 1.000000000000000e+02, 1.000000000000000e+02
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3,3,4,94,93,8432,8433,8524,8523
4,4,5,95,94,8433,8434,8525,8524
5,5,6,96,95,8434,8435,8526,8525
6,6,7,97,96,8435,8436,8527,8526
7,7,8,98,97,8436,8437,8528,8527
8,8,9,99,98,8437,8438,8529,8528
9,9,10,100,99,8438,8439,8530,8529
10,10,11,101,100,8439,8440,8531,8530

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Figure 35. Array of some of the generated recycled concrete aggregates using pyMesomecale [115].

3.4.2 Mesh size

Judgment was made to select a mesh size that would capture the mechanical behavior of our mesoscopic model as best as possible while maintaining a high computational efficiency. It is established in the literature that the standard minimum mesh for concrete models can be taken as 2 mm [1,115,116] while the maximum size should be kept lower than 12 mm. Due to the recent availability of cheap computing resources, such as the cloud-based Google Colab and innovations in computing, e.g., GPUs, this study went a bit lower than the previously recommended minimum, at a mesh size of 1 mm, to better capture the model's mechanical responses.

3.5 Boundary Conditions

For the uniaxial compressive strength test (UCST), the load was applied to the generated mesoscale cubical specimen model via a reference point located at the center of the top and bottom surfaces with a coupling interaction behavior for these surfaces. The bottom surface was firmly restricted from displacements along all directions, and a downward load was applied along the y-axis at the reference point, as illustrated in Figure 36. The load was applied upward for the tensile version of the uniaxial strength test (UTST).

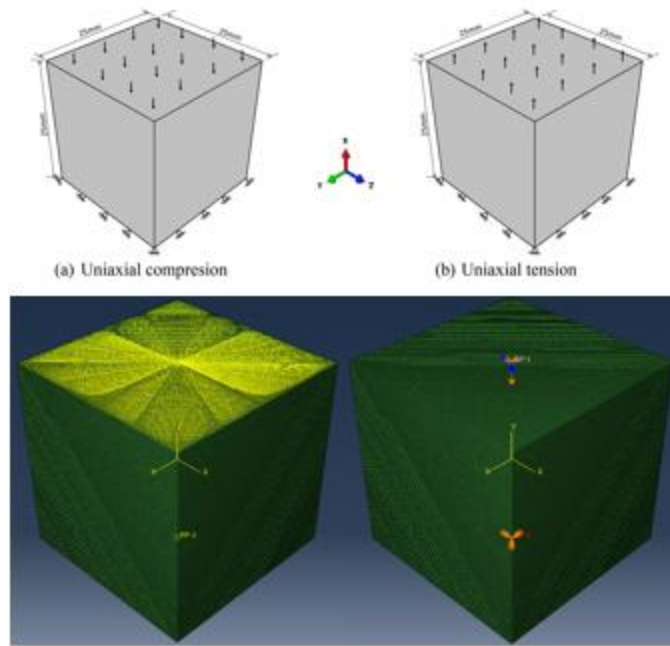


Figure 36. (Top) Depiction of Boundary Conditions [118]; (Bottom) Coupling interaction and application of load and displacement boundary conditions on the upper and lower surfaces of the mesoscopic model in Abaqus CAE [115].

3.6 Finite Element Solver

In many research articles [119–121], explicit solvers are typically favored for quasi-static simulations because they offer a rapid convergence and excel in non-linear calculations [122]. Another advantage of using the dynamic explicit solver is that they can be used in damage and fracture initiation, propagation, and failure studies. A time step of 0.01s was used for consistency with previous research findings on the sensitivity analysis of 3D mesoscale models reported by Huang et al. [123] and Wang et al. [121].

3.7 Constitutive Material Model

The response to mechanical stress of the three phases: attached mortar, ITZ, and matrix was studied using the CDPM. This model has gained quite some popularity in mesoscale modeling studies on recycled aggregates, the most recent of which is Ren et al. [1].

The CDPM was introduced by Lubliner et al. [124,125] and refined by Lee and Fenves [125]. The uniaxial compression responses are made of four (4) major components. The

$\sigma - \varepsilon$ response remains elastic and linear until the point of peak stress is reached at σ_{co} , the yield stress. The plastic region follows, exhibiting a plastic behavior, and then strain hardening until the ultimate compressive stress, σ_{cu} . For the tensile behavior, the relationship between $\sigma - \varepsilon$ remains elastic until tensile failure at σ_{to} , followed by strain softening. The CDPM model is incorporated into ABAQUS and has shown effectiveness in simulating concrete deterioration and fracture while considering both static and kinetic mechanical properties [126–130]. A detailed schematic view is provided in Figure 37.

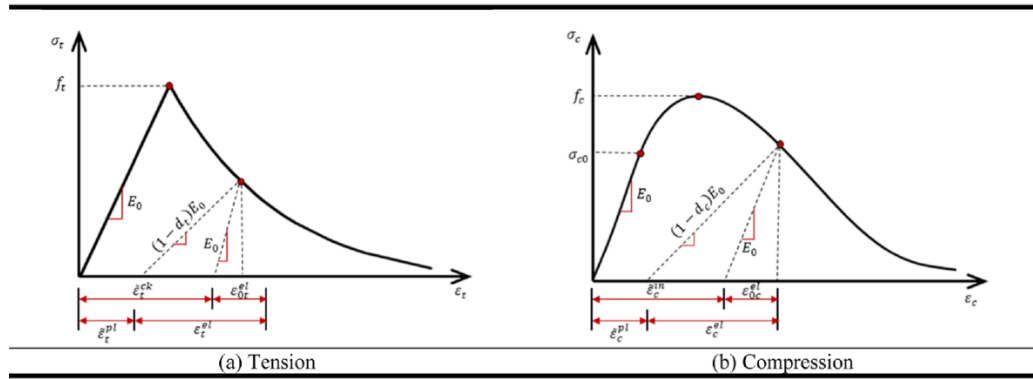


Figure 37. Uniaxial $\sigma - \varepsilon$ as utilized within the Concrete Damage Plasticity Model (CDPM) [1]

The studies by Snozzi et al. [131], Huang et al. [132], and Zhou and Hao [133] entailing the analysis of the tensile and compressive behaviors of concrete under rapid deformation rates have revealed that the aggregates remained undamaged. This is because the aggregates' tensile and compressive resistance properties usually surpass those of the mortar and ITZs. Therefore, this study modeled aggregates as behaving elastically without damage. To simplify the model, the compressive stress-strain behavior of the mortar and ITZs, up to the peak stress, was assumed to be linear elastic. Eq. (30.1) proposed by Guo [134] was employed to describe the post-peak softening behavior. As shown, σ_c and ε represent the compressive resistance and corresponding strain, respectively, while ε_c denotes the compressive strain at the peak strength, f_c . The coefficient $\alpha = 0.157^{0.785} - 0.905$.

$$\frac{\sigma_c}{f_c} = \frac{\frac{\varepsilon}{\varepsilon_c}}{\alpha \left(\frac{e}{\varepsilon_c} - 1 \right)^2 + \frac{e}{\varepsilon_c}} \quad (30.1)$$

For uniaxial stretching, it is presumed that both the mortar and ITZs exhibit linear elastic behavior until the tensile strength is attained. The subsequent exponential decay of the softening curve, as introduced by Hordijk [135], is applied to model the relationship between tensile stress (σ_t) and the displacement resulting from the crack opening (w).

$$\frac{\sigma_t}{f_t} = \left[1 + \left(3.0 \frac{w}{w_0} \right)^3 \right] e^{(-6.93 \frac{w}{w_0})} - 10 \frac{w}{w_0} e^{(-6.93)} \quad (31.1)$$

Here, w_0 refers to displacement due to the crack separation at which the tensile stress reaches zero, and it is determined by the following calculation.

$$w_0 = 5.4 \frac{G_f}{f_t} \quad (32.1)$$

The CDP model defines five additional parameters: the angle of dilation (in degrees), the eccentricity of the flow potential, the proportion of the starting equibiaxial yield stress to the initial uniaxial compressive yield stress, the viscosity coefficient, and the proportion of the second stress invariant to the tension meridian relative to the compressive meridian. For this study, the values of 40, 0.1, 1.16, 0.003, and 0.667 were uniformly applied to both mortar and ITZs.

It is important to emphasize that, in contrast to discrete crack models [136–138], the CDP model, rooted in continuum mechanics, utilizes damage indicators such as DAMAGE-C for compression and DAMAGE-T for tension to simulate crack formation. However, it is unable to accurately capture detailed crack characteristics, such as separation width. Although Equation 2 is commonly applied in simulations, it is based on curve fitting applied to a limited range of prismatic concrete specimens exposed to defined boundary conditions. Their applicability to various geometries, boundary conditions, and materials, such as mortar and ITZs analyzed in this study, remains uncertain, highlighting the need for additional investigation.

3.8 Simulation Matrix

The simulation program evaluates the performance of mortars with different attachment configurations (randomly attached and fully encircled mortars) across various aggregate volume fractions (30%, 40%, 50%, 60%, 70%) and natural and recycled aggregate blends with varying NAC replacement ratios (0%, 30%, 50%, 100%) at 60% aggregate volume fraction. It measures the behavior using two test types: UCT and UTT.

Table 6. Simulation Program

Simulation case	Randomly attached mortar		Fully encircled attached mortar		Simulation case	Natural and recycled aggregate blends	
Test Type	UCT	UTT	UCT	UTT	Test Type	UCT	UTT
Aggregate volume fractions (%)	30, 40, 50, 60, 70		30, 40, 50, 60, 70		NAC replacement ratios (%) at 60% AVF.	0, 30, 50, 100	

CHAPTER 4

RESULTS

4.1 Mechanical Mesoscale Modeling of Randomly Attached Mortar on Recycled Concrete Aggregate.

To investigate the mechanical properties of the concrete cube specimen considered in this study, a 3D mesoscale model was generated with varying aggregate packing densities: 30%, 40%, 50%, 60%, and 70%. The models were subjected to uniaxial compression and tension test simulation using the Abaqus CAE software.

4.1.1 Uniaxial compression test

Figure 38 presents the $\sigma - \varepsilon$ relationship of the various mesoscopic phases across various aggregate packing densities of concrete cube specimens. These values were obtained using the *combine(x,x)*, *abs(x)* and *average([x,x ...])* post-processing functions available in Simulia Abaqus visualization package [115]. Several points across the specimen and the component elements, such as matrix, attached mortar, ITZ, etc., were selected for averaging to obtain the reported quasi-accurate $\sigma - \varepsilon$ relationship of the recycled aggregate concrete specimens.

