

Three-Dimensional Multi-Phase Microscopic Simulation of Service Life of Recycled Large Aggregate Self-Compacting Concrete

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Abstract

Recycled large aggregate self-compacting concrete (RLA-SCC) within multiple weak areas. These weak areas have poor resistance to chloride ion erosion, which affects the service life of RLA-SCC in the marine environment. A three-dimensional multi-phase mesoscopic numerical model of RLA-SCC was established to simulate the chloride ions transportation in concrete. Experiments of RLA-SCC immersing in chloride solution were carried out to verify the simulation results. The effects of recycled large aggregate (RLA) content and RLA particle size on the service life of concrete were explored. The results indicate that the mesoscopic numerical simulation results are in good agreement with the experimental results. At the same depth, the closer to the surface of the RLA, the greater the chloride ion concentration. The service life of RLA-SCC in marine environment decreases with the increase of RLA content. Compared with the service life of 20% content, the service life of 25% and 30% content decreased by 20% and 42% respectively. Increasing the particle size of RLA can effectively improve the service life of RLA-SCC in chloride environment. Compared with the service life of 50 mm particle size, the service life of 70 mm and 90 mm increased by 61% and 163%, respectively.

Keywords

Recycled Large Aggregate Self-Compacting Concrete, Mesoscopic Mode, Chloride Ion Diffusion, Numerical Analysis

1. Introduction

RLA-SCC is developed on the basis of rockfill concrete and recycled concrete. It

inherits the advantages of small amount of cement in rockfill concrete and no need to vibrate. At the same time, it can effectively utilize waste concrete resources and reduce environmental pollution. Therefore, it has a very broad application prospect.

Chloride ion erosion accelerates the corrosion of steel bars, which leads to a decrease in the service life of concrete [1]. It eventually leads to concrete cracking and spalling, affecting the overall stability and safety of reinforced concrete structures. The content of chloride ion in the marine environment is more, and the corrosion of reinforced concrete structures is more serious [2]. In the marine environment, the durability failure of reinforced concrete structures is very common. The structure has been seriously aged before reaching the design service life and cannot be used normally, which has caused huge economic losses.

Recycled aggregate has low strength, high water absorption [3] [4], many micro-cracks and porosity, which leads to poor resistance to chloride ion erosion of recycled concrete. The service life of recycled concrete is shorter than that of natural concrete, which is not conducive to its application in marine environment. At present, many studies on RLA-SCC mainly focus on mechanical properties [5] [6], while there are few studies on chloride ion transportation. Due to the limitation of time, it is difficult to study the long-term chloride ion transportation in concrete by physical experiments. Therefore, this research established a numerical model of RLA-SCC, and uses COMSOL Multiphysics to simulate the influence of particle size of RLA on the service life of RLA-SCC.

2. Three-Dimensional Multiphase Mesoscopic Model

RLA-SCC is divided into natural aggregate, old interfacial transition zone (ITZ), old mortar, new ITZ, self-compacting concrete (SCC) five-phase materials.

2.1. Theory of Chloride Ion Transportation

Concrete structure is immersed in the ocean for a long time and is completely saturated. Chloride ion transportation is generally dominated by diffusion. The diffusion equation is expressed by Fick's second law [2], and its expression is shown in Equation (1).

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \,. \tag{1}$$

where: *C* is chloride ion concentration, g/m^3 ; *t* is time, s; *x* is the distance between the calculated position and the diffusion surface, m; *D* is chloride diffusion coefficient, m^2/s .

With the increase of concrete age, the hydration continues to make the chloride ion diffusion coefficient decay with time [7]. The chloride diffusion coefficient D(t) was calculated by Equation (2).

$$D(t) = D_0 \cdot \left(\frac{t_0}{t}\right)^m.$$
 (2)

where: D_0 is the initial diffusion coefficient; t_0 takes 28 days; *m* is the age attenu-

ation coefficient, which is 0.44 in this research.

For the mesoscopic model of recycled concrete [8], the initial chloride ion diffusion coefficients of different parts are shown in **Table 1**.

