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A numerical study on chloride diffusion in freeze-thaw affected concrete

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HIGHLIGHTS

- How the freeze and thaw affect chloride penetration is quantitatively investigated.
- The evolution of FTCs-induced damage during chloride diffusion is considered.
- The correlative degrees of various factors influencing chloride diffusivity are ranked.

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ABSTRACT

Existing concrete in cold or coastal regions is attacked by chloride penetration under freeze-thaw cycles (FTCs). The combined deterioration process accelerate the damage evolution of concrete and reduces the service life of concrete structures. This paper presents a mesoscopic numerical model, which is 2-D and 3-phases, to investigate the mechanism of chloride diffusion under FTCs in a quantitative manner. Unlike most of existing models, the present model considers the FTCs-induced damage affected chloride diffusion by adopting a time-dependent variable of porosity, which can not only reflect how freeze-thaw action affects the concrete pore structure, but also couple the freeze-thaw process together with the chloride diffusion process at time scale. The reliability of the proposed model is validated against a third-party experiment. Based on the obtained concentration distribution profiles, a series of significant influencing factors, i.e., w/c ratio, ITZ effects, external chloride concentration, aggregate volume fraction and inner temperature are clarified. A grey relational analysis is further conducted to rank the correlative degrees of influencing factors on diffusivity of chloride under FTCs. The findings of this study can bring insights to the preparation technique of concrete in cold or coastal regions as well as the durability prediction on existing concrete structures suffering chloride attack and freeze-thaw action.

1. Introduction

The durability of existing reinforced-steel concrete (RC) structures is deteriorated by the ingress of chloride ions [1–4]. Once the ratio between the concentration of chlorides and hydroxides near the embedded steel becomes higher than 0.6, the passive film protecting reinforcing steel tends to be destroyed and leads to rebar corrosion [5–7]. This chloride-induced degradation would be even more serious when the RC structures are subjected to freeze-thaw cycles (FTCs) in cold regions where concrete structures adopt de-icing salt or are close to marine environment [8–11]. During freezing-thawing process, the pore solution within concrete freezes into ice and that will generate internal stress [12,13]. When the stress exceeds the strength of the concrete, micro-cracks may occur and provide interconnecting flow channels for penetrating more chlorides [14,15], which reduces the durability of RC structures. For these reasons, in recent years, the studies of combined actions of chloride attack and freeze-thaw action have attracted wide attention [16–18], and it is important to get a better understanding on the mechanism of the chloride diffusion under FTCs in concrete.

Recent results of experiments showed that freeze-thaw action can accelerate chloride diffusion and increase the depth of penetration [19–21]. A good correlation was also found between maximum chloride concentration and the number of FTCs [22]. The reason why freeze-thaw action influences chloride diffusion in concrete mainly attributes to the change of pore structure. The

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porosity of concrete as well as the other relative parameters of pore structure such as size, distribution and connectivity of pores have significant influence on the transport behavior of chlorides. The porosity related to the degree of continuity of the pore structure is regarded as the most significant parameter affecting the transport properties of concrete [23–27]. Some experiments found that the external chloride concentration also has effects on the porosity of concrete due to osmotic pressure caused by the icing of pore solution [28,29]. In view of these circumstances, some measures have been adopted to decrease the porosity of concrete, including reducing water-cement ratio (w/c), increasing curing time, adding mineral admixtures, etc. [30–35]. In these methods, the most effective method is to adjust w/c ratio [36–38]. Lower w/c ratio leads to smaller porosity and more hardened cement paste. During freeze-thaw action, the pores of the hardened cement paste work like a molecular filter and dissolved chlorides are hindered to penetrate into the concrete. In addition, higher w/c ratio leads to more pore solution in the concrete, which generates greater hydraulic pressure caused by ice formation [19,39].

Although experimental work has made great progress in researching the combined deterioration processes, it appears to be time-consuming and costly to conduct tests at pore scale [40]. Besides, as the chloride transport in concrete pore structure is a very complex phenomenon including multiple processes, experiments may confront with high challenge to isolate the influence of single variable. To this end, it is necessary to develop analytical or numerical models to predict the diffusivity of chloride in concrete subjected to freeze-thaw action.