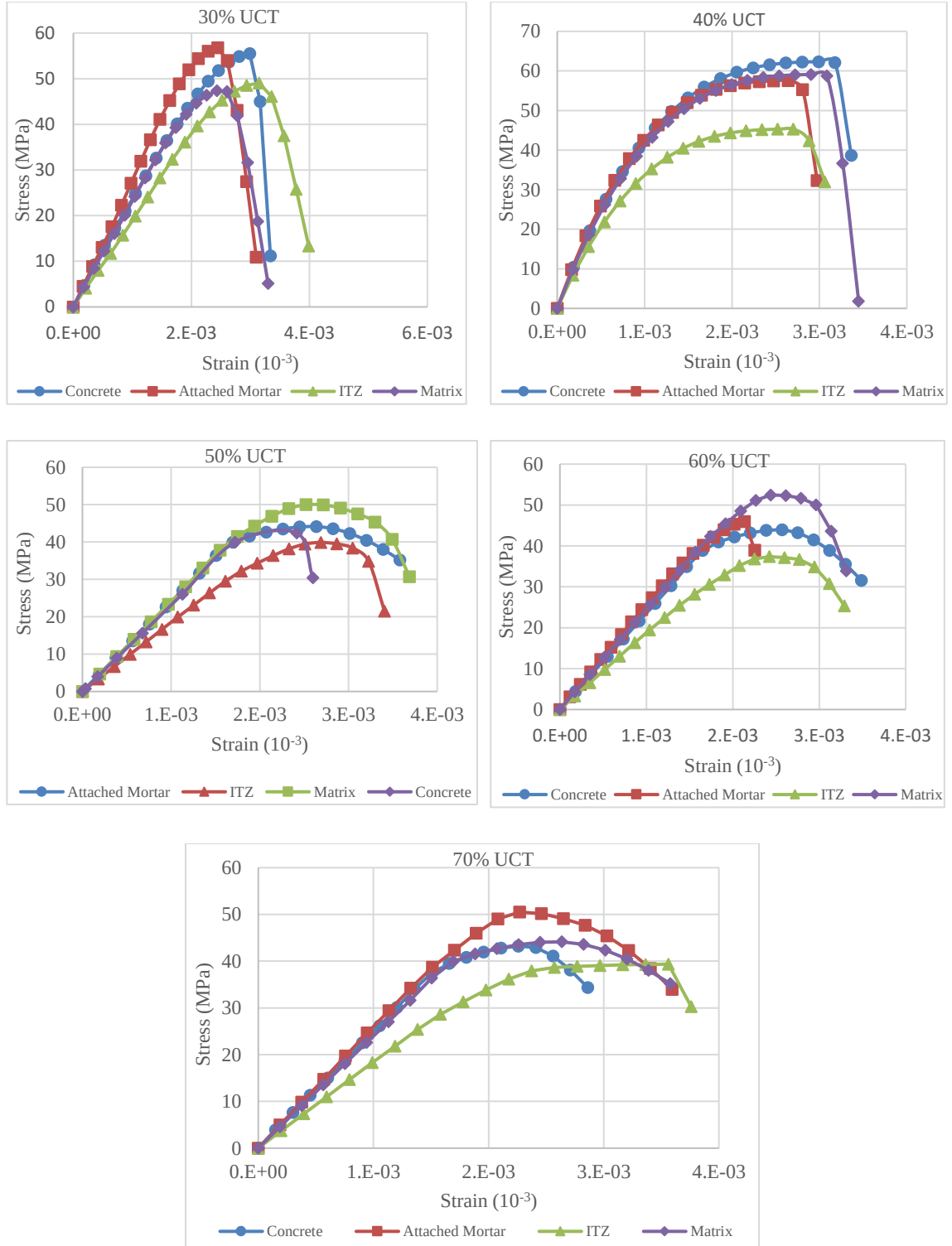


Figure 38. $\sigma - \epsilon$ relationship of various mesoscopic phases at different aggregate packing densities.

Afterward, a comparison was made between the different aggregate packing densities in which the 30-40% recycled aggregate packing density exhibited the highest compressive resistance, as demonstrated in Figure 39. However, higher aggregate volume fractions with a lower compressive strength exhibited a much slower damage deterioration over a much longer duration compared to lower packing densities. The force-displacement relationship is also displayed on the right graph where a peak of 800 kN was recorded across a 1mm compressive displacement length.

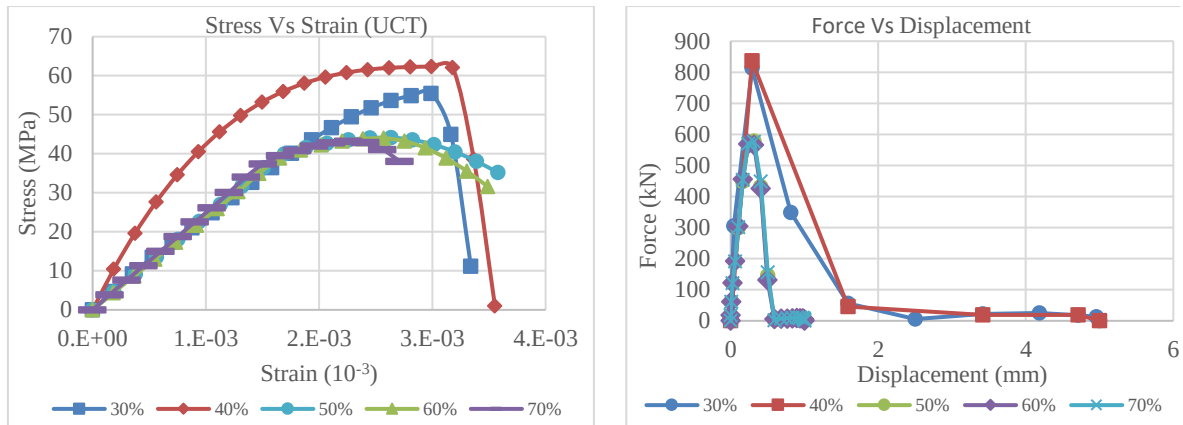


Figure 39. $\sigma - \epsilon$ and force-displacement relationship of UCST for various aggregate packing densities.

Damage evolution studies were conducted to study how the fracture initiates, propagates, and interlinks with other cracks before the eventual failure of the concrete specimen. As demonstrated in Figures 40 and 41, damage mostly initiates in the ITZ and the attached mortar regions, steadily spreading to all the parts of the specimen and causing permanent damage. A large portion of the mechanical strength is lost when the individual cracks interlock to form larger cracks across the specimen.

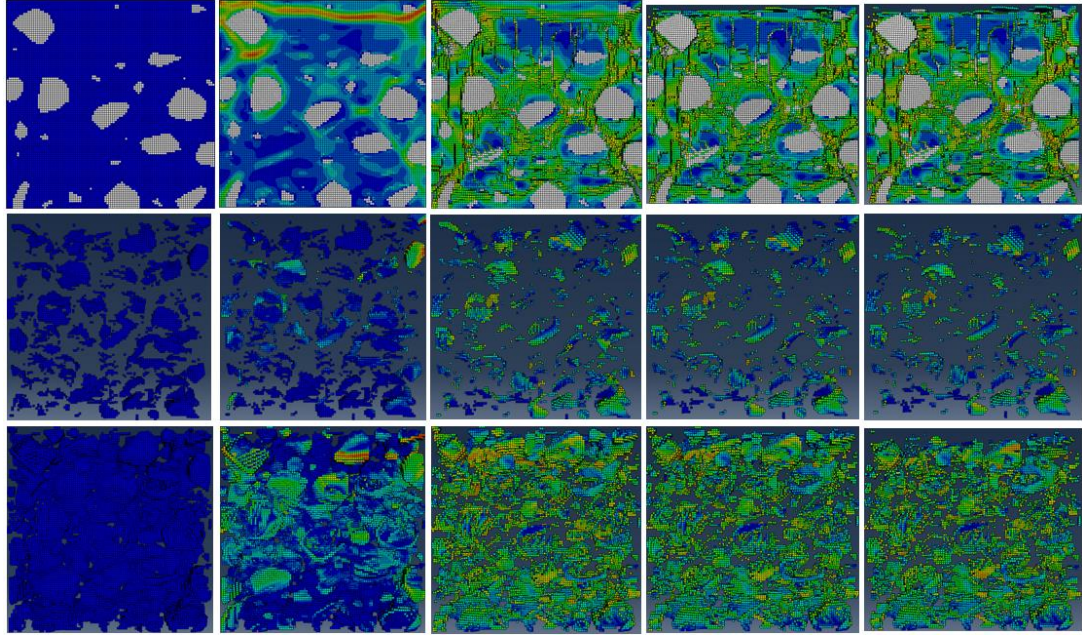


Figure 40. Compressive damage evolution across the RAC specimen, attached mortar, and ITZ (from top to bottom) at an increasing rate of 4 load steps (from left to right).

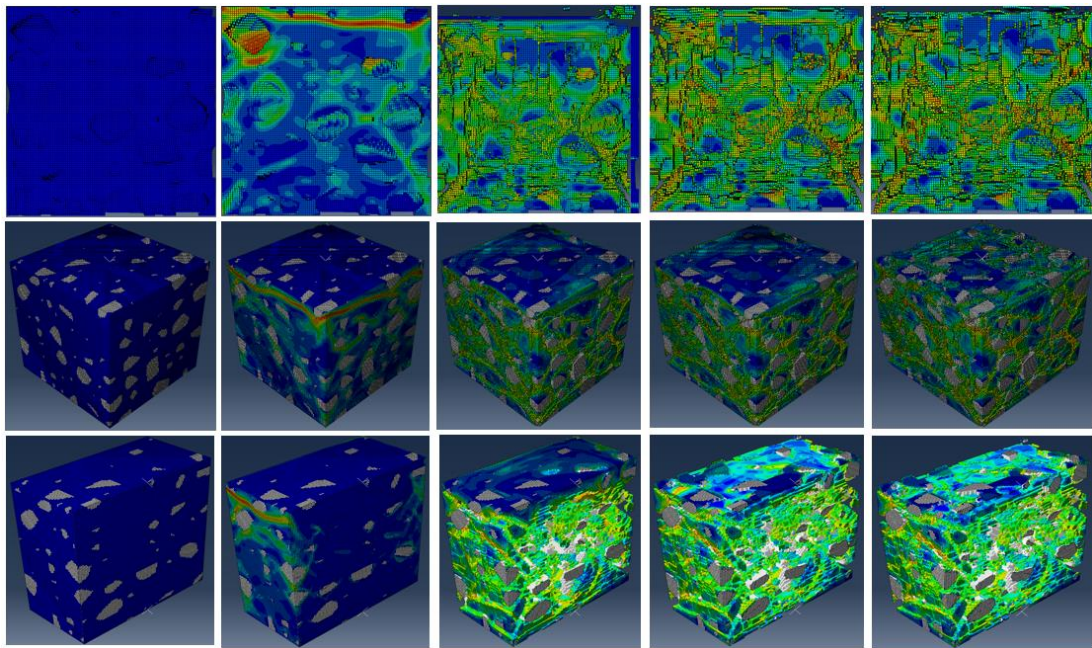
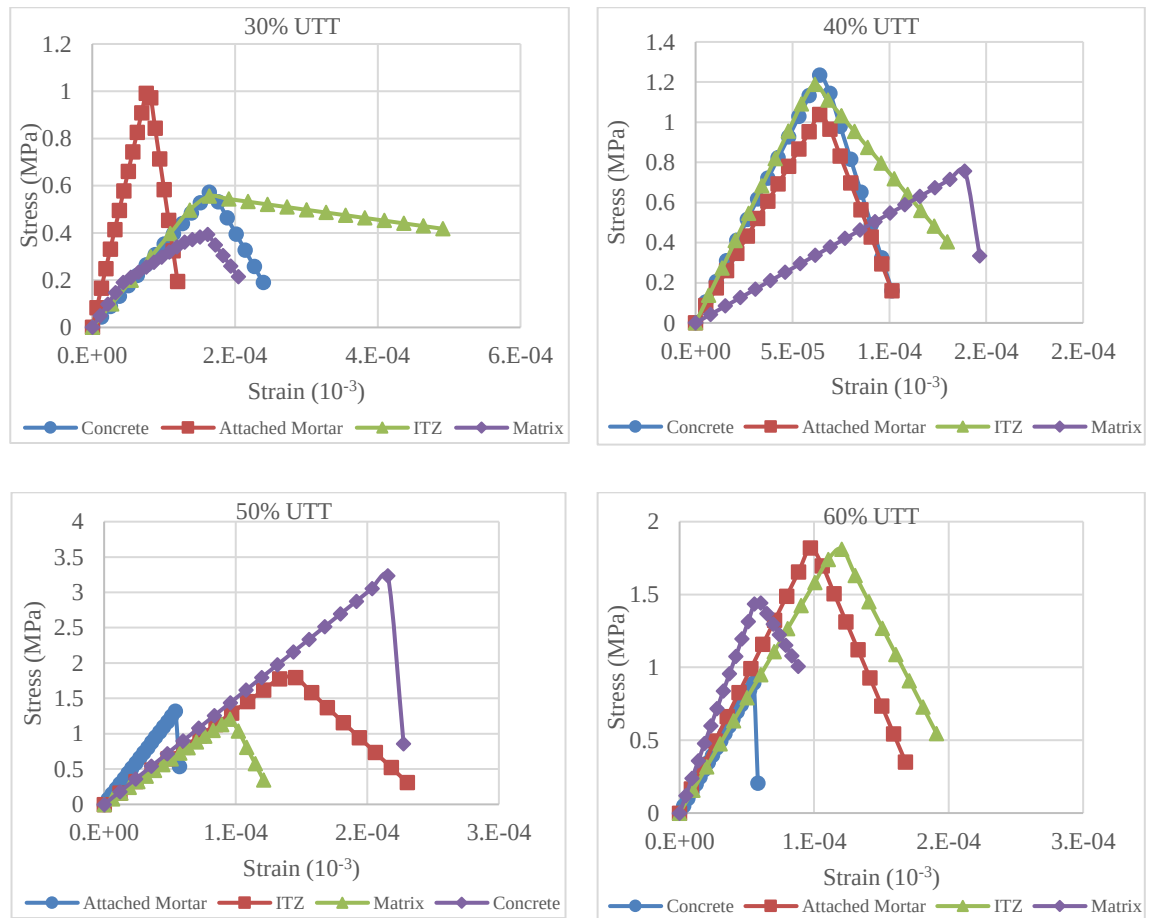