In this research, the SCC wrapped outside the RLA is regarded as a homogeneous phase, and the initial chloride ion diffusion coefficient [7] is calculated by Equation (3).

$$D_{scc,0} = 10^{\left[1.776 + 1.364(W/B)\right]} + \left[5.806 - 18.69(W/B)\right] \left[FA\right].$$
 (3)

where: *W/B* is water binder ratio; [*FA*] is the content of fly ash, %. In this research, the initial chloride diffusion coefficient of SCC is $5.18 \times 10^{-12} \text{ m}^2 \cdot \text{s}^{-1}$.

2.2. Three-Dimensional Multiphase Meso-Stochastic Model

The mesoscopic model size of RLA-SCC is $450 \text{ mm} \times 450 \text{ mm} \times 450 \text{ mm}$, and the particle size is 40 - 100 mm. Based on the Fuller grading curve, the particle size of the aggregate is calculated, and the Monte Carlo method is used to put the aggregate. According to Equation (4), it is judged that the aggregate does not intersect and ends the delivery.

$$\sqrt{\left(x_{i}-x_{j}\right)^{2}+\left(y_{i}-y_{j}\right)^{2}+\left(z_{i}-z_{j}\right)^{2}} \geq \eta\left(r_{i}+r_{j}\right).$$
(4)

where: $(x_{\rho}, y_{\rho}, z_i)$ is the spherical center coordinate of the ith aggregate; r_i is the radius of the ith aggregate; η is the influence range coefficient of aggregate, which is 1.05 in this research.

The equivalent thickness h of the old mortar layer is shown in Equation (5).

$$h = 0.5a \left(1 - \sqrt[n]{1/1 + \overline{\omega}} \right). \tag{5}$$

where: *a* is particle size of aggregate; *n* is the dimension of the model; $\overline{\omega}$ is the ratio of old mortar volume to aggregate volume.

The thickness of the new and old interfacial transition zone of recycled concrete is between 20 - 100 μ m. Considering the size of RLA, the thickness of the ITZ is 100 μ m [9]. Three-dimensional multiphase meso-stochastic model is shown in **Figure 1**.

3. Experiment and Numerical Simulation

3.1. Experimental Materials

The waste aggregates were selected as the concrete pouring material, and the aggregate content was 30% (volume ratio). The basic performance test results of waste concrete aggregate are shown in **Table 2**.

Ordinary Portland cement and grade I fly ash were used as cementing materials in the research. Coarse aggregate chooses gravel with good gradation.

Table 1. Initial chloride diffusion coefficient of different components $[10^{-12} \text{ m}^2 \cdot \text{s}^{-1}]$.

Old Mortar	Old ITZ	New ITZ	Natural Aggregate
30	450	90	0

The particle size distribution is between 5 - 10 mm. Its apparent density is 2680 kg/m³. The fine aggregate is natural river sand, and the fineness modulus is 2.91. 2% polycarboxylate superplasticizer was selected as the admixture. Its water reduction rate is 5%. The mix proportion of SCC is shown in **Table 3**.

3.2. Experimental Method

The RLA-SCC test block with a size of 450 mm \times 450 mm \times 450 mm was made. After curing at room temperature for 28 days, the above concrete test block was cut into a cube test block of 150 mm \times 150 mm \times 150 mm, as shown in **Figure 2**.

The flat surface was taken as the chloride ion erosion surface, and the remaining

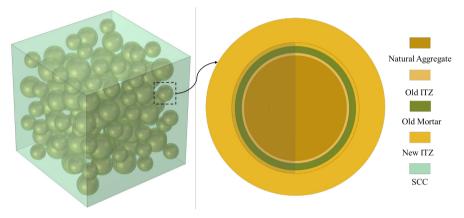


Figure 1. Three-dimensional multiphase meso-stochastic model.

Table 2. Basic properties of waste concrete aggregate.

Particle size [mm]	Apparent density	Water absorption	Concrete strength
	[kg/m³]	[%]	[MPa]
40 - 100	2.30 - 2.65	2.6 - 3.9	27.5

Table 3. The mix proportion of SCC [kg/m³].

