Thermo-mechanic coupled damage simulation of idealized concrete material

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Abstract. Several special concrete structures are subjected to temperature cycling environment. Temperature cycling will influence the physical and mechanical behaviours of concrete material. As the number of loops of temperature cycling increases, the mechanical performance of concrete will decrease. Two different multi-phase composite numerical models for concrete are herein introduced in this paper. Based on damage development and evolution in the mortar and interface transition zone of concrete under temperature cycling, the thermo-mechanic coupled multi-scale behaviours of different groups of concrete were simulated. Afterwards, the failure process and failure mode of concrete material in uniaxial stress state was studied. It is found that the damage within concrete material concentrates on the interface transition zone under temperature cycling, and will develop in mortar as the number of loops of temperature cycling increases. Finally, it is verified that temperature cycling will remarkably influence the internal stress distribution and failure mode of concrete structures. The research findings of the present paper are conducive to improving the mechanical properties of aggregate concrete by optimizing the mix proportion.

1. Introduction.
Industrial chimney, containment of nuclear power plant, cooling tower, high temperature pile and support structures for high temperature equipment are often subjected to the environment with repeated temperature cycling. However, existing literature shows that temperature cycling will influence the mechanical behaviors of concrete, and the mechanical performance of concrete decreases as the number of loops of temperature cycling increases [1-6]. Therefore, this type of structures might fail before the designed age, and the safety in the life cycle would be influenced if temperature cycling is not taken into consideration in structural design. To this end, numerical simulation is performed in this paper to study the influence of temperature cycling on the mechanical performance of concrete and the performance degradation along with the failure mechanism of concrete material under temperature cycling. The coarse aggregates in concrete are often modeled as inclusions in a matrix of mortar. Among different modeling approaches, using modeled concrete was found to be effective to study the cracking process in concrete [7]. It is found that the failure process is related to the relative strength of coarse aggregate and mortar matrix. For modeled aggregate concrete, the first bond cracks appear around both the old and new interfacial transition zones (ITZ), and then propagate into the old and new mortar matrix by connecting each other [8]. Both the idealized meso-scale concrete model and the multi-aggregate model are built to simulate and analyze the degradation process of concrete in meso-scale as a three-phase composite material subjected to temperature cycling, and the evolution rules of internal damage are further studied. The stress distribution of the meso-scale concrete model under axial compression and
the failure mode of concrete model are compared for before and after temperature cycling. This study will provide insights into the failure processes of aggregate concrete.

2. Modelling and simulation methods of concrete in meso-scale

2.1. Geometrical model and boundary conditions

The idealized concrete model [8] and multi-aggregate model [9] can be adopted in the numerical simulation analysis to study the mechanical performance degradation mechanism of concrete in meso-scale under temperature cycling. In the simulation of concrete in meso-scale, concrete material is often regarded as the three-phase composite material including cement mortar, coarse aggregate and ITZ between mortar and aggregate, and the three phases are distributed in the discretization mesh in meso-scale [10]. For simplicity, the idealized concrete and the multi-aggregate model are considered as 2-dimensional models, and the round aggregate is applied. By using the full thermo-mechanical coupling method in the modelling and calculations in ABAQUS software, the response of concrete in meso-scale is simulated under thermal field and force field.

The 9-aggregate idealized model of concrete and its mesh are shown in Figure 1, and the size of the specimen is 100mm×100mm. It is noted that the white circles represent the aggregate with 20 mm diameter which are symmetrically distributed in the model, while the blue parts represent the cement mortar. The ITZ is between the mortar and the aggregate, which is defined as the ring extended 500 μm from the boundary of the aggregate. It should be noted that the width of the ITZ is usually 10~50 μm. However, in this case, the ITZ is assumed to be 500 μm considering the size of the mesh, simulation efficiency and the extension of ITZ after temperature cycling. The size of the mesh on the boundary and inside the aggregate is 4 mm while that of ITZ and mortar is set as 0.5 mm. The multi-aggregate idealized concrete and its mesh are shown in Figure 2, and the overall size of the specimen is 100 mm × 300 mm. The white circles represent round aggregates with the diameter of 5~20 mm while the width of ITZ is 500 μm and the blue part represents mortar, correspondingly. The size of mesh of the aggregate is 4 mm while that of the ITZ and mortar is 0.5 mm. The shape of element of both models is linear triangle, and the CPE3T element is applied in the thermo-mechanic coupled simulation while the CPS3 element is applied in the mechanical simulation model.