Figure 41. Compressive damage evolution across the Matrix, 3D RAC, and Cut section of 3D RAC (from top to bottom) at an increasing rate of 4 steps (from left to right).

4.1.2 Uniaxial tension test

Figure 42 presents the $\sigma - \varepsilon$ relationship of the various mesoscopic phases across various aggregate packing densities of the investigated concrete cubical specimens. The tension strength tests exhibited much higher computational efficiency and speed than UCST, owing to concrete's weakness in tension. A comparison of the strength in tension of RAC models is illustrated in Figure 43. The model with a 50% aggregate volume fraction exhibits a higher tensile strength of 3.4 MPa. The force-displacement relationship is also displayed on the right graph where a peak force of 20 kN was recorded for the 70% aggregate volume fraction at a compressive displacement length of 1 mm due to load exerted on the upper surface of the specimen.

The tensile response and damage evolution of the specimen are more apparent in the upper and lower regions of the RAC specimen, as illustrated in Figures 44 and 45.



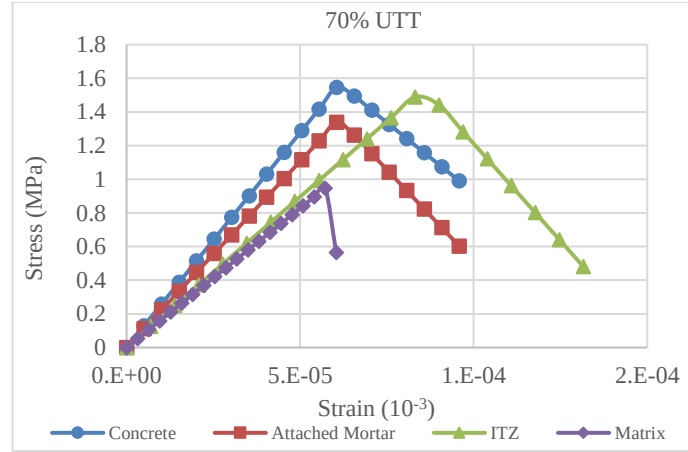


Figure 42. $\sigma - \epsilon$ relationship of various mesoscopic phases at different aggregate packing densities.

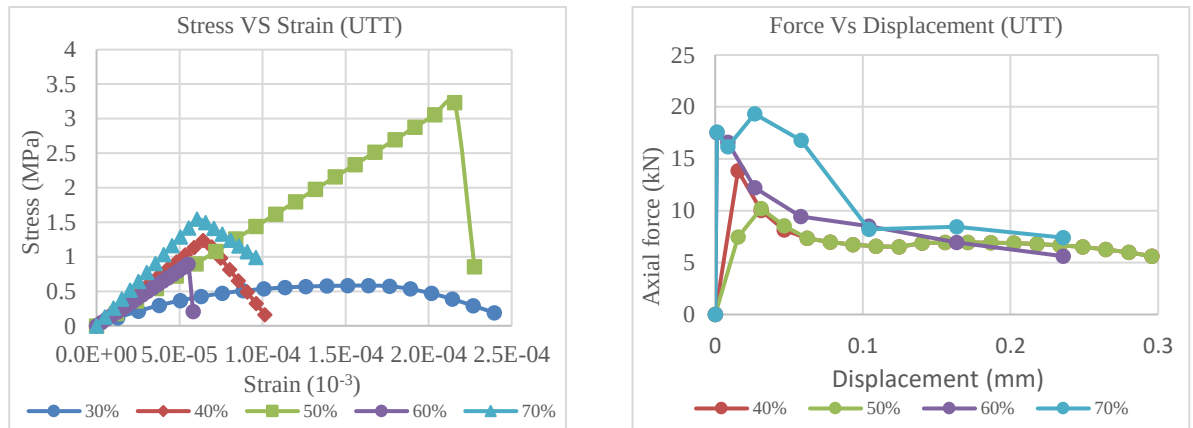


Figure 43. $\sigma - \epsilon$ and force-displacement relationship of UTST for various aggregate packing densities.

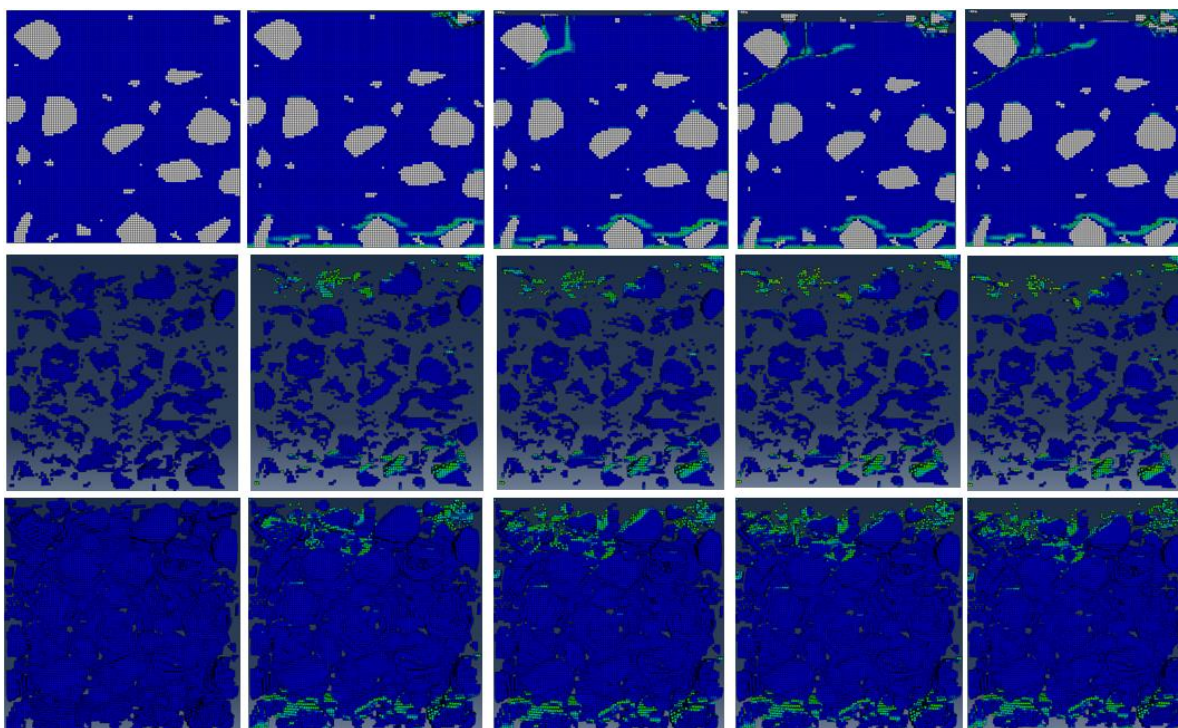


Figure 44. Tensile damage evolution across the RAC specimen, attached mortar, and ITZ (from top to bottom) at an increasing rate of 4 load steps (from left to right).

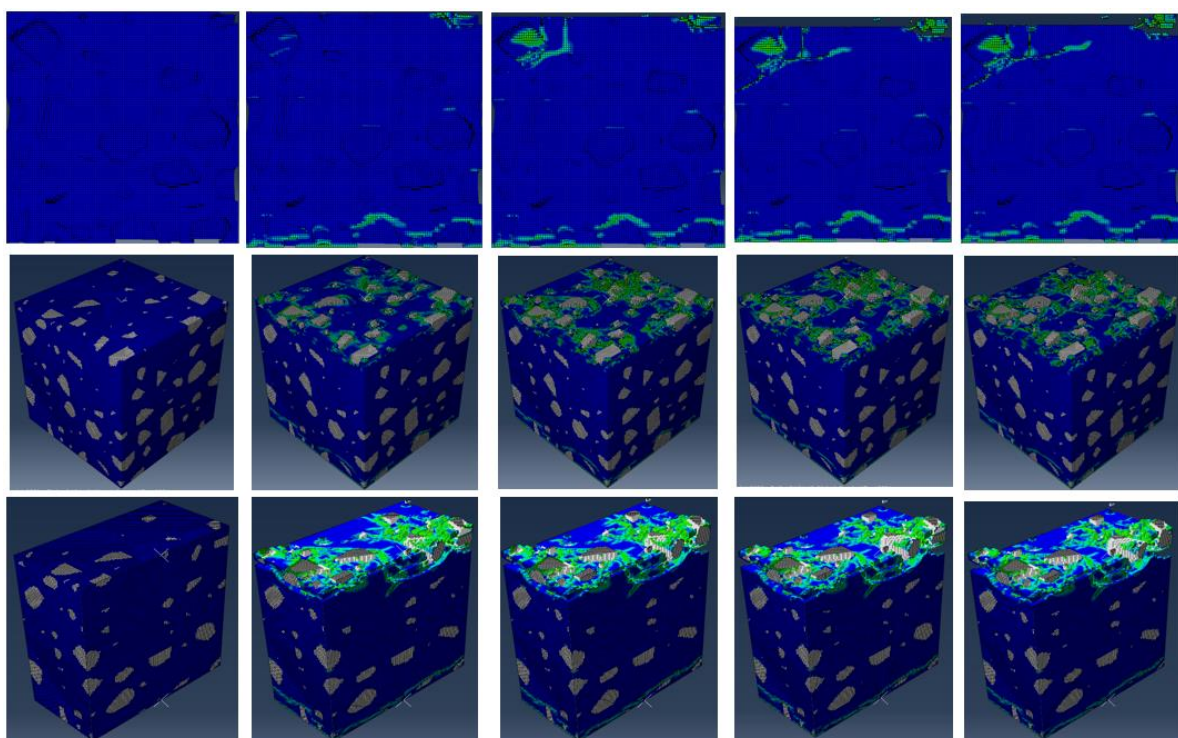


Figure 45. Tensile damage evolution across the RAC specimen (from top to bottom), attached mortar, and ITZ at an increasing rate of 4 steps (from left to right).

