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Scientific paper

Meso-scale Mechanical Model for Mortar Deformation under Freeze Thaw Cycles

Fuyuan Gong¹, Evdon Sicat¹, Tamon Ueda² and Dawei Zhang³

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Abstract

Frost damage mechanism under freezing and thawing cycles is an important issue for service life evaluation of concrete structures in cold regions. In order to simulate the frost damage mechanism, this paper presents a simulation method in meso-scale for coupled mechanical and transfer analysis in which Rigid Body Spring Model (RBSM) is applied. This method can simulate the coupled heat and moisture transfer in mortar, and also the ice formation process based on thermodynamic equilibrium. In addition, a degradation constitutive model is proposed to describe the deformation behavior under several Freezing and Thawing Cycles (FTCs). To evaluate the effectiveness of this method, the simulation results are compared with experimental data of the strain behavior under FTCs and found in satisfactory agreement with the experimental data.

1. Introduction

In cold regions, frost damage is a very common and serious deterioration problem for concrete structures. Frost damage is thought caused by the ice formation process for porous materials like cement, mortar and concrete. When the temperature falls down below the freezing point (usually lower than 0°C due to the super cooling effect (Grübl 1980)) of the water in pore, ice is formed and causes tensile stress in the pore wall. This tensile stress is usually big enough to cause micro cracks inside the concrete materials. For the structures in natural environment, the ice formation usually starts from the surface of the concrete due to some nucleating particles like ice crystals, snowflakes, dust or the uneven parts of the surface (Kaufmann 2002). Once the ice is formed, the thermodynamic equilibrium will be disturbed, thus result in water redistribution and hydraulic pressure. The chemical potential has also been introduced by Kaufman (2002) to explain the water movement. He stated that the chemical potential of formed ice is lower than the surrounding water, and that due to this difference, the liquid water will move towards the ice front. Fagerlund (2002) also stated that the moisture content significantly affects the damage behavior, and there is a critical saturation degree for each specific specimen to have damage, which is expressed as a relative loss in elastic modulus. Therefore the moisture movement and phase transfer of

pore water are two key factors for the deterioration of the materials suffering from freezing and thawing cycles.

The moisture transfer between the environment and the concrete materials, as well as the moisture movement inside the concrete has been discussed during recent several decades. The moisture transfer is controlled by coupled effect of temperature and moisture concentration. The governing equations of this coupled effect have been developed by several researchers, like Luikov (1966), Matsumoto (1978), Kunzel (1993) and so on. However these equations only consider the non-freezing conditions, whose environmental temperature is always above 0°C. Based on these equations, Matsumoto (2001) introduced moisture chemical potential as a quantitative index, and developed a mathematical model for the coupled heat and moisture transfer, in which the freezing condition had also been considered. In this paper, Matsumoto's equations will be mainly adopted for the heat and moisture transfer simulation program.

To simulate the mechanical behavior of the concrete under FTCs, the meso-scale analysis is useful for concrete materials, in which the concrete is considered as a composite material with three phases: aggregates, mortar and interfacial transition zones between them. Analysis in this scale level is relatively precise for simulation each components, such as mortar and aggregate and their interface. In recent years, there are many studies on the meso-scale analysis and simulation of concrete structures. For example, Nagai *et al.* (2004, 2005) succeeded in simulating the failure mechanism and failure modes of mortar and concrete specimens using both two and three dimensional models. Ueda *et al.* (2009) also proposed a meso-scale constitutive model for frost damaged concrete subjected to mechanical loading. However, there is no constitutive model for frost damage impact itself, for which the failure of material is considered caused by internal freezing. Further, there is no meso-scale constitutive model for deterioration with increase in FTCs.

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According to the reviews and discussions above, in this paper, the objectives are as follows. First, computational analysis of heat and moisture transfer and ice formation process will be developed. Then, according to the linear relation assumption (Oiwa 2008; Johannesson 2010) between ice amount and macro deformation, the strain curve will be predicted. Finally, a mathematical constitutive model will be developed to explain the deterioration strain behavior of mortar with increase in FTCs.

2. Method of the Analysis

2.1 Mechanical model

The Rigid Body Spring Model (RBSM) is a discrete numerical analysis method, which is first developed by Kawai (1977) and applied for computer programming by Kawai and Takeuchi (1990). Unlike the continuum methods such as Finite Element Method or Finite Difference Method, RBSM is a more proper way to simulate splitting and cracking in cement-based materials like mortar and concrete. And also compared to other discrete method like Distinct Element Method, RBSM is more suitable for small deformation and tiny cracks which often occurs in concrete structures. There have been a lot of researches using RBSM to analyze the behavior of cement-based materials (Ueda *et al.* 1988; Nagai *et al.* 2004).

The analytical model is divided into polyhedron elements, and the mesh is arranged randomly using a Voronoi diagram (Okabe 2000) (see Fig. 1). Each Voronoi cell represents a mortar element in the model. This Voronoi mesh is automatically divided using a geometric computational software developed by Sugihara (1998).