![Figure 1. The 9-aggregate model and mesh.](image1)

![Figure 2. Multi-aggregate model and mesh.](image2)

In the thermal-mechanical coupled simulation of concrete model, two types of boundary conditions should be defined, including the thermal boundary condition in the temperature field analysis and the displacement boundary condition in the uniaxial loading process. The initial temperature of the thermal field in the model is set as 30℃, and the Stefan-Boltzmann constant is taken as $5.6697 \times 10^{-8}$. The effect of thermal convection and radiation are considered in all of the boundaries of concrete specimen in the simulation of thermal field. The coefficient of thermal convection is taken as 462 J/min·m²·℃ while the coefficient of thermal radiation is 0.5 J/min·m².
Both constraint boundary and displacement boundary conditions should be considered in the uniaxial loading model. In order to limit the influence of boundary conditions on the mechanical state in the loading process, the lower left corner of the model is set as hinge connection and the vertical degree of freedom of the lower bound of the specimen is constrained. The displacement is uniformly loaded on the specimen with the displacement rate being $1.333 \times 10^{-2}$ m/min for the idealized concrete model and $4 \times 10^{-5}$ m/min for the multi-aggregate model.

2.2. Constitutive laws for different phases in concrete

Generally, the aggregate in the meso-scale concrete model are considered as elastic material. Similar to concrete, the mechanical performance of cement mortar is quasi-brittle, and its stress-strain relation is close to that of concrete. The actual material of ITZ is the same as the mortar. However, the ITZ is relatively loose with more micropores. Therefore, the ITZ and the mortar are considered as the same kind of material in the modelling of concrete while the ITZ locates around the aggregate, and the elastic modulus and hardness of the ITZ can be accessed by nano-indentation technology to represent the macro mechanical behaviour of the ITZ [11]. The thermal parameters and the mechanical parameters are involved in the meso-scale thermal-mechanical simulation of concrete, and the values of these parameters can be referenced from literatures [12-17] which are shown in Table 1.

### Table 1. Thermal and mechanical parameters of different phases in concrete.

| Material property | Thermal conductivity (J/min·m²·°C) | Specific heat capacity (J/kg·°C) | Density (kg/m³) | Coefficient of thermal expansion (10⁻⁵) | Elastic modulus (GPa) | Poisson’s ratio | Tensile strength (MPa) | Compressive strength (MPa) | Fracture energy (N/m) |
|-------------------|-----------------------------------|---------------------------------|----------------|----------------------------------------|----------------------|----------------|-----------------------|------------------------|------------------|
| Aggregate         | 186                               | 1000                            | 2700           | 0.8                                    | 80                   | 0.16          | --                    | --                     | --               |
| Cement mortar     | 60                                | 800                             | 2200           | 1.8                                    | 30                   | 0.2           | 5                     | 50                     | 93               |
| ITZ               | 30                                | 800                             | 2200           | 0.8                                    | 15                   | 0.2           | 3                     | 65                     | 31               |

The compressive stress-strain relation of cement mortar is analogically taken from the design code for concrete structures of China currently in effect. Because the ITZ is usually under triaxial compressive state, the compressive softened effect is herein ignored. The scale of ITZ is at micro-meter, hence the compressive deformation is relatively small and the mechanical property of ITZ is considered to be perfectly elastoplastic. The tensile stress-strain relations of cement mortar and ITZ is considered as linearly softened. To avoid the mesh sensitivity, the softened effect of cement mortar and ITZ were adjusted based on the fracture energy and the size of the mesh.

3. Meso-scale simulation of idealized concrete

3.1. Damage cumulation in temperature cycling

Under the effect of temperature cycling, the softening of strength and reduction of stiffness exhibited due to the thermo induced cumulative damage. With the inhomogeneity of thermal field in concrete and the divergency of the material properties in different phases, the damage develops in the ITZ and cement mortar, and it will gradually extend from ITZ to the inside of the cement mortar as the number of loops of temperature cycling increases. The cumulative damage states of mortar and ITZ at 1~5 loops of temperature cycling are shown in Figure 3. In the process of rising temperature, damage starts to occur at around 40 min, and the meso-scale structural damage of concrete concentrates in the ITZ at the first loop of temperature cycling. The damage starts to develop in the mortar from the 2nd loop, and starts to extend from the surface to the inner part while it bridges the gaps between aggregates. The area of damage grows as the loops of temperature cycling increases, and the damage develops towards the mortar. In such uniformly distributed aggregate model, the damage of mortar distributes in a
symmetrical grid pattern, and it is relatively small compared with the damage in the ITZ. The first crack appeared around the ITZ, and then propagated into the mortar matrix.

