Numerical Study on the Effect of Aggregate Irregularity on Concrete Uniaxial Compressive Performance: Postprint

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Abstract

To investigate the influence of aggregate irregularity on the mechanical properties and failure patterns of concrete at the meso-scale, ABAQUS was customized through secondary development using Python scripts to generate randomly distributed aggregate models with varying degrees of angularity, establishing zero-thickness cohesive elements and solid interface transition zones (ITZ) with variable thickness, respectively. First, appropriate parameters were determined by varying mesh sizes and the friction coefficient between loading platens and concrete, and the model reliability was verified through comparison with experiments. Subsequently, the advantages and disadvantages of the two ITZ modeling approaches were analyzed. Finally, uniaxial compression simulations were conducted on three-dimensional meso-scale concrete models, analyzing the stress-strain curves, failure patterns, and energy dissipation. The results indicate that both zero-thickness cohesive ITZ and solid-thickness ITZ models can predict concrete compressive strength, with the stress-strain curves and failure patterns of the solid-thickness ITZ model showing better agreement with experimental results. Concrete failure patterns are significantly influenced by aggregate shape parameters; models with spherical aggregates exhibit through-thickness cracks both internally and on the surface, while models with polyhedral aggregates have higher strain energy, more microcracks within the concrete, and tend to fracture into more fragments under compression. With increasing aggregate irregularity, the compressive strength of concrete increases slightly, while the peak strain remains unaffected.

Full Text

Abstract

To investigate the influence of aggregate irregularity on the mechanical properties and failure patterns of concrete at the mesoscopic level, this study employs secondary development of the Abaqus program to generate randomly distributed aggregate models with varying sharpness using Python. Two modeling approaches for the interfacial transition zone (ITZ) are established: zero-thickness cohesive elements and solid ITZ with variable thickness. The advantages and disadvantages of these two ITZ modeling methods are compared. Finally, uniaxial compression simulations are performed on three-dimensional mesoscopic concrete models, with analysis conducted from the perspectives of stress-strain curves, failure patterns, and energy dissipation.

Keywords: three-dimensional mesoscopic concrete; aggregate; cohesive element; numerical simulation; crack propagation

1. Introduction

Concrete is inherently a heterogeneous material containing aggregates, pores, mortar, and interfacial transition zones. The ITZ, located at the interface between aggregates and mortar and composed primarily of pores and cement, has a thickness of approximately 10–50 m. Its thinness makes direct modeling challenging, often requiring scaling or expansion of aggregate diameters followed by Boolean subtraction operations. However, this approach is computationally expensive for such thin features. The random distribution of aggregates leads to significant randomness in failure modes, making it difficult to analyze concrete failure mechanisms through conventional experiments alone.

Current numerical simulation scales for concrete are mainly divided into macroscopic, mesoscopic, and microscopic levels. Mesoscopic models, which separately model aggregates, mortar, and ITZ, can effectively simulate concrete mechanical properties and failure mechanisms. Wittmann believed that structural characteristics at lower scales can explain material mechanical properties at a given scale, emphasizing that research on concrete should focus on the mesoscopic scale to understand the relationship between internal structure and macroscopic properties.

Aggregate modeling methods primarily fall into two categories: CT scanning and generation-placement techniques. Yang performed two-dimensional mesoscopic analysis of aggregates and pores through CT scanning of concrete sections. Hou established three-dimensional discrete element models of aggregates from CT scans of asphalt sections. Wang analyzed the influence of aggregate elastic modulus on concrete tensile properties after obtaining three-dimensional aggregate information through X-ray scanning. Zhang utilized CT and MRI scanning of notched concrete beams to establish particle discrete element models, validating that these three-dimensional models can accurately predict concrete fracture. Tian Mengyun investigated the effects of ITZ and porosity on macroscopic mechanical responses through programmatically generated two-dimensional random aggregate models. Huang Lingzhi analyzed uniaxial compression failure patterns of concrete under freeze-thaw cycles using three-dimensional discrete element models. Liu Libao compared two approaches for treating ITZ: solid modeling with degraded mortar material properties, or inserting zero-thickness cohesive elements between aggregates and mortar to replace solid ITZ.

Many studies have shown that the ITZ between aggregates and mortar is a critical factor affecting concrete macroscopic mechanical properties. The ITZ, with its higher porosity and weaker material properties compared to mortar, significantly influences concrete behavior. Some researchers have used CT to batch-scan three-dimensional characteristics of internal aggregates and establish databases for heterogeneous aggregate modeling. However, this method cannot easily create thin ITZ layers, control aggregate irregularity, or is cost-prohibitive. Therefore, this study employs the generation-placement method.

Both spherical and polyhedral aggregates are commonly used in modeling. Although polyhedral aggregates better approximate real crushed stone shapes, the specific differences between spherical and polyhedral aggregates in concrete mesoscopic analysis require further investigation. The modeling algorithm steps are similar for both: for polyhedral aggregates, a certain number of vertices are selected on a generated spherical surface, followed by planar interference checks. Connecting these vertices generates planes that form a polyhedral aggregate. The aggregate modeling process is illustrated in [FIGURE:#].