Cement	River Sand	Gravel	Fly Ash	Admixture	Water
348	785	860	147	6.96	213



Figure 2. Test cube.

surfaces were smeared with epoxy resin. After being completely immersed in NaCl solution (mass fraction of 5%) for 180 days, the test blocks were taken out and dried in the sun. Four points were selected on the chloride ion erosion surface, and the powder sample was taken every 5 mm borehole inward. Weigh 3 g powder samples at the same depth in 30 ml of distilled water and stir well. The free chloride ion concentration of each sample was tested by a rapid chloride ion content detector.

3.3. Model Validation

The comparison between the simulated data and the experimental data is shown in **Figure 3**. It can be seen from the graph that the distribution of chloride ion in concrete shows a downward trend along the depth direction, which is consistent with the experimental data. Before 20 mm, the chloride ion concentration of the simulated data is more than that of the experimental data. After 20 mm, the simulated data is less than the experimental data. The numerical simulation results of the model are in good agreement with the experimental data. The proposed multiphase mesoscopic chloride ion diffusion model of RLA-SCC has high reliability.

The concentration distribution of chloride ion at service age of 100 a is shown in **Figure 4**. It can be seen that the chloride ion concentration near the RLA is higher. This is due to the Old ITZ, new ITZ and the old mortar around the RLA are conducive to the formation of rapid diffusion channels, which accelerates the erosion of chloride ion.

4. Analysis of Influencing Factors on Service Life of Concrete

The effects of coarse aggregate on the diffusion of chloride ion in concrete mainly include tortuosity effect and ITZ effect. The tortuosity effect hinders the diffusion of chloride ion. The ITZ effect accelerates the diffusion of chloride ion. This research mainly studies the influence of RLA content and particle size on

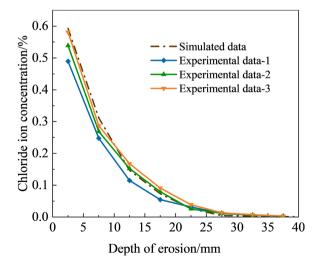


Figure 3. Comparison of simulated data and experimental data.

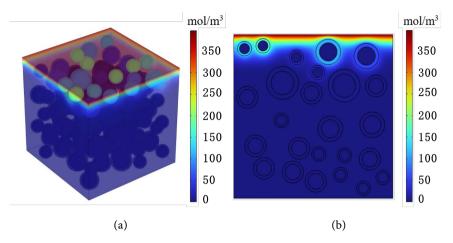


Figure 4. Concentration distribution of chloride ion at service age of 100 a: (a) whole model; (b) model cross section.

the service life of RLA-SCC. Considering the need of safety reserve of concrete structure, the time of steel bar depassivation is taken as the time node of durability failure limit state of RLA-SCC. The thickness of the protective layer is 60 mm. The critical chloride ion concentration that causes the surface of the steel bar to depassivate in concrete is 0.5% (42.74 mol/m³) of the cementitious material [10]. The chloride ion concentration on the surface of concrete is related to the environmental conditions, the water-binder ratio of concrete and the type of cementitious materials. The expression of the mean value [11] is shown in Equation (6).

$$C_s = A_c \cdot (W/B). \tag{6}$$

where: A_c is the fitting coefficient, which is 10.8% in this research; W/B is water binder ratio. The surface chloride concentration C_s is expressed by the relative ratio of the mass of the cementitious material in each square of concrete.

4.1. Effect of Recycled Large Aggregate Content on Service Life

Considering the influence of different RLA content, two groups of models with aggregate contents of 20%, 25% and 30% were set up respectively. In each group of models, only the random placement positions of RLA are different, and the aggregate gradation is the same. A set of model settings is shown in **Figure 5**.

Figure 6 shows the change of chloride ion concentration with time in different aggregate content. With the increase of diffusion time, the concentration of chloride ion is increasing. Under the same thickness of protective layer, the service life of concrete decreases with the increase of aggregate content. When the protective layer thickness is 60 mm, the service life of RLA-SCC with 20%, 25% and 30% RLA content is 25.1, 20.2 and 14.5 years, respectively. Compared with the service life of 20% content, the service life of 25% and 30% content decreased by 20% and 42% respectively. The ratio of reduction is roughly linear with the aggregate content.