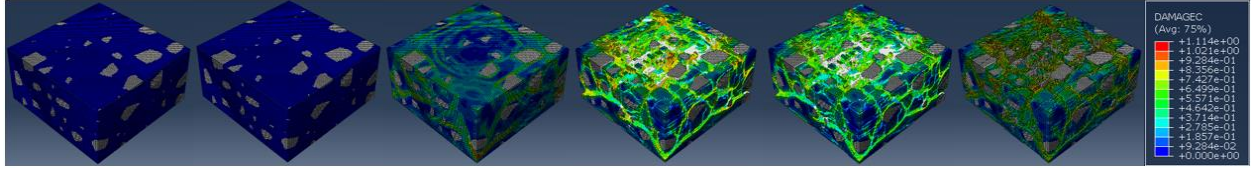


Figure 46. DAMAGEC evolution through our mesoscale model with 60% aggregate volume fraction with randomly attached mortar on RCA varying at 4-step intervals (from left to right).

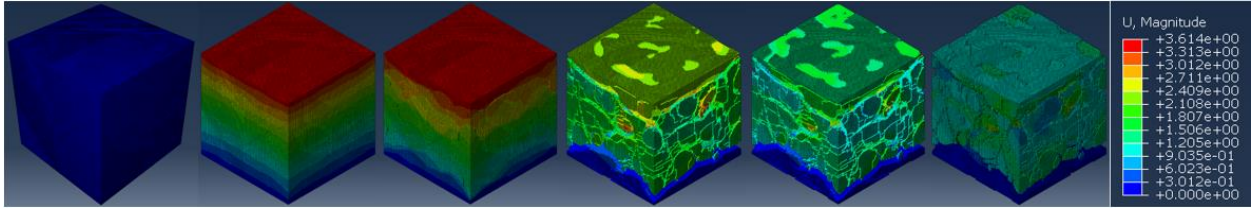


Figure 47. Translations and Rotations at 60% aggregate volume fraction for randomly attached mortar on recycled concrete aggregate varying at 4-step intervals (from left to right).

4.2 Mechanical Mesoscale Modeling of Fully Enclosed Attached Mortar on RCA.

4.2.1 Uniaxial compression strength test

Previous Mesoscale modeling research of recycled aggregate concrete involves generated aggregates with attached mortar covering the entire geometry of the base aggregate [1,22,138]. Accordingly, this study sought to examine the significance of the present results, which were based on the algorithmic generation of mesoscopic models with randomly attached mortars on aggregates. To achieve this, mesoscopic models were generated with the base polygonal aggregates' surfaces coated with uniformly attached mortar and then subjected to uniaxial compression as done with the previously discussed models.

The $\sigma - \varepsilon$ relationship of models with varying aggregate volume fractions is presented in Figure 48, along with a comparison of these model cases shown in Figure 49. The highest three compressive strengths were 70, 65, and 63 MPa corresponding to the models with 70%, 40%, and 60% aggregate volume fractions, respectively. Surprisingly, these values are higher than their counterparts with randomly bonded mortar. This can be explained by

the randomly attached mortar having varying thicknesses, unlike in the fully enclosed cases where the attached mortar is uniform, ultimately leading to a higher attached mortar content.

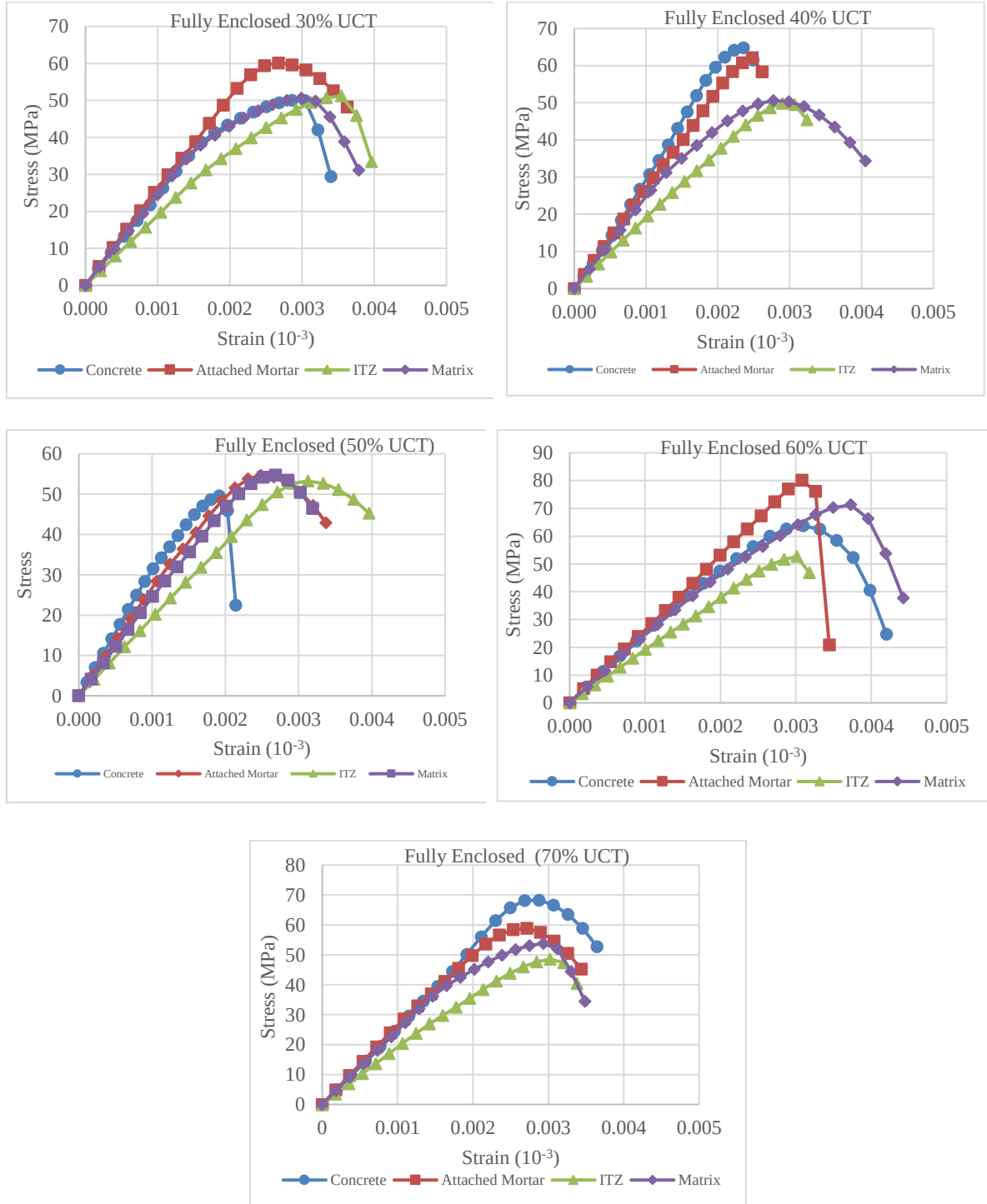


Figure 48. Compressive (fully enclosed) $\sigma - \varepsilon$ relationship of various mesoscopic phases at different aggregate packing density.

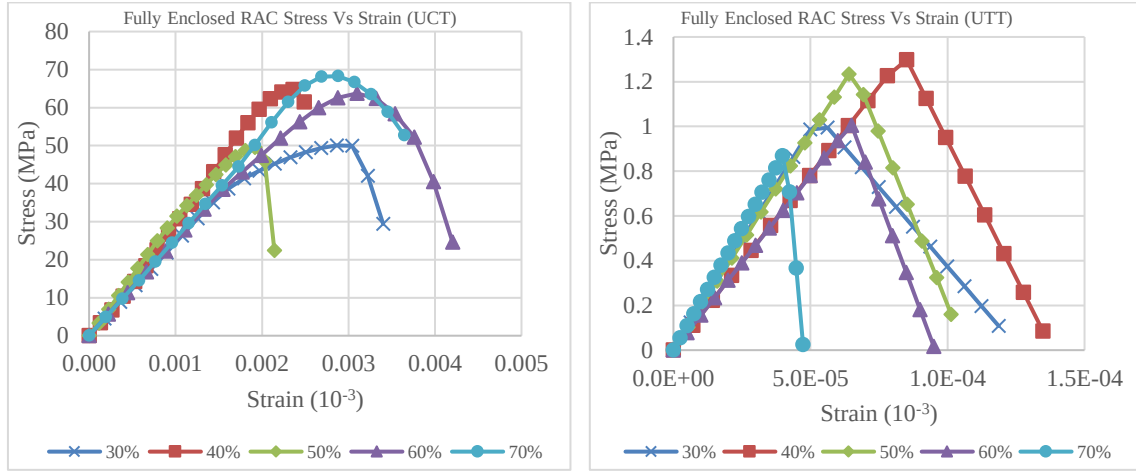
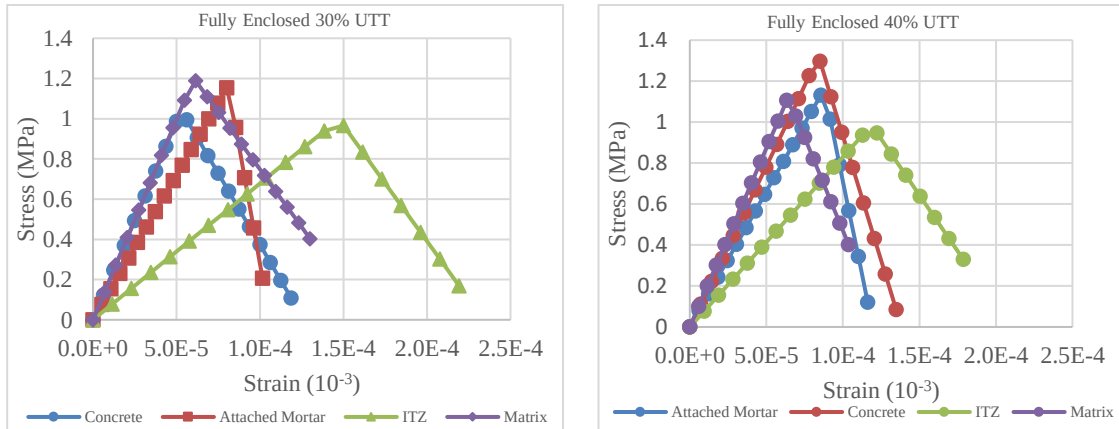


Figure 49. Compressive & Tensile (Fully Enclosed) $\sigma - \varepsilon$ relationship at different aggregate packing densities.

4.2.2 Uniaxial tensile strength test

The tensile $\sigma - \varepsilon$ response for fully enclosed recycled concrete aggregate is shown in Figure 50, where the mesoscopic model with a 40% aggregate volume fraction claims the highest tensile strength of 1.3 MPa, closely followed by the 50% case.