For two adjacent elements, there are two springs connecting them: normal spring and shear spring, which are placed at the boundary of the elements (see Fig. 2). Each element has two translational and one rotational degree of freedom at the center of gravity.

The value of normal and shear elastic modules between two elements are calculated based on plane stress assumption (Nagai *et al.* 2004):

$$\begin{aligned} k_n &= k_{nsp} \frac{l}{h_1 + h_2} \\ k_s &= k_{ssp} \frac{l}{h_1 + h_2} \end{aligned} \quad (1)$$

where, l is the length of boundary [mm], and h_1, h_2 are the perpendicular length from the center of gravity to the boundary [mm]. k_{nsp} and k_{ssp} are the modules of normal and shear springs [MPa], which can be derived:

$$\begin{aligned} k_{nsp} &= \frac{E_{elem}}{1 - \nu_{elem}^2} \\ k_{ssp} &= \frac{E_{elem}}{1 + \nu_{elem}} \end{aligned} \quad (2)$$

where E_{elem} and ν_{elem} are the element elastic modulus

Fig. 1 Element mesh of analysis.

Fig. 2 Elements, degree of freedom and springs.

[MPa] and Poisson's ratio, which should be derived from the macroscopic elastic modulus E [MPa] and Poisson's ratio ν (Nagai *et al.* 2004).

$$\nu_{elem} = 20\nu^3 - 13.8\nu^2 + 3.8\nu \quad (0 \leq \nu \leq 0.3) \quad (3)$$

$$E_{elem} = (-8\nu_{elem}^3 + 1.2\nu_{elem}^2 - 0.2\nu_{elem} + 1)E \quad (4)$$

Despite the fact that the compressive failure occurs in macro-scale, there are many meso-cracking caused by the tensile and shear stresses. Therefore only the tensile and shear strength stress are set as material strength. Because of consisting of different components like sand, cement paste and air voids, the mortar is not a homogeneous material. Here a normal distribution was assumed for the tensile strength of the normal spring (Nagai *et al.* 2004).

$$\begin{aligned} f(ft_{elem}) &= \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(ft_{elem} - \mu)^2}{2\sigma^2}\right] \\ \mu &= ft_{average} + 1.5 \\ \sigma &= -0.2ft_{average} + 1.5 \end{aligned} \quad (5)$$

when $f_{t_{elem}} < 0$, then $f_{t_{elem}} = 0$.

where $f_{t_{elem}}$ is the distributed tensile strength [MPa] and $f_{t_{average}}$ is the average tensile strength of mortar at meso-scale level [MPa].

And the shear strength of mortar is given based on the failure criterion suggested by Taylor and Brom (1964) and Kosaka *et al.* (1975) as follows:

$$\tau_{max} = \pm(0.11f_{t_{elem}}^3(-\sigma + f_{t_{elem}})^{0.6} + f_{t_{elem}}) \quad (\sigma \leq f_{t_{elem}}) \quad (6)$$

For the macroscopic material parameters, in this simulation program, we use macro-scale compressive strength of mortar f'_{cm} as the only known parameter. Other parameters can be derived using the relationships between the compressive strength and the w/c ratio (Eq. (7)), the elastic modulus (Eq. (8)) and the static tensile strength (Eq. (9)) (Kosaka *et al.* 1975).

$$c/w = 0.047f'_{cm} + 0.5 \quad (7)$$

$$E_m = 1000\{7.7\ln(f'_{cm}) - 5.5\} \quad (8)$$

$$f_{tp} = 1.4\ln(f'_{cm}) - 1.5 \quad (9)$$

where E_m is elastic modulus of mortar [MPa], f_{tp} is the pure tensile strength of mortar [MPa], and c/w is the inverse of water cement ratio.

2.2 Ice formation analysis

The governing equations for coupled heat and moisture transfer analysis in this paper will use Matsumoto's model, which is able to calculate the water content, ice content and temperature at any location of mortar. Before these governing equations are derived, there are some important prerequisite assumptions. For example, it is assumed that each phase of water is in local equilibrium with each other. And also the bulk flow of dry air does not exist, so that the total pressure of the vapor phase is constant inside the materials. Finally, this model does not consider the dissolved salts, which would also affect the chemical potential equilibriums. The governing equations are as follows:

$$\frac{\partial \rho_i \psi_i}{\partial \mu} \frac{\partial \mu}{\partial t} = \nabla \cdot \{ \lambda'_r \nabla T \} + \nabla \cdot \{ (\lambda'_{\mu g} + \lambda'_{\mu l}) \nabla \mu \} - \frac{\partial \rho_i \psi_i}{\partial t} \quad (10)$$

$$C\rho \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + H_{\mu} \{ \nabla \cdot (\lambda'_{\mu g} \nabla T) + \nabla \cdot (\lambda'_{\mu l} \nabla \mu) \} + H_{\mu} \frac{\partial \rho_i \psi_i}{\partial t} \quad (11)$$

$$\mu_i = H_{li} \ln \frac{T}{T_0} \quad (12)$$

where, μ is chemical potential of moisture [J/kg], ρ is density for each phase [kg/m³], T is absolute temperature [K], C is specific heat [J/kgK], t is time [s], ψ is moisture content, λ is thermal conductivity [J/sm²K], $\lambda'_{\mu l}$ is moisture transfer ratio in gas and liquid phase caused by chemical potential gradient [kg/ms(J/kg)],