This is due to a large amount of old mortar with high porosity and loose structure

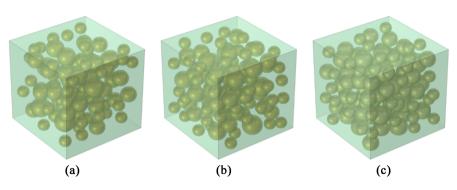


Figure 5. A set of models with different aggregate content: (a) 20%; (b) 25%; (c) 30%.

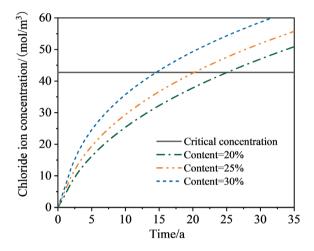


Figure 6. Change of chloride ion concentration with time in different aggregate content.

is attached to the surface of the RLA, and its chloride ion diffusion coefficient is larger than that of the general cement mortar. Therefore, old mortar becomes the weak part of the RLA-SCC. At the same time, the volume of the double-layer ITZ will increase with the increase of the content of RLA, and the effect of ITZ will be enhanced. Chloride ion is more likely to diffuse into the deep, thereby increasing the diffusion capacity of chloride ion in concrete. With the increase of aggregate content, the diffusion rate of chloride ions inside the concrete increases. Chloride ion is more likely to diffuse deeper, resulting in a decrease in the service life of RLA-SCC. The service life of RLA-SCC in chloride environment can be improved by reducing RLA content in practical engineering, but it cannot reach the life expectancy of concrete structures in the general marine environment. Therefore, RLA-SCC should not be used in major projects in the marine environment.

4.2. Effect of Recycled Large Aggregate Particle Size on Service Life

Considering the influence of different RLA particle size, two groups of models with RLA particle sizes of 50 mm, 70 mm and 90 mm were set up respectively. In each group of models, only the random placement positions of RLA are different, and the aggregate content is the same. A set of model settings is shown

in Figure 7.

Figure 8 shows the change of chloride ion concentration with time in different particle size. With the increase of diffusion time, the concentration of chloride ion is increasing. Under the same protective layer thickness, the service life of concrete increases with the increase of aggregate particle size. When the thickness of the protective layer is 60 mm, the service life of RLA-SCC with RLA particle size of 50 mm, 70 mm and 90 mm is 8.3, 13.4 and 21.8 years, respectively. Compared with the service life of 50 mm particle size, the service life of 70 mm and 90 mm increased by 61% and 163%, respectively.

This is due to chloride ion cannot pass through the aggregate and can only be transmitted along the aggregate surface. With the increase of the particle size of the RLA, the chloride ion diffusion path is prolonged. The tortuosity effect is dominant [12] and the migration time is increased. The hindering effect of chloride ion diffusion in RLA-SCC is enhanced, which leads to the decrease of chloride ion diffusion rate and the increase of service life of concrete. Increasing the particle size of RLA can prolong its service life to a certain extent. But it cannot reach the life expectancy of concrete structures in the general marine environment.

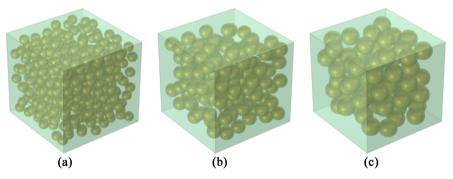


Figure 7. A set of models with different aggregate particle size: (a) 50 mm; (b) 70 mm; (c) 90 mm.

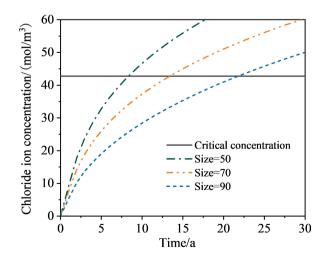


Figure 8. Change of chloride ion concentration with time in different aggregate particle size.