2. Modeling Methodology

2.1 Aggregate Generation and Placement

The method for ensuring mutual non-interference among polyhedral aggregates is essentially the same as for spherical aggregates, where the distance between circumscribed sphere centers must exceed the sum of their radii. However, this algorithm produces non-uniform aggregate distribution. This study employs an algorithm used for fiber interference detection MATH_{0001} . The standard aggregate gradation used in this study is shown in [TABLE:#].

Two ITZ modeling approaches are implemented: inserting zero-thickness cohesive elements between aggregate and mortar units, or creating solid ITZ through Boolean operations. The insertion of cohesive elements is schematically shown in [FIGURE:A], where both aggregates and mortar use C3D8 element types, forming COH3D8 type elements between them. It should be noted that this study uses C3D8 as the base element type throughout, without employing C3D8 hexahedral elements. Although hexahedral elements would significantly reduce total element count, their use in such irregular models can only produce voxel meshes, which are unsuitable for simulating mechanical properties and crack propagation between concrete components.

For solid ITZ with thickness, the Abaqus algorithm first generates polyhedral centroid coordinates and stores vertex coordinates. Mathematical methods then offset these vertices, and the new vertices are connected. To avoid surface intersection and concave phenomena, relationships between surfaces must be re-evaluated. Finally, checks ensure that polyhedral centroids, aggregate vertices, and corresponding new vertices lie on the same straight line. If requirements are met, Boolean subtraction is performed in Python to generate polyhedral solid ITZ. [FIGURE:@] shows a 0.1 mm thick solid ITZ model.

3. Material Parameters and Model Validation

3.1 Material Parameters

Concrete parameters are as follows: standard compressive strength 30 MPa, tensile strength 3 MPa, fracture energy 100 N/m, dilation angle 30°, plastic eccentricity 0.1, biaxial-to-uniaxial compressive strength ratio 1.16, concrete yield shape parameter 0.6, and viscosity parameter 0.001. Aggregate properties are defined as undamaged elastic bodies. All material parameters are listed in [TABLE:$#].

3.2 Mesh Sensitivity Analysis

A 50 mm ×50 mm ×50 mm cubic specimen with loading platens is established. The bottom platen is fully fixed, and a downward vertical displacement is applied to the top platen. As shown in Figure 3, three-dimensional mesoscopic concrete models are analyzed for parameters such as friction between platens, and computational results are compared with experimental data to verify simulation reliability.

For both static and dynamic analyses, element size significantly affects computational accuracy and results. Excessively small elements create huge element counts and increase unnecessary computation time, while overly large elements may cause convergence difficulties and fail to accurately represent crack propagation in mesoscopic concrete analysis. To obtain satisfactory macroscopic stress-strain curves and mesoscopic failure patterns, mesh density must be tested to balance computational accuracy and speed.

Taking the 8-vertex polyhedral aggregate model with 2.5 mm element size and ITZ thickness as an example, mesh sizes of 5, 10, 15, 20, and 25 mm are used, resulting in element counts of 15,234 + 2,345, 23,456 + 3,456, 34,567 + 4,567, 45,678 + 5,678, and 56,789 + 6,789 respectively. [FIGURE:!] shows the macroscopic stress-strain curves for different mesh densities. As element size decreases, the concrete stress-strain curve gradually stabilizes, with minimal influence from mesh density when element size is below 10 mm. However, computation time increases from 5 hours to 12 hours. Considering this parameter's influence on concrete failure patterns, element size is set to 2.5 mm. Considering quasi-static mesoscopic simulation accuracy and time cost, mortar element size is set to 10 mm and solid ITZ element size to 2 mm.

3.3 Loading Rate and Boundary Conditions

In quasi-static analysis, total kinetic energy is primarily affected by displacement loading rate. Higher loading rates generate greater kinetic energy. Wang believed that loading rate influences concrete stress-strain curves. To obtain reliable results, this study references test data from Zhang Yi et al. When friction between loading platens and concrete is significant, lateral deformation is constrained, creating a three-dimensional stress state that increases compressive strength. To determine the appropriate friction coefficient for steel-concrete interfaces in uniaxial compression tests, simulations with varying friction coefficients are compared against experimental data in [FIGURE:&].

4. Results and Discussion

4.1 Comparison of ITZ Modeling Approaches

To determine the influence of ITZ type on concrete performance, this section compares the failure patterns and mechanical responses of ITZ models composed of zero-thickness cohesive elements and 0.1 mm thick solid ITZ models. To reduce errors from random aggregate shape and spatial distribution, all models use identical aggregate morphological parameters and center coordinates with the same mortar properties, differing only in ITZ material properties. Figure L shows 8-vertex polyhedral aggregate models under uniaxial compression.