$\lambda'_{\mu g}$ is moisture transfer ratio in gas phase caused by chemical potential gradient [kg/ms(J/kg)], λ'_r is moisture transfer ratio in gas and liquid phase caused by temperature gradient [kg/msK], λ'_{Tg} is moisture transfer ratio in gas phase caused by temperature gradient [kg/msK], T_0 is freezing temperature of free water (273.16K), ψ_i is ice content, H_{gl} is the evaporation heat [J/kg], H_{li} is melting heat [J/kg]. Eq. (10) shows the mass equilibrium and Eq. (11) shows the energy equilibrium within the elements. Eqs. (10) and (11) can be solved by difference method within the time domain. For each time step, use the chemical potential and temperature as indexes, calculate the heat and moisture movement between every two adjacent elements. Here only the first orders of the difference equations are used for calculating. Eq. (12) is the criteria of the ice initiation, which is derived by thermodynamic analysis (Matsumoto, 2001). The chemical potential of ice μ_i was developed based on the vapor-liquid-solid equilibrium, therefore this chemical potential is the value shared by the whole system (vapor, liquid and solid) if the equilibrium condition was achieved. The moisture with the same phase (gas and liquid) will move automatically to the place whose chemical potential is lower. Besides, the phase transfer can also be controlled by the chemical potential of each phase. For example, if the chemical potential of liquid water is higher than that of ice (calculated using Eq. (12)), the liquid water will change to solid phase until the chemical potential of two phases become the same.

In the governing equations above (Eqs. (10), (11) and (12)), there are four unknowns: chemical potential μ , temperature T , liquid and solid water content ψ_l and ψ_i , so one more equation is needed to satisfy the solvability of the simultaneous equations. Here we use the $\mu - \psi_l$ curve as the fourth equation, which shows the equilibrium water content under any given moisture chemical potential. The $\mu - \psi_l$ curve can be calculated from water adsorption isotherm, which gives a relationship between equilibrium water content and relative humidity of the environment. The equilibrium condition requires that the liquid phase and vapor phase share the same value of chemical potential ($\mu_l = \mu_v$). The chemical potential of vapor can be calculated as:

$$\mu_v = RT \ln \frac{p}{p_s} \quad (13)$$

where R is the gas constant, which equals to 8.314 J/mol·K or 461.89 J/kg·K. T is the absolute temperature. p and p_s are local vapor pressure and saturated vapor pressure respectively [Pa]. p/p_s is the relative humidity (RH), which can be measured experimentally. The water adsorption isotherm can be drawn from experiment, and also can be calculated using Xi *et al.*'s mathematical model (1994). Combining Xi *et al.*'s model and chemical potential equilibrium, the $\mu - \psi_l$ curve can be calculated as (Gong *et al.* 2012):

$$\psi_i = \frac{(1-k)[1+(C-1)k]\exp(\frac{\mu}{RT})}{(1-k\exp(\frac{\mu}{RT}))[1+(C-1)k\exp(\frac{\mu}{RT})]} \quad (14)$$

where C and k are parameters which can be decided according to Eq. (15). (Xi *et al.* 1994):

$$\begin{cases} k = \frac{(1-\frac{1}{n})C-1}{C-1} \\ n = (2.5 + \frac{1}{15})(0.33 + 2.2\frac{w}{c}) \times 1.5 \\ C = \exp(\frac{855}{RT}) \end{cases} \quad (15)$$

where t is the age of specimen in days and w/c is water cement ratio. If taking $t=28$ day, $T=293$ K, the $\mu-\psi_i$ curve for different water cement ratio can be drawn (Fig. 3). Here we need to pay attention to the fact that the water adsorption isotherm used for Fig. 3 is a curve under constant temperature (20°C), while temperature during real experiment is always changing. But Xi *et al.* (1994) has proved that the temperature variation has very little influence on the adsorption isotherm so that this influence can be neglected.