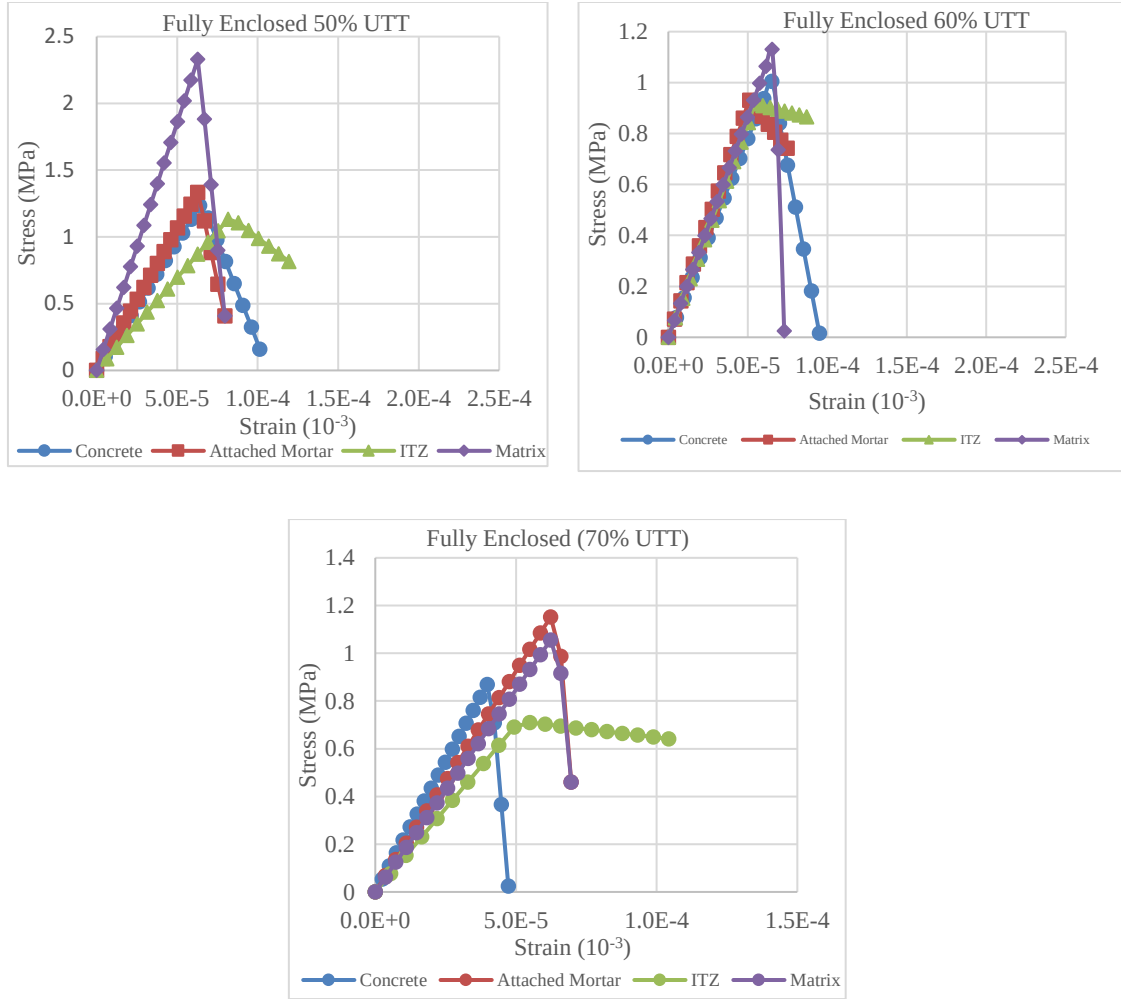


Figure 50. Tensile $\sigma - \epsilon$ relationship of various mesoscopic phases at different aggregate packing density.

4.2.3 Comparison of fully enclosed and randomly attached recycled concrete aggregate

As depicted in Figure 51, the values predicted by the randomly and fully enclosed AM tend to vary, although not with a huge difference, except for the 40% aggregate case which arrived at the same value of about 63 MPa. Also, the value of the fully enclosed AM tends to be much higher. The same thing can be said for the uniaxial test for tensile strength with the exception of the 50% random AM case in tension, which overshoot to 3.4 MPa.

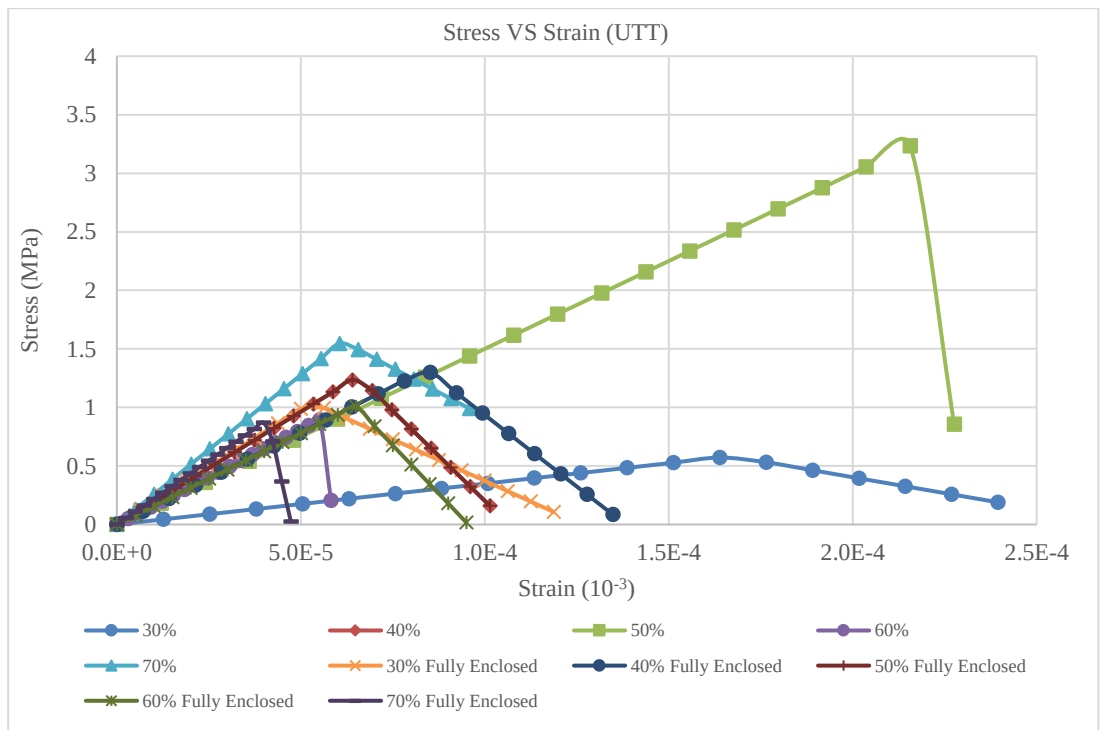
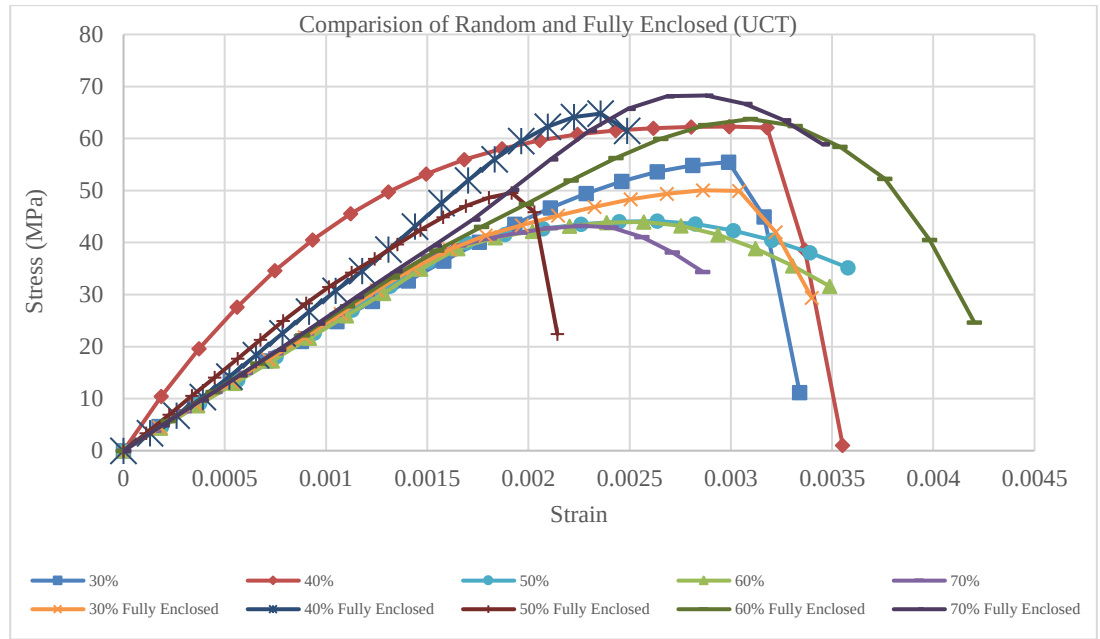


Figure 51. Compressive and Tensile σ - ϵ relationship of randomly attached and fully enclosed recycled concrete aggregate at different aggregate packing density.

4.3 Mechanical Mesoscale Modeling of Combinations of Natural And Recycled Concrete Aggregates.

4.3.1 Uniaxial compression strength test

Simulation for UCT was carried out to determine the responses of mesoscopic models with various blends of natural and recycled concrete aggregates, including 100% natural and recycled aggregates. Figure 52 shows the σ - ϵ of the various natural and recycled aggregate blends.

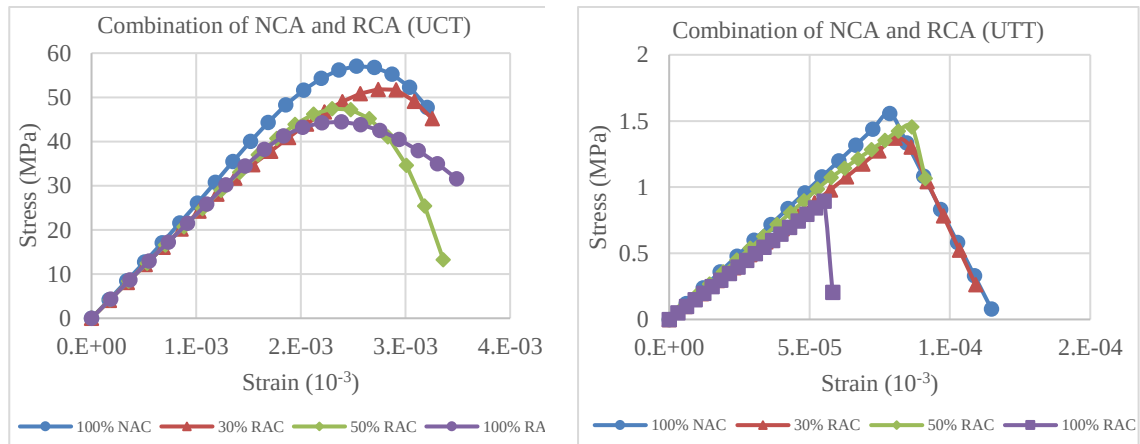


Figure 52. Compressive σ - ϵ relationship of UCST at different natural and recycled concrete aggregate blends.

4.3.1 Uniaxial tensile strength test

The simulation for UTST was also conducted, as illustrated in Fig. 52. In tension, there appears to be negligible differences in the mesoscopic models' tensile responses for 100% natural aggregate and 100% recycled aggregate.

CHAPTER 5

DISCUSSION

5.1 Comparison of the Effect of Aggregate Volume Fraction and Randomly Attached Mortar on the Mechanical Properties of Recycled Aggregate Concrete

It was observed from the results that the compressive strength of recycled aggregate concrete peaks at a 40% aggregate volume fraction with a value of $\sigma_c = 63 \text{ MPa}$, followed by the 30% aggregate volume fraction, and eventually decreases with increasing aggregate volume fraction. Figure 53 compares the $\sigma - \varepsilon$ relations of this study's mesoscopic phases of the 60% aggregate volume fraction (dotted lines) with those reported by Ren et al. [1] (solid lines).