3.2. The uniaxial tension model
To validate the failure mode, the uniaxial tensile loading case is simulated on the model for before and after temperature cycling, and the effects of temperature cycling on tensile failure modes of the idealized concrete are compared. The results of direct tension test and the result of uniaxial tensile test after 1 loop of temperature cycling are shown in Figure 4. It is found that slight damage occurs in the ITZ and the edge of aggregates along the tensile direction, and failure concentrates on a single crack band where the damage develops first and gradually drives through the whole specimen. However, in the tension test after temperature cycling, larger damage develops in the ITZ from temperature cycling. After the tension test, the shape of the crack of this specimen is close to the one in the direct tension test. The difference between the two tests reflects on the location of the crack. In the direct tension test, the crack is on the edge of the bottom row of aggregates, while in the tension test after temperature cycling, the crack is on the edge of the middle row of the aggregates. The simulation result illustrates that temperature cycling changes the location of the weakest part, and influences the failure mode.

3.3. The uniaxial compression model
The uniaxial compression model for idealized concrete is built and simulated after 0, 1, 3 and 5 loops of temperature cycling. The stress and damage evolution of idealized concrete in uniaxial compression test is studied by numerical simulation and the influence of different number of loops of temperature cycling on the failure mode of idealized concrete is discussed.

1) The propagation of stress
The vertical compressive stress distributions of idealized concrete in 4 cases are shown in Figure 5. In the elastic stage, since the elastic modulus of aggregate is relatively large, the vertical stress mainly propagates along the aggregates and uniformly distributes. After 1 loop of temperature cycling, as relatively large damage has developed in the ITZ, in the compression test, the vertical stress is not uniformly distributed even through the propagation of stress is still along the aggregates. However, at the elastic stage, the distribution of vertical stress in the specimen gradually becomes uniform after 3 and 5 loops of temperature cycling. This is because the damage develops into the mortar as the number of loops of temperature cycling increases, and in the elastic compression loading, the stress gradually becomes uniformly distributed. By comparing the 4 cases, it is seen that the vertical stress in idealized concrete mostly propagates by aggregates with larger strength. The influence of temperature cycling on the stress propagation is mainly found after the first cycling loop. And as the number of loops increases, the damage smears in the mortar, and the path of stress propagation becomes clearer.

The corresponding horizontal stress at the same moments with the vertical stress is shown in Figure 6. It is clearly seen that the path of propagation of the horizontal stress is along the aggregates on the
horizontal direction. But due to the constraint on the bottom of the specimen, the propagation of the horizontal stress is influenced. By comparing Figure 5 and Figure 6, a similar pattern can be found. The propagation pattern of horizontal stress becomes blurry after the first loop of temperature cycling, and the regulation returns as the number of loops increases.

Figure 5. The vertical stress distribution in 4 loading conditions.

Figure 6. The horizontal stress distribution in 4 loading conditions.

2) Failure mode
The failure modes of the 4 cases are shown in Figure 7. The corresponding strain is 0.008. The crack of the initial specimen concentrates on a local zone in ITZ. Afterwards, the crack penetrates through the mortar to form a failure surface. After 1 loop of temperature cycling, initial damage develops in the ITZ before the compression test. Therefore, this failure mode differs greatly from the previous specimen. The crossing cracks are mainly formed in the test, and the cracks cross and converge in the ITZ around the aggregates, while the “X” shaped cracks are found in the mortar between aggregates. Besides, after the damage state caused by 3 and 5 loops of temperature cycling, in the compression test, the concentration of the damage is lower than that in the previous loading conditions. By comparing several different failure modes, it is found that the smaller the distribution area of the initial damage in the mortar is before compression, the more concentrated the cracks are distributed in the failure mode after the compression test, but the length of the crack will be longer. From the characteristics of the damage distribution, it is inferred that as the number of loops of temperature cycling increases, the distribution zone of the initial damage will extend; and after the compression test, the damage distribution will be more homogenous, forming the damage area in a network shape. It is intuitively explained by the simulation result that as the number of loops of temperature cycling increase, the elastic modulus of concrete will decrease.