Eq. (14) and Fig. 3 show the equilibrium water content under different value of chemical potential, which can also be rewritten as $\mu_v = \mu_i = f(\psi_i)$. When the temperature falls down below 0°C, and if the chemical potential of ice calculated using Eq. (12) is equal or less than μ_i , the ice can form; otherwise there should be no ice even below 0°C. So if we combine two equations below:

$$\begin{cases} \mu = H_{li} \ln \frac{T}{T_0} \\ \mu = f(\psi_i) \end{cases} \quad (16)$$

a relation between ice initiation temperature and liquid water content can be obtained. The sum of volume fraction of the pore space filled by three phases should be $\psi_i + \psi_l + \psi_v = 1$. When ice initiates, $\psi_i = 0$, so the saturation degree S_r equals to ψ_l . Then from Eq. (16), the relation of ice initiation temperature T_{ini} regarding saturation degree can be obtained:

$$T_{ini} = T_0 \cdot \exp(\frac{f(S_r)}{H_{li}}) \quad (17)$$

As the temperature continuously falls down, the volume of ice will increase. Usually the growth rate of ice is much faster than the speed of evaporation or condensation. So we can regard the saturation degree as constant. Then, the amount of ice should be:

$$\psi_i = 1 - \psi_l - \psi_v = S_r - \psi_l \quad (18)$$

Solving Eq. (16), it brings $\psi_i = f^{-1}(\mu) =$

Fig. 3 Relationship between equilibrium liquid water content (volume fraction of pore space filled with water) and chemical potential.

$f^{-1}(H_{li} \ln(T/T_0))$ Substituting ψ_i into Eq. (18), the ice content depending on local saturation degree and temperature will become clear as follows:

$$\psi_i = S_r - f^{-1}(H_{li} \ln \frac{T}{T_0}) \quad (19)$$

3. Mechanical Constitutive Model

3.1 Model for damaged concrete

The constitutive law for RBSM program is first developed by Nagai *et al.* (2004, 2005), which is for undamaged concrete and mortar. In Nagai's model (Fig. 4(a)), before reaching the tensile strength, the normal spring behaves elastically and shares the same elastic modulus under both compressive and tensile conditions. After reaching the tensile strength, the normal stress falls linearly with increasing crack width. The maximum crack width at which tensile stress can be transferred is constant and assumed to be 0.03mm in Nagai *et al.* (2004). The normal spring in Nagai's model is assumed to be

Fig. 4 Unloading-reloading path: (a) Nagai's model; (b) Ueda's model.

have elastically based on an elastic-fracturing concept, which allows the linear unloading and reloading path passing through the origin. However, based on the experimental fact that there are remaining strains under both compression and tension in macro-scale, Ueda *et al.* (2009) modified the unloading-reloading path (**Fig. 4(b)**), which is based on an elastoplastic and fracture behavior. A strain of ε_{pa} was adopted to describe this phenomenon: once the tensile strength is exceeded, the unloading paths will intersect with the initial stress-strain curve at the same point whose strain is equal to ε_{pa} . As a result, the unloading paths will not pass through the origin, but have some plasticity. And at the same time, the elastic modulus of the reloading path will also decrease due to the irreversible tensile deformation inside the material.

The behavior of frost damaged concrete materials can be described using this constitutive model well. Due to the hydraulic pressure caused by ice formation, tensile stress is generated inside the material, which is big enough to cause internal micro cracking, thus result in macro expansion of the concrete. This tensile deformation is irreversible, which can be represented by the remaining plastic tensile strain of concrete after any internal or external loading has been removed. In Ueda *et al.*'s (2009) paper, this remaining plastic tensile strain of the normal spring is referred to as “meso-scale plastic tensile strain” ε_{pf} .

In tension, if the stress exceeds the tensile strength f_t , the stiffness will decrease (k_1), accompanying with a plastic residual strain ε_{pf} even in the stress-free condition. In compression, a bilinear stress-strain relationship is assumed by Ueda *et al.* (2009). The stiffness is k_1 until reaching the envelop of the stress-strain relationship for undamaged concrete at ε_{pa} . After that, the micro cracks are assumed fully closed and the stiffness will also be fully recovered (**Fig. 5(a)**). Before the analysis under mechanical loading (internal or external), the residual strain during FTC is removed for convenience (see **Fig. 5(b)**).

The value of residual strain ε_{pf} depends on the degree of internal micro cracking, which is directly related to the maximum tensile stress that has been experienced. From the Ueda *et al.*'s model, this relationship can be derived as follows:

Fig. 5 Constitutive relationships for normal spring of frost-damaged concrete.

$$\varepsilon_{pf} = \frac{\varepsilon_{\max}(\varepsilon_{ta} - \varepsilon_0)}{(\varepsilon_0 + \varepsilon_{pa})(\varepsilon_{\max} - \varepsilon_0) - \varepsilon_0(\varepsilon_{ta} - \varepsilon_0)} \varepsilon_{pa} \quad (20)$$

where the constant ε_{pa} is assumed to be 400μ (Ueda *et al.* 2009). ε_0 is the strain corresponding to the tensile strength. $\varepsilon_{\max}$ is the strain corresponding to maximum crack width beyond which no stress is transferred. Since $w_{\max}$ is assumed to be 0.03mm (Nagai *et al.* 2004), and according to the element size in this simulation program (average length of elements $L \approx 4$ mm), then,

$$\varepsilon_{\max} = w_{\max} / L = 7500\mu \quad (21)$$

3.2 Constitutive model under frost action

Ueda *et al.*'s model has successfully simulated the strain-stress behavior of “damaged” concrete after subjected to internal forces, such as frost action. But the frost action itself has not been clearly explained yet. And the deterioration model for the mortar subjected to several FTCs is also needed to be developed.