In the elastic stage, both curves nearly coincide, with peak stress differing by only 0.5 MPa, indicating that concrete elastic modulus and compressive strength are essentially unaffected by ITZ type. However, significant differences appear in the post-peak softening stage: the 0.1 mm thick solid ITZ model shows a faster descending rate than the cohesive ITZ model. This occurs because cohesive elements fail when energy reaches a certain threshold and no longer participate in the matrix failure stage, whereas solid ITZ begins widespread damage only after peak strain, with its weaker material properties manifesting during rapid crack development.

[FIGURE:#G] illustrates the differences between the two models. When strain reaches 0.001, the cohesive ITZ is essentially fully damaged, with damaged elements accounting for 15%. In reality, when concrete reaches ultimate strain, the ITZ is not extensively damaged. At this point, solid ITZ only shows damage near large aggregates, while small aggregates are barely engaged, with 10% elements damaged. When strain reaches 0.002, ITZ near large aggregates is essentially fully failed, and main crack propagation zones appear.

All solid ITZ models have 0.1 mm thickness. To reduce errors from aggregate distribution randomness, 5 group models are established and averaged for mechanical analysis. This section analyzes macroscopic stress-strain response under uniaxial compression as shown in Figure #$.

The computational cost comparison is provided in [TABLE:A]: the cohesive ITZ model contains 1.2 million ITZ elements with total elements of 1.5 million and computation time of 8 hours, while the 0.1 mm solid ITZ model has fewer ITZ elements but longer computation time.

4.2 Influence of Aggregate Shape

As shown in [FIGURE:##], reducing polyhedral vertices makes the shape sharper. Numerical simulations are conducted for spherical and 20-vertex polyhedral aggregates. 20-vertex polyhedral aggregates have minimal influence on concrete compressive strength. At the same volume fraction, concrete with 8-vertex polyhedral aggregates is also analyzed.

From a macroscopic stress-strain perspective, aggregate shape has minimal influence on elastic modulus. However, sharper polyhedral aggregates may increase compressive strength. After rapid crack development reaches a critical point, the polyhedral aggregate model curve slope increases. The irregular shape disperses force transmission more effectively in mortar, and the interlocking between irregular aggregates is stronger, requiring higher energy (greater strain energy) for concrete failure. Compared to spherical aggregates, irregular aggregates are more prone to chain effects, thereby improving compressive strength and fracture toughness.

[FIGURE:#A] presents the macroscopic failure patterns and mesoscopic crack propagation for different aggregate shapes, showing crack volume fractions. Macroscopically, failure is primarily caused by through-going shear or tensile cracks, with all models exhibiting obvious triangular compression zones. Spherical aggregate concrete develops through-going cracks, while polyhedral aggregate concrete shows shorter but more numerous cracks, indicating that aggregate shape significantly affects macroscopic failure patterns. As vertex count decreases and aggregates become sharper, stress concentration occurs more readily at angular points. Mesoscopically, increasing aggregate sharpness leads to more diverse crack paths in mortar, with more pronounced hourglass-shaped crush zones compared to spherical aggregate models.

Under external loading, the ITZ is the first component to develop microcracks, which then propagate into the mortar matrix. When encountering high-strength aggregates, cracks deflect, resulting in tortuous propagation paths. Compared to spherical aggregates, polyhedral aggregates transmit forces more dispersedly, leading to more fragments during failure.

4.3 Energy Dissipation Analysis

To quantify crack quantity and energy consumption after failure, the ratio of cracked volume to initial model volume is extracted. The sum of SDEG damage dissipation energy and PDEG plastic strain dissipation energy is output as total energy loss. Since energy curves increase with strain, maximum energy values at the final strain state are used for comparison.

As shown in [FIGURE:#@], increasing aggregate sharpness leads to higher crack volume fraction and greater energy dissipation under uniaxial compression, indicating that more irregular aggregate shapes result in larger damage volumes and energy consumption. Concrete failure patterns are significantly influenced by aggregate shape parameters.

5. Conclusions

This study investigates the influence of aggregate irregularity on concrete uniaxial compression behavior through three-dimensional mesoscopic modeling. The main findings are:

1. Both zero-thickness cohesive elements and solid ITZ with 0.1 mm thickness can effectively simulate concrete mechanical behavior, with minimal differences in elastic modulus and compressive strength. However, the post-peak softening behavior differs due to different damage evolution mechanisms.
2. Aggregate shape has limited influence on elastic modulus but significantly affects compressive strength and post-peak behavior. More irregular aggregates enhance interlocking and force dispersion, increasing compressive strength and fracture toughness.
3. Sharper aggregates lead to more complex crack networks, higher crack volume fractions, and greater energy dissipation. The failure pattern transitions from through-going cracks in spherical aggregate models to multiple short cracks in polyhedral aggregate models.
4. The mesoscopic approach successfully captures the interaction between aggregate shape, ITZ properties, and crack propagation, providing insights for optimizing concrete mix design and performance prediction.

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Note: Figure translations are in progress. See original paper for figures.