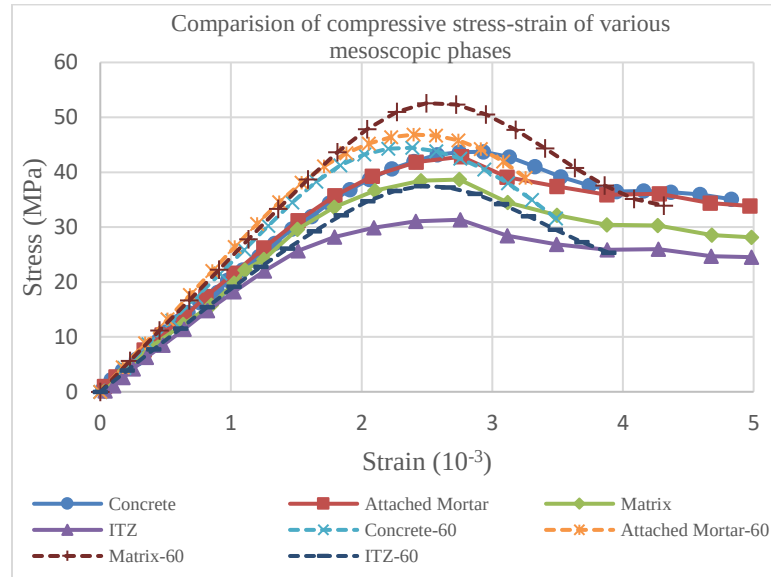


Figure 53. Comparison with compressive $\sigma - \varepsilon$ relations of mesoscopic phases compared with Ren et al. [1]

Regarding the uniaxial tensile tests, the 50% aggregate volume fraction yielded the highest tensile strength of $\sigma_t = 3.4 \text{ MPa}$. An illustration of the tensile response of different phases

of 60% aggregate volume fraction (dotted) compared with the corresponding ones of Ren et al. [18] is shown in Figure 54.

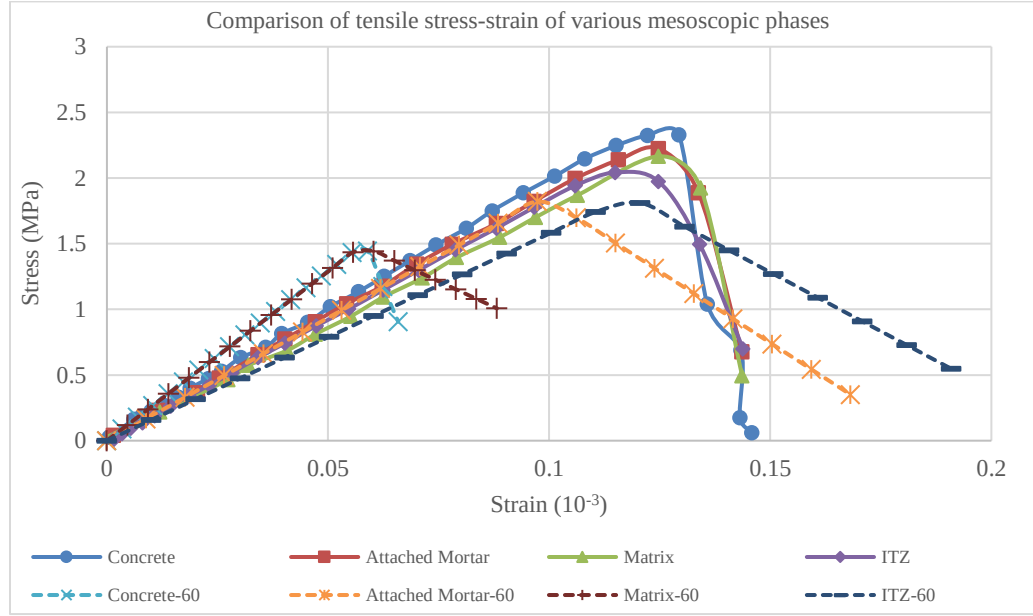


Figure 54. Comparison with tensile $\sigma - \epsilon$ relations of mesoscopic phases compared with Ren et al. [1]

5.2 Comparison between the Simulated Uniaxial Compression Strength Tests with Experimental Results from Literature

In Figure 55 (top) a comparison of our results (dotted lines) using the 60% aggregate packing density was made with previous research conducted. Where our study demonstrates calibration with a compressive strength value of 45 MPa which approximately tallies with that of the 2010 fib model code [140], 3D and 2D mesoscale modeling results from Ren et al. [18]. The experimental results that were used to calibrate our model is as result of Xiao et al. [112] where the characteristics of the ITZ is studied using the nanoindentation technique. Figure 55 (bottom) demonstrates and compares the experimental ($\sigma - \epsilon$) of the 65% aggregate packing density for both NAC and RAC of Gonzalez et al. [141] which also demonstrated a compressive strength of ~41 MPa for NAC and ~38 MPa for RCA. This is completely reasonable as an increase in aggregate density leads to less mechanical properties which in this case represents a 5% increase.

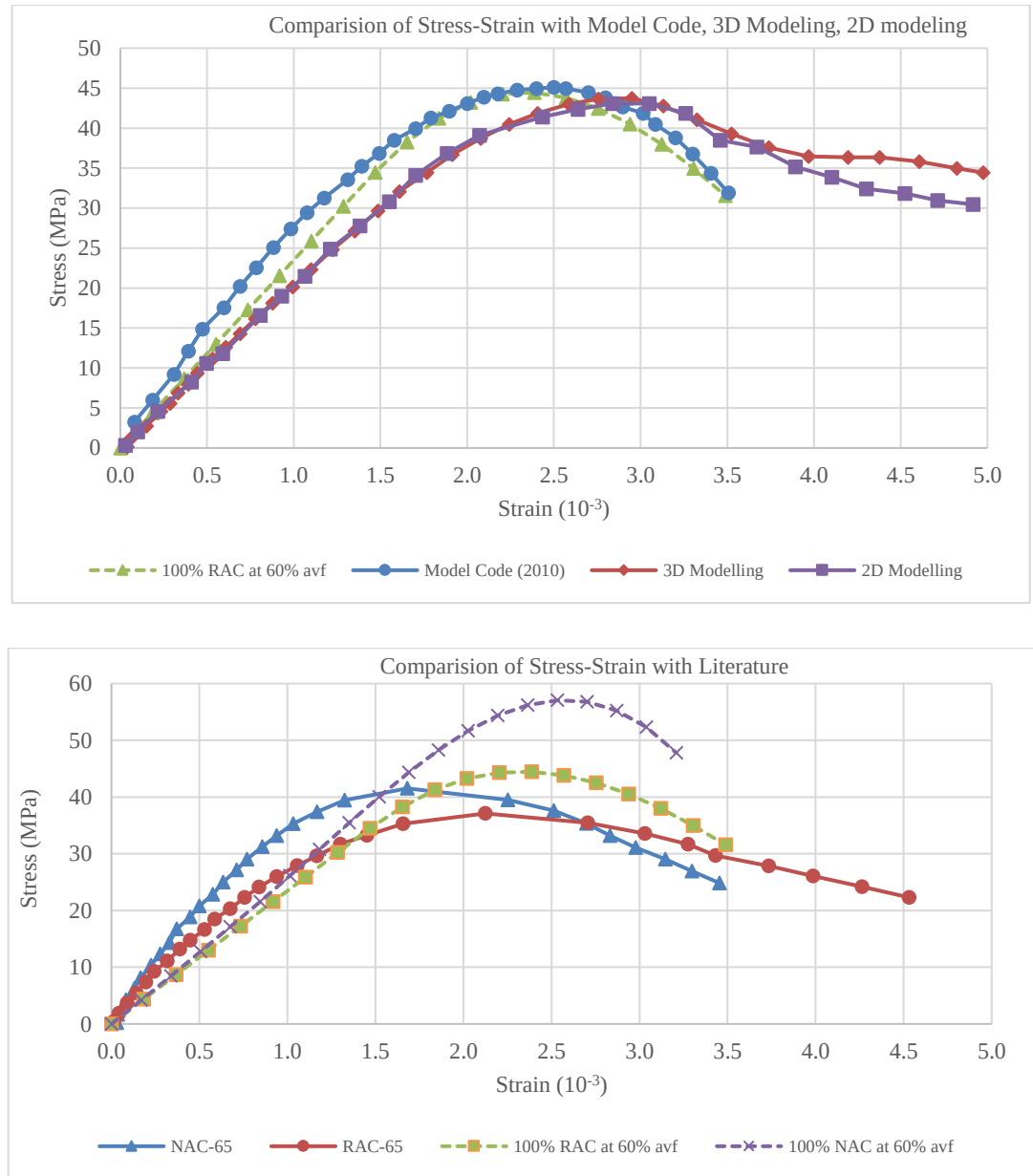


Figure 55. Comparison of simulated, experimental, fib code compressive tensile $\sigma - \epsilon$ relations of recycled aggregate concrete [18,112,141,142]

This aligns with some of the established theory in the study of recycled aggregate concrete from the previously reported studies, such as:

1. Both the upper and lower ends of the cubic specimen are quite intact compared to the other surfaces. This can be attributed to the Poisson effect, which is because of

triaxial confinement created by the friction between the sample and the loading plates [1], as illustrated in Figure 56.

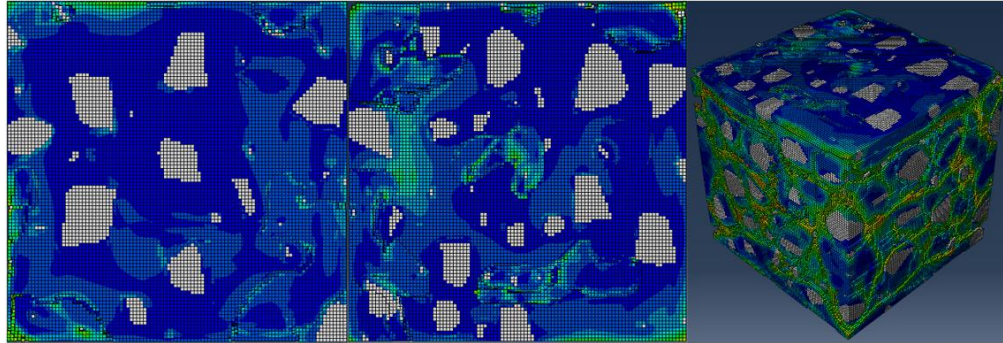


Figure 56. Less damaged upper and lower portions of cubic recycled aggregate concrete specimen.

2. The simulated sample exhibits angled cracks, as indicated in the sectional view in Figure 57. This type of cracking pattern is also observed in experimental results of Zhuo et al. [143] as shown in right after.

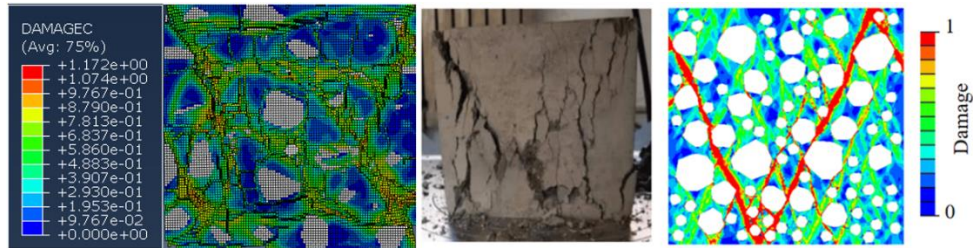


Figure 57. Angled cracks as demonstrated in the simulation and experiments of Zhuo et al. [143]

3. The primary damage of the simulated specimen occurs in the central region, which aligns with the expected outcome (e.g. BS EN 12390-3:2019). This is shown in Figure 58.