3.2.1 Single freezing and thawing cycle

The internal force during frost action is caused by the additional pressure generated when ice forms. But as the tensile strain increases, the stress applied on the pore wall caused by ice should be released, thus finally the strain and stress between pore walls and the ice-liquid system will achieve an equilibrium condition. There are some basic assumptions about this equilibrium:

1. The strain of concrete material is induced by the stress due to ice formation, that is, when ice forms suddenly, there is an initial stress due to this rapid ice formation σ_0 (assuming the pore network has not started to deform yet). The value of this initial stress corresponds to the amount of ice formed and the saturation degree.
2. Due to σ_0 applied on the pore wall, material starts to deform. At the same time, because of the volume increase of local pore space, the hydraulic stress will be released (**Fig. 6(a)**). Here we assume a linear stress-strain relation and the slope k is the stress releasing rate.

From the above assumptions:

$$\sigma = \sigma_0 - k\varepsilon \quad (22)$$

where ε is the tensile radial strain of both pore and ice (ice fully occupies pore). According to the compatibility of deformation, the strain of ice should always be equal to that of the concrete. But the difference is, as the tensile strain ε increase, the tensile force applied on pore structure by the ice is decreasing from the initial value, while the compressive force applied on the ice by pore structure is decreasing from the maximum value. Finally, the stress equilibrium and deformation compatibility will be satisfied at the same time (**Fig. 6**).

Fig. 6 Stress-strain relations and equilibrium condition: (a) Relationship between stress acting on ice from pore wall and strain of ice (and pore); (b) Stress-strain relationship of mortar.

In order to determine **Fig. 6(a)**, at least we need two known points or one point plus the slope. The initial stress σ_0 is relatively difficult to estimate due to the complex condition. But the stress releasing rate k and the maximum strain ε_m are rather clear. Since the final equilibrium owes to the stress-strain balance between pore wall and ice network, k should be closely related to the stiffness of ice:

$$k = \phi \cdot \psi_i \cdot k_i \quad (23)$$

where ϕ is the void ratio, ψ_i is the ice volume fraction which is the pore volume fraction of the pore space occupied by ice and k_i is the stiffness of ice, which can be calculated as:

$$k_i = \frac{E_i}{1 - \nu_i^2} \quad (24)$$

where E_i and ν_i is the elastic modulus and Poisson's ratio of ice crystal respectively. The parameters of material property can be found in **Table. 1**. The ε_m in **Fig. 6(a)** means the maximum strain that the formed ice ψ_i can cause if there is no restriction at all. If the local saturation degree is not high enough to satisfy that the increased ice volume occupies all of the pores:

$$\psi_i \cdot \left(\frac{\rho_l}{\rho_i} - 1 \right) + S_r < 1 \quad (25)$$

where ρ_l and ρ_i are the density of liquid and solid phase respectively. Then, there should be no volume expansion for the whole material $\Delta V_{\max} = 0$. The critical value of saturation degree to have expansion is:

$$(S_r)_{\text{critical}} = 1 - \psi_i \cdot \left(\frac{\rho_l}{\rho_i} - 1 \right) \quad (26)$$

Since ψ_i is a variable depending on the temperature T . So as temperature goes down, the critical saturation degree will also decrease, which means more possible to have damage. If saturation degree is high enough, then the maximum volume change would be:

$$\Delta V_{\max} = \phi \cdot \left(\psi_i \cdot \left(\frac{\rho_l}{\rho_i} - 1 \right) - (1 - S_r) \right) \quad (27)$$

A general expression of maximum volume change should be:

$$\Delta V_{\max} = \begin{cases} \phi \cdot \left(\psi_i \cdot \left(\frac{\rho_l}{\rho_i} - 1 \right) - (1 - S_r) \right) & S_r > (S_r)_{\text{critical}} \\ 0 & S_r < (S_r)_{\text{critical}} \end{cases} \quad (28)$$

The strain in one dimension should be:

$$\varepsilon_m = \sqrt[3]{1 + \Delta V_{\max}} - 1 \approx \frac{\Delta V_{\max}}{3} \quad (29)$$

In the elastic region, $\varepsilon \leq \varepsilon_0$, where,

$$\varepsilon_0 = \frac{f_t}{k_n} \quad (30)$$

where f_t is the tensile strength, and k_n is the elastic modulus of undamaged normal spring, the value of stress and strain for ice and mortar can be obtained by solving the following equations:

$$\begin{cases} \sigma = \sigma_0 - k\varepsilon \\ \sigma = k_n \varepsilon \end{cases} \quad (31)$$