In previous theoretical studies, the diffusion coefficient of chloride in Fick's second law was always served as the primary parameter to evaluate the chloride diffusivity under FTCs [41–45]. This coefficient is a changing value in the coupling processes between chloride penetration and freeze-thaw action, which needs to be functioned. Yuan et al. presented fitting curves for chloride diffusion coefficient under FTCs to predict the residual service life of a bridge [46]. Zhang et al. found the linear relationship between the diffusion coefficient of chloride and the number of FTCs [16]. Chen et al. declared that both hydration of concrete and sulfate-induced damage would affect the coefficient [47,48]. Temperature variation during freeze-thaw processes is deemed to have a significant influence on chloride diffusivity, which can be combined in the term of diffusion coefficient by using Arrhenius equation [49,50]. High temperature will increase ionic mobility and decrease the resistivity of concrete; whereas low temperature during freezing process may lead to the formation of ice, which can be served as a type of "pore filler" to block chloride transport [51–53]. In addition, some studies also presented analytical methods to investigate the permeability change of concrete from the strain behavior caused by freeze-thaw action [54–57].

For further understanding of the influence caused by individual phase of concrete such as cement matrix, aggregate particles and interfacial transition zone (ITZ), meso/micro-scope numerical models have been adopted to study chloride transport when subjected to FTCs. The aggregates are the main phase affecting the tortuosity property of concrete at *meso*-scale level. The results of a series of transport models found that the volume fraction of aggregates has significant influence on chloride diffusivity [58–61] and the shape of aggregates has smaller impact [43,62]. ITZ is a narrow region around aggregates, which has a higher w/c ratio and effectively increases the chloride diffusivity, especially during FTCs [63,64]. Some models also showed that chloride diffusivity in concrete degrade significantly because of binding effect [65–68]. Note that all above findings are obtained based on a freeze-thaw free environment and appear to be significant during chloride diffusion when subjected to FTCs as well.

During freeze-thaw action, icing in the pores generates increasing stress in the concrete. Thus, the models of chloride transport in cracked concrete are supposed to have some similarities with those in concrete affected by FTCs. For cracked concrete, finite element analysis with a smeared cracking approach was conducted to investigate the associated concrete cracking process [69]. Some researchers also utilized lattice models to simulate the process of chloride penetration through cracks in concrete [70–72]. However, cracks in concrete are mainly attributed to external stress, most common ones of which being shrinkage and mechanical loading. The stress caused by freeze-thaw action is a type of internal stress, which firstly results in the change of pore structures. Wang further developed a mesoscopic truss network model to evaluate the diffusivity of chloride focusing on the damage induced by FTCs against the experiment results of Jacobsen [73]. The crack-free mortar during freezing and thawing is taken into account to calculate the capillary porosity [74]. Li et al. established a new mesoscopic model with freeze-thaw stress based on the pore size variation and presented the diffusion coefficient as a function of chloride concentration and the number of FTCs. Their model theoretically proposed a coupling acceleration coefficient based on microscopic elastic-plastic mechanics to reflect the effects of external chloride concentration and freeze-thaw action on chloride diffusion [29]. In their models, the freeze-thaw effect was mainly represented by the influence on pore structure.

The literature survey shows that only very few numerical models consider both chloride attack and FTCs simultaneously. Existing models also lack of information on chloride diffusivity combining the successive frost-induced porosity evolution as well as systematic studies on the aforementioned influencing factors, which are vital for evaluating the service life of concrete structures in cold regions where concrete structures adopts de-icing salt or are close to marine environment. In this study, a multi-phase numerical model is established to investigate the mechanism of chloride diffusion under FTCs in a quantitative manner. Note that the FTCs-induced damage evolution considered herein is defined until the time when cracks appear. Unlike most of existing models, the model presented in this work considering the FTCs-induced damage during the freeze-thaw affected chloride diffusion by adopting a time-dependent variable of porosity, which can not only reflect how freeze-thaw action affects the concrete pore structure, but also couple the freeze-thaw process together with the chloride diffusion process at time scale - the time-varying porosity leads to a time-varying diffusion coefficient of chloride. Thus, the chloride transport in concrete can be prudently described herein via considering this non-linear diffusion coefficient, as well as binding effect, temperature effect and tortuosity effect (based on aggregates and ITZs), etc. The reliability of the proposed model is validated against a third-party experiment. Based on a systematic parametric analysis, a series of significant influencing factors, i.e., w/c ratio, ITZ effects, external chloride concentration, aggregate volume fraction and inner temperature are clarified. A grey relational analysis is further conducted to examine the correlative extent of the influencing factors. The degrees of their influences on chloride permeability under freeze-thaw action are ranked. The findings of this study can bring insights to the preparation technique of concrete in cold or coastal regions as well as the prediction on the service-life of existing structures suffering chloride attack and freeze-thaw action.

2. Theoretical background

Concrete is highly heterogeneous and complex compared with other porous materials, and the chloride diffusivity is strongly dependent on the microstructure of concrete. It is confirmed that