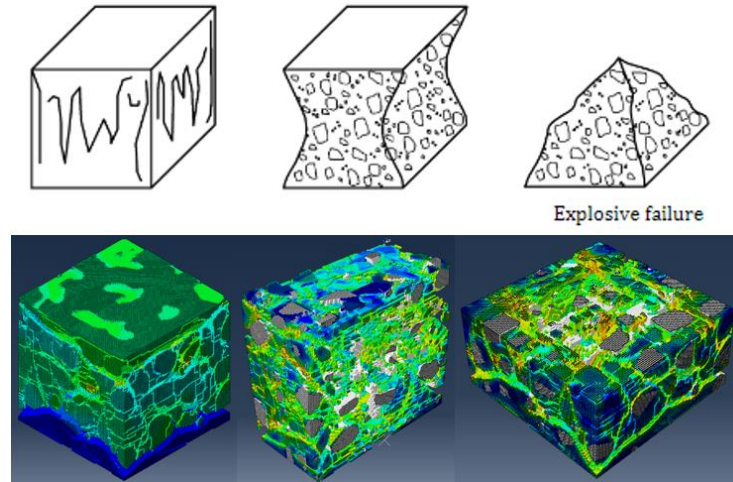


Figure 58. Uniaxial compression strength test failure pattern of simulated cubic sample (below) and that of BS EN 12390-3:2019 [144].

5.3 Comparison between the Simulated Uniaxial Tension Test with Experimental Results

Both the simulated (dotted lines) and fib Model Code [140] stress-strain relationships exhibit elastic behavior before reaching the peak stress, after which the tensile stress, σ_t , drops sharply. However, the stiffness (f_t) and failure strain values for the simulated recycled aggregate concrete are lower than those predicted by the fib Model Code except for the 50% aggregate volume fraction producing a similar tensile strength as that of the Model code. This discrepancy arises because the inclusion of recycled aggregate reduces both the tensile strength (f_t) and stiffness, as captured in the illustrious RCA incorporated work of Liu et al. [145], although at a lower aggregate packing density.

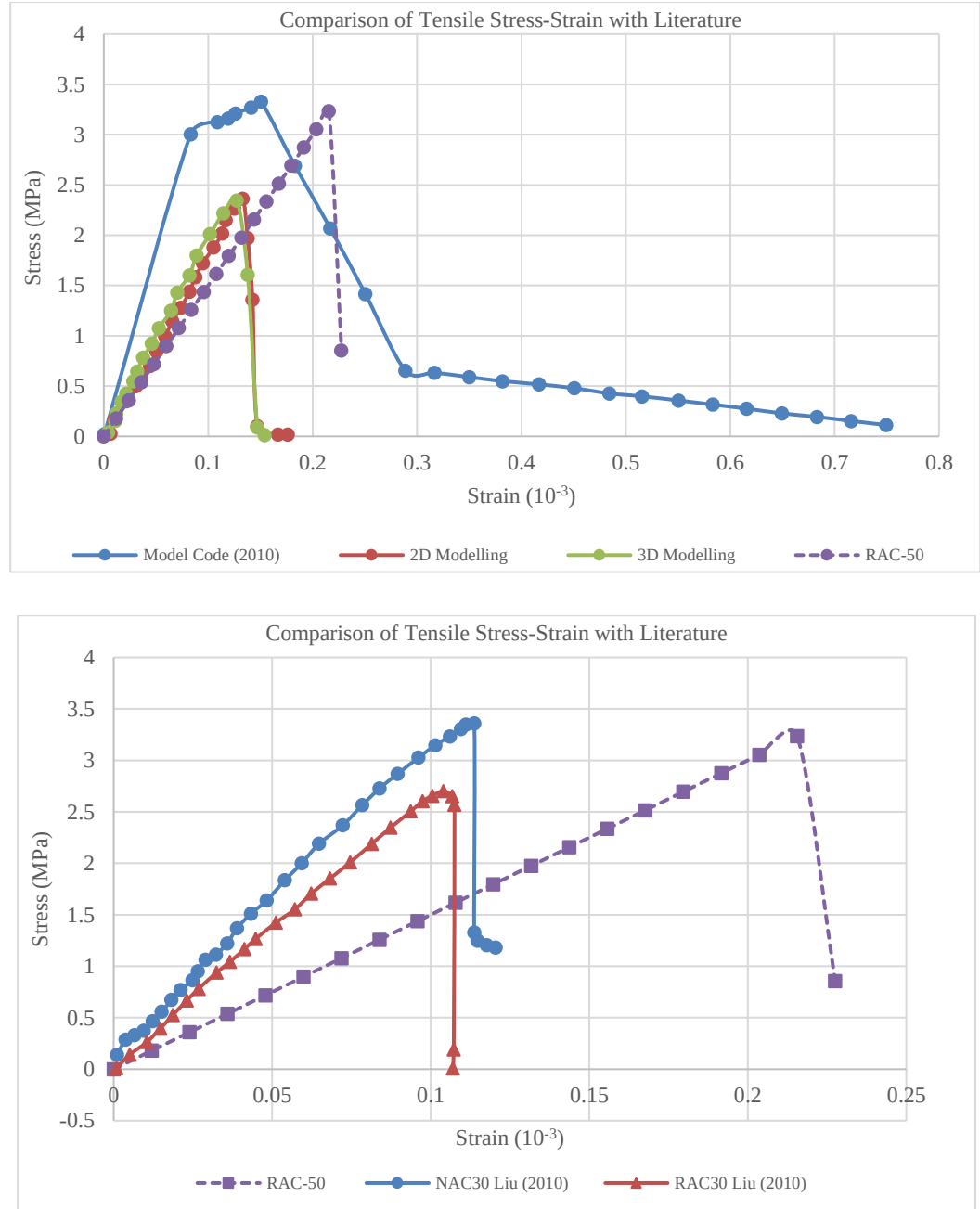


Figure 59. Uniaxial tensile strength test as available in fib Model Code [140], Liu et al. [145], Ren et al. [1] and this study simulated cubic concrete specimen.

5.4 Comparison between the Randomly Attached Mortar and Fully Enclosed Mortar of Simulated Specimens

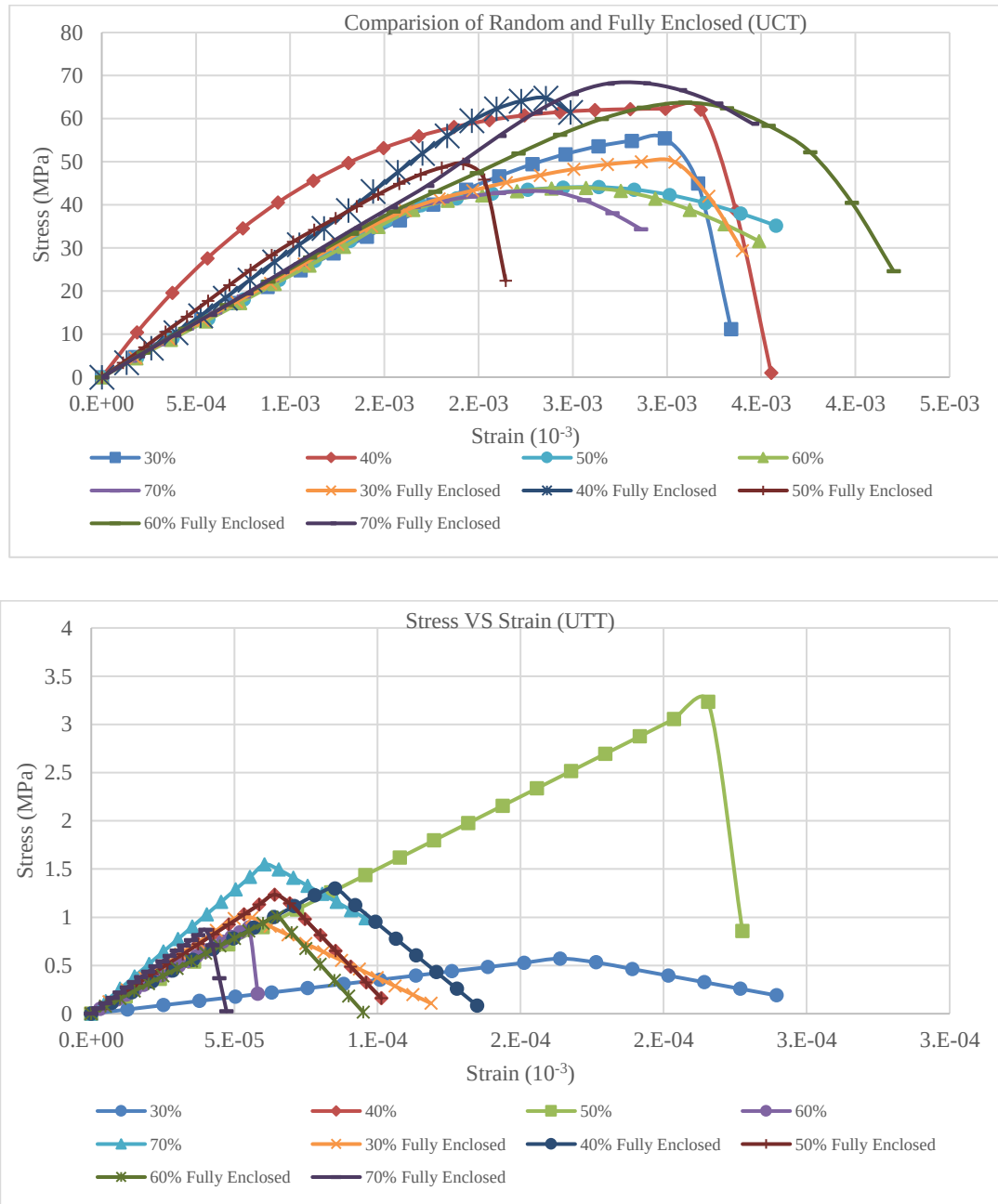


Figure 60. Randomly attached and fully enclosed simulation $\sigma - \varepsilon$ relationship in compression and tension.

Results show that mechanical behavior exhibited by the randomly attached and fully enclosed RCA were quite similar although the fully enclosed aggregate came out on top

with the highest compressive strength with a value of 70MPa close to the highest of 63MPa of the randomly attached mortar. Although the aggregates are fully enclosed with attached mortar of a **uniform** thickness, the randomly attached mortar had various thicknesses which could ultimately lead to a higher attached mortar content reducing mechanical strength.

5.5 Combination of Natural and Recycled Aggregate Concrete

To satisfy the final objective of this paper which is to study the mechanical response of our mesoscopic model by replacing a fraction of the recycled aggregate with natural aggregate. We did a 30%, 50%, and 100% replacement of recycled aggregate with natural aggregate to compare their response with established sources from the literature. According to Faisal et al. [146], as the RCA content increased, the mechanical properties of concrete worsened, suggesting that the decline in physical and mechanical properties negatively affected the hardened concrete. This deterioration is due to the porous mortar attached to RCA, which leads to higher water absorption, ultimately weakening the concrete's resistance to mechanical stresses compared to the control sample made with only natural aggregates.