Then the strain is:

$$\varepsilon = \frac{\sigma_0}{k_n + k} \quad (32)$$

So, if $\sigma_0 \leq \varepsilon_0(k_n + k)$, there will be no micro cracks,

Table 1. Input Material Properties (Ueda *et al.*, 2009; Parameswaran, 1987)

Parameters	f_t (MPa)	E (GPa)	ν
Mortar	4.09	25	0.18
Ice	—	10.56	0.3

the material will stay elastic. If $\sigma_0 > \varepsilon_0(k_n + k)$, the plastic strain will occur:

$$\begin{cases} \sigma = \sigma_0 - k\varepsilon \\ \sigma = f'_t - k_p\varepsilon \end{cases} \quad (33)$$

where k_p is the stiffness of the softening curve. f'_t is the intersection of the extended tension-soften curve and the vertical axis as shown in **Fig. 6(b)**, which is equal to:

$$f'_t = \varepsilon_0(k_n + k_p) \quad (34)$$

Solving Eq. (33), we can get:

$$\varepsilon = \frac{\sigma_0 - \varepsilon_0(k_n + k_p)}{k - k_p} \quad (35)$$

3.2.2 Multiple freezing and thawing cycles

After the first freezing and thawing cycle, there is a residual plastic strain left if the maximum stress caused by ice formation is larger than the tensile strength of mortar. For the calculation convenience, the origin should be shifted so that the loading path of the 2nd FTC can go through it. The relationships between symbols of the first and second FTC are as follows (The meaning of symbols doesn't change, while the number of FTC is labeled on upper right) (**Fig. 7**):

$$\varepsilon_0^{(2)} = \varepsilon_{ta}^{(1)} - \varepsilon_{pf}^{(1)} \quad (36)$$

$$k_n^{(2)} = \frac{f_{ta}^{(1)}}{\varepsilon_{ta}^{(1)} - \varepsilon_{pf}^{(1)}} \quad (37)$$

$$\varepsilon_{ta}^{(2)} = \frac{\sigma_0 - \varepsilon_0^{(2)}(k_n^{(2)} + k_p)}{k - k_p} \quad (38)$$

$$\varepsilon_{\max}^{(2)} = \varepsilon_{\max}^{(1)} - \varepsilon_{pf}^{(1)} \quad (39)$$

$$f_{ta}^{(2)} = k_p(\varepsilon_{\max}^{(2)} - \varepsilon_{ta}^{(2)}) \quad (40)$$

Fig. 7 Stress-strain relationship for several FTCs.

$$\varepsilon_{pf}^{(2)} = \frac{\varepsilon_{\max}^{(2)}(\varepsilon_{ta}^{(2)} - \varepsilon_0^{(2)})}{(\varepsilon_0^{(2)} + \varepsilon_{pa}^{(2)})(\varepsilon_{\max}^{(2)} - \varepsilon_0^{(2)}) - \varepsilon_0^{(2)}(\varepsilon_{ta}^{(2)} - \varepsilon_0^{(2)})} \varepsilon_{pa} \quad (41)$$

In general, for the i_{th} freeze thaw cycle (FTC_i), the parameters for the next FTC (FTC_{i+1}) will be:

$$\varepsilon_0^{(i+1)} = \varepsilon_{ta}^{(i)} - \varepsilon_{pf}^{(i)} \quad (42)$$

$$k_n^{(i+1)} = \frac{f_{ta}^{(i)}}{\varepsilon_{ta}^{(i)} - \varepsilon_{pf}^{(i)}} \quad (43)$$

$$\varepsilon_{ta}^{(i+1)} = \frac{\sigma_0 - \varepsilon_0^{(i+1)}(k_n^{(i+1)} + k_p)}{k - k_p} \quad (44)$$

$$\varepsilon_{\max}^{(i+1)} = \varepsilon_{\max}^{(i)} - \varepsilon_{pf}^{(i)} \quad (45)$$

$$f_{ta}^{(i+1)} = k_p(\varepsilon_{\max}^{(i+1)} - \varepsilon_{ta}^{(i+1)}) \quad (46)$$

$$\varepsilon_{pf}^{(i+1)} = \frac{\varepsilon_{\max}^{(i+1)}(\varepsilon_{ta}^{(i+1)} - \varepsilon_0^{(i+1)})}{(\varepsilon_0^{(i+1)} + \varepsilon_{pa}^{(i+1)})(\varepsilon_{\max}^{(i+1)} - \varepsilon_0^{(i+1)}) - \varepsilon_0^{(i+1)}(\varepsilon_{ta}^{(i+1)} - \varepsilon_0^{(i+1)})} \varepsilon_{pa} \quad (47)$$

The parameters calculated above are based on the adjusted coordinate system. So to get the real strain at the maximum tensile stress and the residual plastic strain for each FTC, the adjusted value of previous FTCs should be added in. Thus, the maximum strain for each FTC is:

$$\varepsilon_t^{(n)} = \varepsilon_{ta}^{(n)} + \sum_{i=1}^{n-1} \varepsilon_{pf}^{(i)} \quad (48)$$

where $\varepsilon_t^{(n)}$ is the maximum tensile strain during FTC_n . And the residual plastic strain at the end of each FTC is:

$$\varepsilon_p^{(n)} = \sum_{i=1}^n \varepsilon_{pf}^{(i)} \quad (49)$$

where $\varepsilon_p^{(n)}$ is the total residual plastic strain after previous n FTCs.