Figure 7. The damage and failure mode of the idealized concrete in 4 loading conditions.

4. Meso-scale simulation of multi-aggregate model
The uniaxial compression model of multi-aggregate concrete after temperature cycling is built. Based on the comparison with that of the 9-aggregate idealized model, the stress distribution and correctness of failure laws of the idealized concrete before and after temperature cycling are verified.
1) The stress distribution
The vertical and horizontal stress of the multi-aggregate model in the elastic stage of compression test with and without 1 loop of temperature cycling are shown in Figure 8 and Figure 9, respectively. By comparison of the compressive stress before and after temperature cycling, it is found that the stress propagation path of the specimen without temperature cycling is clearer, and the compressive stress propagates along the aggregates with relatively larger stiffness, which is consistent with the results of the 9-aggregate idealized concrete model. After 1 loop of temperature cycling, stress still propagates along the aggregates. However, the stress propagation path is relatively less clear, and the stress distribution within the specimen is relatively more homogenous with some tensile stress states in certain locations. The horizontal stress distribution is similar to the vertical stress distribution for the multi-aggregate model. After temperature cycling, the horizontal stress of the specimen is more homogenous and the stress concentrates on the mortar between aggregates, which is consistent with the idealized concrete model.

2) Failure mode
The failure modes of the specimen with and without temperature cycling are shown in Figure 10, where the initial specimen, the direct uniaxial compression loading failure and the compression failure after 1 loop of temperature cycling are shown from left to right accordingly. The loaded displacement corresponding to the failure is 4mm. Considerable difference can be seen between the failure mode of direct compression test and the compression test after temperature cycling by comparing the simulation results. The failure mode of the direct compression test is duo-shear failure with a “V” shaped crack formed in the specimen, and the failure concentrates in a local area. In the meanwhile, in the compression test after 1 loop of temperature cycling, as the initial damage has developed in the ITZ, the range of the crack is larger, and a network shaped crack surface is formed similar to the idealized concrete model. As shown in Figure 10, the failure mode of the compression test after temperature cycling is shear failure, and crisscrossing network shaped cracks are formed in the lower part of the specimen after a single penetration crack has developed, while the upper part of the specimen is rarely cracked.

Based on the comprehensive comparison of numerical simulation results in the multi-aggregate model and the 9-aggregate idealized concrete model, it is verified that the two are mostly consistent in terms of the stress propagation and failure mode, and that the failure characteristic of the multi-aggregate model is subject to that of the latter. In practice, the aggregate inside the concrete is more irregular than the multi-aggregated model with diversified shapes, more nonhomogeneous distribution of the aggregate and 3-dimensional structures. However, based on the comparison of the simulation results of multi-aggregate model and the idealized model, it can be inferred that the stress propagation and failure mode of the concrete in reality still follow the same law. The concentration of failure surface in the specimen in direct compression test is higher, and the failure surface of the specimen with temperature cycling is larger with larger damage in the mortar and the crisscrossing shaped cracks being easier to form. The stress distribution in the elastic stage is non-uniform and stress mainly propagates along the aggregates.
5. Conclusions
Modelled cement-based materials were designed to investigate the failure processes of aggregate concrete under uniaxial compression. By means of the numerical simulation method, the 9-aggregate idealized concrete model and the multi-aggregate model are established in this paper. The structural stress distribution characteristics and failure mode in meso-scale structure of concrete loaded by external force and temperature are studied. Major conclusions can be drawn as follows:

1) In the process of temperature cycling, damage develops within the concrete and concentrates mainly in ITZ and mortar. As the number of cycling loops increases, the damage extends to the mortar. The global cracks basically developed along the loading direction for all the modelled cement-based materials. The first crack appeared around the ITZ, and then propagated into the mortar matrix.

2) As initial damage is induced by temperature cycling within the concrete, the temperature cycling effect will influence the failure mode and stress distribution in the concrete structures. Understanding of the failure processes can provide insights into the failure mechanism of aggregate concrete. Such understanding can be used to improve the mechanical properties of aggregate concrete through optimization of the mixture proportions.

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