Researchers such as Fan et al. [147], Pedro et al. [148], Pereira et al. [149], Kim et al. [150] and many more, who have studied the mechanical behavior of recycled aggregate while proportionately replacing the natural aggregate with RCA at different ratios have concluded that mechanical properties decrease with an increase in natural aggregate replacement. However, they also discovered that a replacement of the natural aggregate with about 30% had little effect on the mechanical properties of the concrete. This behavior is tacitly captured by our mesoscopic model where the 100% natural aggregates had a 59 MPa compressive strength followed by a 30% replacement of NCA with RCA as shown in Figure 60. The tensile response also expresses the same behavior, although it's not as apparent as that of compression. Our 100% NAC came out on top with a tensile strength of 1.6 MPa.

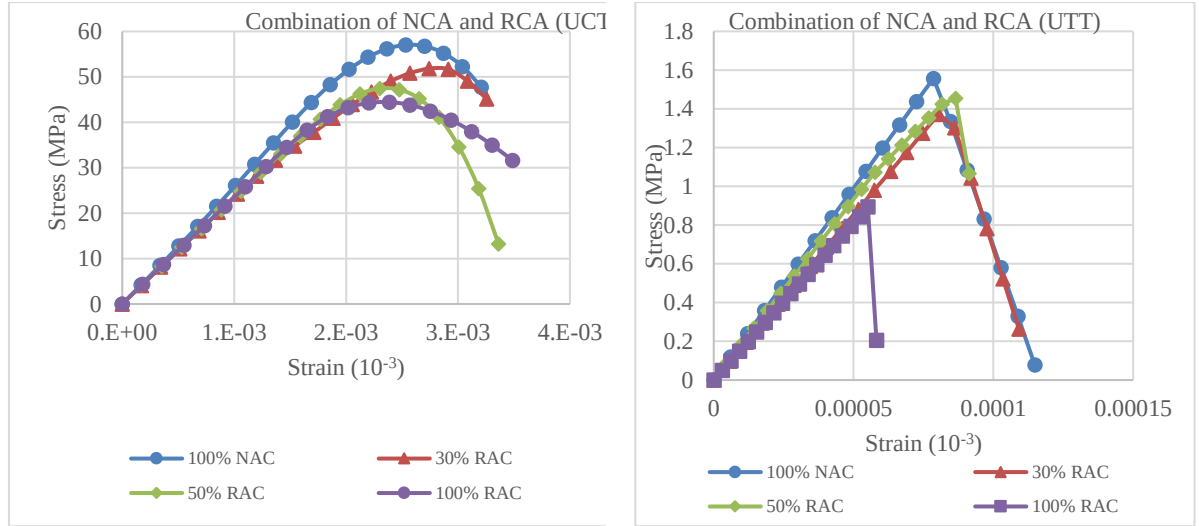


Figure 61. Randomly attached and fully enclosed simulation $\sigma - \varepsilon$ relationship in compression and tension.

This behavior is captured in various research as demonstrated in Table 7.

Table 7: Compressive strength of concrete at various replacement rates of recycled aggregate [146]

Reference	Concrete		Concrete Compressive Strength 28 days					
	Type	kg/m ³	0 %	5 %	25 %	30 %	50 %	100 %
Pedro et al. [148]	CEM 1 42.5N	380	59.3	-	-	57.1	58.8	54.8
Fan et al. [147]	OPC	449	56.3	-	51.4	-	47.4	37.8
Fan et al. [147]			56.3	-	53.3	-	51.3	49.6
Fan et al [147]			34.1	-	28.6	-	24.6	17.8
Fan et al. [147]			34.1	-	31.3	-	29.1	27.3
Kim et al. [150]	OPC	392	31.5	-	-	29.9	-	27.4
Pereira et al. [149]		350	39.5	-	-	38.6	37.6	38.6
Pereira et al. [149]			53.3	-	-	51	47.8	45.1
Pereira et al. [149]			65.2	-	-	65.4	63.2	63
Pliya et al. [151]	CEM 1	345	40	-	0	42	-	40.1
Kou et al. [152]			53.7	-	64.3	-	62.3	53.2

5.6 Comparison of the Efficiency of pyMesoscale with Existing Approaches

As mentioned earlier, spherical and ellipsoidal aggregates have been traditionally utilized in mesoscale modeling due to their generation efficiency and simplicity [12,59,139]. Yet, spherical and ellipsoidal particle shapes fail to accurately capture the stress concentrations present at the sharp edges of crushed aggregates [11]. Polyhedrons are used to model the true shape of crushed aggregate particles, capturing the local stress concentrations and crack initiation caused by their angular form and mechanical interlock [57]. However, they are known to have limitations, such as complex generation algorithms, high computational cost, experimental calibration difficulties, and parametrization [11,117]. However, this premise no longer holds as the pyMesoscale library has demonstrated the generation of polygonal aggregates at high aggregate volume fractions in lesser times available in previous literature. It also includes a computation segment for an additional element, i.e., attached mortar, which was not considered in some previous mesoscopic models. This phenomenon is shown in Table 8 and visualized in Figure 62.

Table 8: Comparison of computation time vs aggregate volume fraction of pyMesoscale with popular mesoscale generation methods from literature [110].

Aggregate Content	Voronoi-based methods	Traditional random aggregate method			Local Background grid method	pyMesoscale
		Generation	Meshing	Total		
15	817	101	157	258	4	122
20	2518	135	221	356	5	128
25	-	216	290	506	8	149
30	-	407	344	751	12	138
35	-	1080	420	1500	20	154
40	-	2708	501	3209	50	142
45	-	5087	651	5738	153	140
50	8936	-	-	-	763	152
60	-	-	-	-	-	164
70	-	-	-	-	-	182

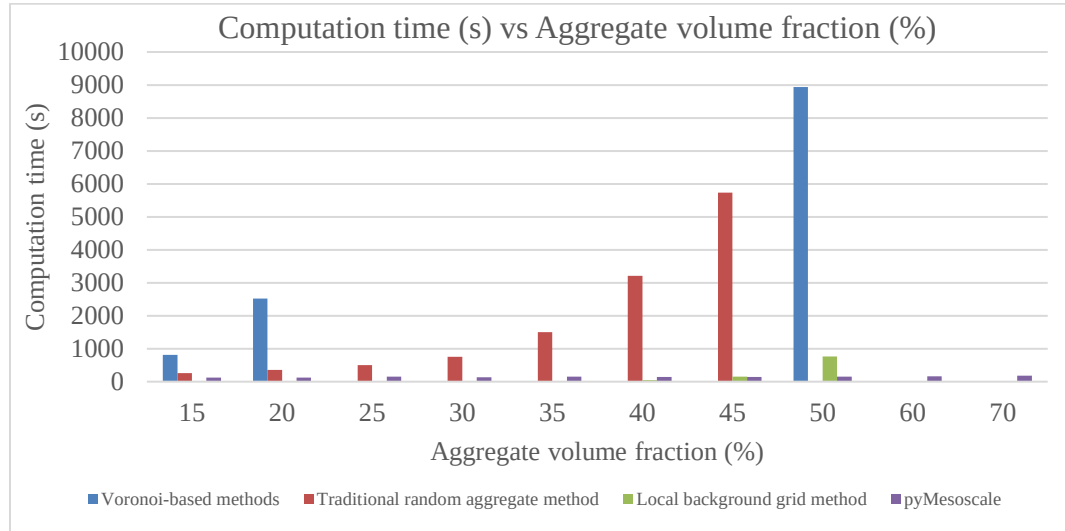


Figure 62. Computation time vs aggregate volume fraction of pyMesoscale and other mesoscale generation techniques [110].

The foundational objective of this study was to implement an efficient way of generating mesoscale models for recycled aggregate concrete. This has been achieved by employing the low-level tensor manipulation library NumPy within the Python programming environment, resulting in a much better generation time compared to previous work, as reported by Ouyang et. al [110] and illustrated in Figure 61. In addition to pyMesoscale not exhibiting an exponential generation time increase with increasing aggregate packing density, it also generates mesoscopic models in an import-ready format for simulations on the Abaqus CAE platform.

CHAPTER 6

CONCLUSION AND RECOMMENDATIONS

6.1 Conclusions

This study aimed to develop an efficient method for generating 3D recycled aggregate mesoscopic models, leading to the development of the pyMesoscale Python library. Mesoscopic models incorporating varying aggregate volume fractions, and random and fully attached mortar configurations were investigated and validated using experimental data and literature on combined blends of natural and recycled aggregates. The key conclusions derived from this study are summarized as follows:

- 1) The developed pyMesoscale Python library, utilizing the local-background-grid method, demonstrated exceptional efficiency in generating mesoscopic models of polyhedral aggregates at high packing densities. This achievement marks a significant advancement, overturning prior claims about the intractability of packing polyhedral aggregates to high densities. Advances in computing power, graphics card performance, and cloud-based interactive development environments, such as Google Colab, have been pivotal in enabling this breakthrough.
- 2) This study found that increasing the proportion of recycled concrete aggregate (RCA) as a replacement for natural aggregate (NA) reduces the compressive load-carrying capacity. However, 30–40% replacement levels result in only modest strength reductions, making them suitable for practical applications.
- 3) For the randomly attached mortar (AM) cases, the 40% aggregate packing density achieved the highest compressive strength. However, the 60% and 70% packing densities also exhibited relatively high strength despite their greater AM content. This behavior reflects the interplay between two opposing factors: increased

attached mortar content, which reduces mechanical strength, and higher aggregate packing density, which enhances it.

- 4) Models with fully encircled RCA exhibited higher compressive strength than their randomly attached mortar (AM) counterparts. This can be attributed to the lower aggregate content, though it may seem counterintuitive. The encircled attached mortar forms a uniform thickness across the aggregate surface, whereas in real-life RCAs, the attached mortar (AM) varies in thickness and adheres to parts of the surface, leading to a greater AM volume. The results from the randomly attached mortar model more closely matched experimental data from the literature, suggesting it provides a more accurate representation.
- 5) Damage initiation, propagation, and interlocking primarily occur in the attached mortar and interfacial transition zone (ITZ) due to their relatively weaker mechanical properties. However, the recycled aggregate concrete (RAC) continues to carry the load until significant cracks have interlocked, forming larger cracks that ultimately lead to failure. This finding aligns with established literature.

6.2 Recommendations

The following are some recommendations for some opportunities for further research in this area:

- 1) The developed library is currently limited to cubical specimen models and does not account for the vertical aggregate segregation phenomenon. It is recommended that future research extend the library to include more complex specimen shapes and incorporate the vertical segregation phenomenon to better reflect real-world conditions.
- 2) Additionally, it is recommended that future studies explore alternative methods, such as motion simulation techniques, and compare their computational speed with that of the local-background-grid method.
- 3) Further studies could consider how environmental factors, such as temperature and moisture content, influence the behavior of recycled aggregate concrete (RAC) models, as these factors play a significant role in real-world applications.
- 4) Investigating advanced models for the interfacial transition zone (ITZ) between the recycled aggregate and mortar could provide a more accurate representation of the material behavior, especially under stress and during cracking.
- 5) It may also be valuable to investigate the long-term durability of RAC using your mesoscopic models, especially under cyclic loading or in aggressive environments, to understand how the material behaves over time.

CHAPTER 7

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Publications

1. Influence of Bonded Mortar on Recycled Aggregate Concrete Properties: A reviewPublished on the 20th of May, 2024. Construction and Building Materials, Elsevier.
2. pyMesoscale: A friendly python library for generating 3D concrete mesoscale models. Accepted for publication, oral presentation and Poster Session at the 16h World Congress on Computational Mechanics / 4th Pan American Congress on Computational Mechanics (WCCM2024) to be held July 21-26, 2024 in Vancouver, BC, Canada.

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