4. Results and Discussion

4.1 Experiment and simulation model

The mortar specimens in this experiment (Sicat *et al.* 2010) used ordinary Portland cement with density of 3.14 g/cm³, fine aggregate which is 1.2mm or less in size with density of 2.67 g/cm³ at 1467.6 kg/m³ of concrete without air entraining agent to promote damage. Mix proportion for specimens is 1:2:6 (water: cement: fine aggregate). After curing, specimens were cut into size of 40mm x 40mm x 2mm (see **Fig. 8(a)**). Strain gauges used were self-temperature compensation gauges having base size of 4 x 2.7 mm, gauge length of 1 mm and gauge resistance of 120Ω, lead wires were 3-wire cable, and adhesive was made of polyurethane, all were designed for low temperature strain measurement. Specimens were submerged underwater until mass was constant to attain full saturation. Finally, the specimens were sealed

Fig. 8 Specimens used in experiment (a) 40 x 40 x 2mm cut specimens; (b) attachment of strain gauges; (c) sealed specimens.

with vinyl tape to prevent water uptake or loss. The preparation of the specimens is shown in Fig. 8. The 2D simulation model for mortar is a 40mmx40mm square with unit thickness, and is divided into 100 elements.

Since the specimens were sealed during the experiment process, and also the thickness is very small, then it can be practically assumed that the moisture and temperature condition are uniform, so that the heat and moisture transfer in the specimen is negligible. The bottom boundary is fixed for both vertical and horizontal direction (Fig. 1).

Initial condition of mortar: relative humidity=0.99, temperature=10°C

Time for one FTC: 10hrs

Time step: 1s

The temperature history is as shown in Fig. 9:

4.2 Ice formation

As shown in Fig. 9, the temperature falls down from 10°C to -28°C and for the local areas, the ice initiation depends on both temperature and saturation condition. Once we know the temperature at the moment of ice initiation for a given saturation degree, an ice initiation curve can be drawn for different w/c ratio based on Eq. 17 (see Fig. 10), which shows the critical condition between two status. According to Fig. 10, the following conclusions can be drawn:

1. For a given saturation degree, there is an ice initiation temperature. The lower saturation degree is, the lower ice initiation temperature will be.
2. For a given lowest temperature, there is a limit saturation degree. If below this limit, no ice will form.
3. The mortar with higher w/c ratio has a wider range of temperature and saturation set for ice formation. This means that the higher w/c ratio is, the more easily ice can initiate.

Fig. 9 Temperature history of one freezing and thawing cycle.

Although Fig. 10 show the macro behavior of the mortar under different combinations of temperature and saturation degree, the phenomenon itself is closely related to the micro pore structure. The cement-based material contains different sizes of pore. The water in larger pores is more “active” due to the higher chemical potential. That is, the water in larger pores freezes more easily than smaller pores. So if the mortar is fully saturated, meaning that even the biggest pores are occupied with water, then the freezing point of the water in the biggest pores should be 0°C. But if the saturation degree is lower, the water occupies only the smaller pores before freezing. It is because the chemical potential of pore water can be calculated as (Gong *et al.* 2012):

$$\mu_l = \frac{2\gamma \cos \theta}{r - \delta} \cdot v_l \quad (50)$$

where $\gamma = 0.072 \text{ J/m}^2$ is the surface energy of water; θ is the contact angle of the water surface with the pore walls; r is the radius of pores; δ is the thickness of the adsorbed film of water on the pore wall, which is approximately equal to 0.9nm (Scherer *et al.* 2005). v_l is the molar volumes and equals to $18 \times 10^{-6} \text{ m}^3/\text{mol}$. So it can be seen that the chemical potential is lower for smaller pores. Then if the mortar is partially saturated, the stable condition is that all the water fills in smaller pores. For example, if the saturation degree is 70%, there is no liquid water in the biggest 30% pores before freezing. And since the freezing point of pore water is decreasing with smaller pores, the ice initiation temperature will decrease to nearly -11°C for w/c=0.5 case.

As the temperature continuously decreases, the ice

Fig. 10 The critical conditions for ice initiation.

amount will also increase. **Fig. 11** shows the relationship between ice content and temperature under four different saturation conditions with different w/c ratio based on Eq. (19). Here assume there is no moisture exchange in the local area (like sealed specimens), the absolute value of the slope is decreasing gradually as the temperature decreases. If the saturation degree is lower enough, like 50% in **Fig. 11**, theoretically the ice will not initiate unless the temperature falls down to near -36°C for $w/c=0.3$, -22°C for $w/c=0.5$ and -17°C for $w/c=0.7$. It is rather difficult to have frost damage under this saturation condition.