5. Conclusion

The numerical simulation results of the multiphase mesoscopic numerical model of RLA-SCC are in good agreement with the experimental data. The model reproduces the diffusion of chloride ion in RLA-SCC. At the same depth, the closer to the surface of the RLA, the greater the chloride ion concentration. With the increase of the content of RLA, the weak position inside the concrete increases. The ITZ effect dominates, and the service life of concrete decreases. With the increase of the particle size of RLA, the tortuosity effect dominates. The increase of aggregate size hinders the diffusion of chloride ions in concrete. Increasing the particle size of RLA can prolong its service life to a certain extent, but it cannot reach the life expectancy of concrete structures in the general marine environment. The RLA in RLA-SCC weakens its resistance to chloride ion erosion. In order to promote the use of this environmentally friendly concrete material, RLA should be further treated to improve its service life.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- Ivan, H. and Juraj, B. (2018) Effect of Chloride-Induced Steel Corrosion on Working Life of Concrete Structures. *Solid State Phenomena*, **4634**, 226-231. <u>https://doi.org/10.4028/www.scientific.net/SSP.272.226</u>
- [2] Bao, J., Wei, J., Zhang, P., Zhuang, Z. and Zhao, T. (2022) Experimental and Theoretical Investigation of Chloride Ingress into Concrete Exposed to Real Marine Environment. *Cement and Concrete Composites*, **130**, 10451. <u>https://doi.org/10.1016/j.cemconcomp.2022.104511</u>
- [3] Fawzy, A., Elshami, A. and Ahmad, S. (2023) Investigating the Effects of Recycled Aggregate and Mineral Admixtures on the Mechanical Properties and Performance of Concrete. *Materials (Basel, Switzerland)*, 16, 14. https://doi.org/10.3390/ma16145134
- [4] Janani, S., Kulanthaivel, P., Nidharshana, S., Nithesh Kumar, S.M. and Narendhiran, J. (2022) Performance Evaluation of Mechanical Behaviour of Concrete with Recycled Aggregate and M-Sand. *Materials Today: Proceedings*, 65, 1867-1872. https://doi.org/10.1016/j.matpr.2022.05.047
- [5] Li, J., Zhang, Jun., Ni, S., Liu, L. and Walubita Lubinda, F. (2021) Mechanical Performance and Environmental Impacts of Self-Compacting Concrete with Recycled Demolished Concrete Blocks. *Journal of Cleaner Production*, 293, 126129. <u>https://doi.org/10.1016/j.jclepro.2021.126129</u>
- [6] Wang, J.C., Guan, Z.Z., Qiu, Z.M. and Hou, W. (2021) Experimental Study on Short Steel Tube Columns Filled with Recycled Large Aggregate-Self Compacting Con-

crete Subjected to Compression. *Science of Advanced Materials*, **13**, 991-1002. https://doi.org/10.1166/sam.2021.3998

- [7] Aruz, P. (2013) Time Dependent Models of Apparent Diffusion Coefficient and Surface Chloride for Chloride Transport in Fly Ash Concrete. *Construction and Building Materials*, **38**, 497-507. <u>https://doi.org/10.1016/j.conbuildmat.2012.08.041</u>
- [8] Zheng, B., Li, T., Qi, H., Gao, L., Liu, X. and Yuan, L. (2022) 3D Meso-Scale Simulation of Chloride Ion Transportation in Cracked Concrete Considering Aggregate Morphology. *Construction and Building Materials*, **326**, 126632. https://doi.org/10.1016/j.conbuildmat.2022.126632
- [9] Fang, G., Chen, J., Dong, B. and Liu, B. (2023) Microstructure and Micromechanical Properties of Interfacial Transition Zone in Green Recycled Aggregate Concrete. *Journal of Building Engineering*, 66, 105860. <u>https://doi.org/10.1016/j.jobe.2023.105860</u>
- [10] Li, C, Jiang, L. and Li, S. (2020) Effect of Limestone Powder Addition on Threshold Chloride Concentration for Steel Corrosion in Reinforced Concrete. *Cement and Concrete Research*, 131, 106018. <u>https://doi.org/10.1016/j.cemconres.2020.106018</u>
- [11] Rajamallu, C., Chandrasekhar Reddy, T. and Arunakanthi, E. (2021) Service Life Prediction of Self Compacted Concretes with Respect to Chloride Ion Penetration. *Materials Today: Proceedings*, **46 P1**, 677-681. https://doi.org/10.1016/j.matpr.2020.11.746
- [12] Jeonghyun, K. (2022) Influence of Quality of Recycled Aggregates on the Mechanical Properties of Recycled Aggregate Concretes: An Overview. *Construction and Building Materials*, **328**, 127071. <u>https://doi.org/10.1016/j.conbuildmat.2022.127071</u>