4.3 Deformation and residual plastic strain

The tensile strain during FTCs is thought caused by the volume expansion when liquid water freezes to solid phase. Combining the ice amount, which can be measured during the freezing and thawing process by using calorimetric tests, with the length change of the specimens, Johannesson (2010) concluded that there is a linear relationship between the tensile deformation and the ice amount. Oiwa *et al* (2008) also used a linear expression as follows:

$$\varepsilon_i = \alpha_i \times \psi_i \quad (51)$$

where ε_i is the expansion strain caused by phase transfer, ψ_i is the percentage ice content, which is the ratio of the

ice volume to the total pore volume, α_i is the constant. In this experiment, when the temperature reaches the minimum value (-28°C), the ice content calculated is 0.44, then k and ε_m in **Fig. 6(a)** can be obtained. ($k = 1.16\text{GPa}$ and $\varepsilon_m = 4320\mu$). According to Eq. (35), the strain at the minimum temperature should be 243μ . So the constant α_i equals to 5.5×10^{-4} .

According to Eq. (51), the strain caused by ice formation can be calculated. And applying this tensile strain to the constitutive model discussed in Section 3.2, the strain behavior during the freezing and thawing process can be simulated. **Fig. 12** shows the simulation result and comparison with the authors' former experiment (Sicat *et al.* 2010). Here the thermal strain is removed for both the simulation and experimental result. From **Fig. 12**, the strain behavior is basically in accordance with the temperature history. But during the thawing process, there is residual plastic strain even after the temperature returns to above 0°C . It can be also seen from the experimental results that during the first cycle, there is a drop in strain and soon recovered at the end of melting process. It might be due to the sudden melting of a large amount of ice, and there is no enough time for the liquid water to redistribute to achieve an equilibrium condition. So the effect of melting will be enlarged and then recovered a little as time passes. But as the number of FTCs increases, the permeability becomes higher due to the micro cracking, and results in more rapid movement of liquid

Fig. 11 Ice amount at different temperatures (a) $w/c=0.3$ (b) $w/c=0.5$ (c) $w/c=0.7$.

Fig. 12 Strain changes during one freezing and thawing cycle (the solid black curve is the average of three samples).

water. Therefore, such phenomenon is only significant during the first cycle (see Fig. 13).

Since the physical and mechanical process during FTCs is rather complex, there are other influences such as the shrinkage caused by liquid water movement. As a result, the strain curve measured by experiment is not smooth and has some fluctuation. The simulation cannot exactly reflect all influences, but the result is in satisfactory agreement.

Figure 13 shows the strain behavior of the mortar subjected to 5 FTCs. After the first FTC, other than the remaining tensile strain, the stiffness will also decrease due to micro-cracking inside the mortar. Thus, during the next FTC, bigger deformation will be caused by the same internal stress, and result in bigger residual plastic strain. As the number of FTCs increases, the peak tensile strain and residual plastic strain will also increase gradually.

There is also a linear relationship between the peak strain of each FTC and the residual strain at the end of that FTC (Fig. 14). Such phenomenon was also observed by the study of Sicat *et al* (2010) and Ueda *et al* (2010). The slope is 0.473 and 0.534 respectively. This phenomenon can be explained by the constitutive model in

this paper as well. Eq. (48) and Eq. (49) are the peak tensile strain and residual plastic strain of each FTC respectively. So the slope β should be:

$$\beta = \frac{\varepsilon_p^{(n)}}{\varepsilon_t^{(n)}} = \frac{\sum_{i=1}^n \varepsilon_{pf}^{(i)}}{\varepsilon_{ta}^{(n)} + \sum_{i=1}^{n-1} \varepsilon_{pf}^{(i)}} \quad (52)$$

5. Conclusions

- (1) Based on the governing equations of heat and moisture transfer analysis and ice formation process in mortar, a simulation program is developed. After setting the temperature history, initial condition and boundary condition. The ice initiation temperature under different saturation condition as well as the ice content can be calculated. The calculating results only has theoretical basis at this moment, further experimental verification will be conducted in the next step.
- (2) The mechanical constitutive model of mortar in meso-scale is presented for single and multiple freezing and thawing cycles. According to this model, the relationship between the peak tensile strain and residual plastic strain can be clearly explained. In addition, the deterioration mechanism,

Fig. 14 Peak strain and residual strain relationship in analysis.

Fig. 13 Strain changes during 5 FTCs.

such as residual plastic strain and the stiffness changes during several FTCs can also be explained using this constitutive model.

- (3) Due to the complexity of the physical and mechanical process during FTCs, the simulation result cannot match the experiment process very precisely. However they are still in satisfactory agreement.
- (4) The physical model for ice formation and constitutive law for mechanical behavior can be used for the modeling and simulation of larger structure members with different local conditions, which will be conducted in the next study.

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