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# Mesoscale influence on the macroscopic material behavior of concrete

Volker Hirthammer[1]*, Jörg F. Unger[1] and Josko Ozbolt[2]

**Micro Abstract**
The heterogeneous mesostructure of concreted causes local stress concentrations. Stress dependent phenomena like damage and creep as well as their interactions are effected by those stress concentrations. Therefore a material model's macroscopic behavior will differ whether the mesoscale structure is considered or not. The differences between the mesoscale approach and an homogeneous approach will be presented. The results are discussed with focus on the true materials behavior.

[1]Safety of Structures, Federal Institute for Materials Research and Testing, Berlin, Germany
[2]Institute for Construction Materials, University of Stuttgart, Stuttgart, Germany
***Corresponding author**: volker.hirthammer@bam.de

## Introduction

Concrete is a highly heterogeneous material composed of aggregates and the surrounding cement paste. The varying material characteristics of the two components result in complex interactions which influence the macroscopically observable material behavior. Stress concentrations caused by the stiffer aggregates lead to damage initiation and crack propagation as well as increased creep deformations in the cement paste. Additionally, the moisture transport through the porous mortar matrix is disrupted by aggregates. The shrinkage of the cement paste is influenced by the resulting inhomogeneous moisture content in the pore system and causes a complex stress distribution in the material.

A mesoscale finite element approach is used to investigate the interactions between the heterogeneous material structure of concrete and the deformations caused by creep and shrinkage. The results of the mesoscale calculation and a homogeneous approach are compared in order to evaluate the aggregates impact on the mentioned phenomena and their interactions.

## Material model

### Mesoscale

The heterogeneous structure of concrete is considered during the mesh generation. The Aggregates' size distribution is specified by the desired grading curve. An event driven molecular dynamics algorithm [5] is used to randomly place the spherical shaped aggregates inside the mesh's domain. While the aggregates are assumed to behave linear elastic without any contribution to the moisture transport, the constitutive model for the cement paste considers creep, shrinkage and moisture transport.

### Moisture transport

The employed moisture transport model was proposed by Johannesson and Nyman [3]. Equations (1) and (2) describe the transport of liquid water and moist air through the pore system of the cement paste.

$$\rho_{\mathrm{w}} \frac{\partial \eta_{\mathrm{w}}}{\partial t} = \mathrm{div}\left(D_{\mathrm{w}}\left(\eta_{\mathrm{w}}\right) \mathrm{grad}\eta_{\mathrm{w}}\right) + \bar{R}(\eta_{\mathrm{w}}^{\mathrm{eq}} - \eta_{\mathrm{w}}) \tag{1}$$

$$\rho_{\mathrm{g}}^{\mathrm{sat}}\left(\eta_{\mathrm{p}} - \eta_{\mathrm{w}}\right) \frac{\partial \phi_{\mathrm{g}}}{\partial t} - \rho_{\mathrm{g}}^{\mathrm{sat}} \phi_{\mathrm{g}} \frac{\partial \eta_{\mathrm{w}}}{\partial t} = \mathrm{div}\left(D_{\mathrm{g}}\left(\eta_{\mathrm{w}}\right) \mathrm{grad}\phi_{\mathrm{g}}\right) - \bar{R}(\eta_{\mathrm{w}}^{\mathrm{eq}} - \eta_{\mathrm{w}}) \tag{2}$$

The index "w" refers to the liquid water and "g" to the moist air. $\phi_{\mathrm{g}}$ is the relative humidity, $\rho$ and $D$ are the phase specific density and the diffusion coefficient, $\rho_{\mathrm{g}}^{\mathrm{sat}}$ the density of saturated moist air and $\bar{R}$ the mass exchange rate between both phases. $\eta_{\mathrm{p}}$ and $\eta_{\mathrm{w}}$ are the volume fraction of the pores and the liquid water related to the specimens total volume. The equilibrium water volume fraction $\eta_{\mathrm{w}}^{\mathrm{eq}}$ can be obtained from concrete specific sorption curves and is responsible for the mass exchange between both phases.

## Shrinkage

When concrete dries, its volume decreases. This phenomena is called shrinkage. As published in [4], several microscale processes are responsible for this kind of behavior. While it is necessary to consider them all in order to match experimental data as exactly as possible, concentrating on one of the major effects is still sufficient for the purpose of this paper. We will focus on capillary shrinkage which is caused by increasing capillary pressure with decreasing water content of the pore system.

The capillary pressure $p_{\mathrm{c}}$ can be calculated in dependency of the relative humidity by the well known Kelvin-Laplace equation (3) as written in [1].

$$p_{\mathrm{c}} = p_{\mathrm{g}} - p_0 - \frac{\rho_{\mathrm{w}} R T}{M_{\mathrm{w}}} \ln \phi_{\mathrm{g}} \tag{3}$$

$p_{\mathrm{g}}$ and $p_0$ are the pressures of the pore systems' gas phase and the atmosphere. Most of the times both can be assumed to be equal which further simplifies the equation. $R$ is the ideal gas constant, $T$ the temperature and $M_{\mathrm{w}}$ the molar mass of water. The capillary shrinkage strains $\varepsilon_{\mathrm{c}}$ are obtained by eq. (4) [4].

$$\varepsilon_{\mathrm{c}} = \frac{S_{\mathrm{w}} p_{\mathrm{c}}}{3}\left(\frac{1}{K} - \frac{1}{K_{\mathrm{s}}}\right) \tag{4}$$

$K$ is the macroscopic bulk modulus and $K_{\mathrm{s}}$ the solid phases bulk modulus. $S_{\mathrm{w}}$ is the water volume fraction related to the specimens total pore volume. The obtained strains are directly applied to the structure.

## Creep

A Kelvin-Chain model as shown in fig. 1 is employed to describe creep as linear viscoelastic material behavior. By using an arbitrary number of $N$ spring-dashpot combinations, also referred to as Kelvin-Units, experimentally obtained creep curves can be matched as exact as necessary.

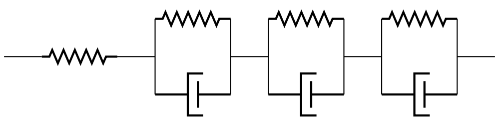

**Figure 1.** Kelvin Chain

A "non-aging" version of the exponential algorithm described in [2] is used to calculate the time dependent states of each Kelvin-Unit with respect to the loading history. Each Kelvin-Unit is defined by two parameters. The spring's stiffness $\mathrm{E}_i$ and the retardation time $\tau_i$. For every timestep the eqs. (5) and (6) are solved.

$$\Delta\varepsilon'' = \sum_{i=1}^{N} (1-\beta_i)\,\gamma_i^n \tag{5}$$

$$\Delta\sigma = \bar{\mathrm{E}}\mathbf{D}_\nu \left(\Delta\varepsilon - \Delta\varepsilon''\right) \tag{6}$$

$$\beta_i = \exp\left(-\frac{\Delta t}{\tau_i}\right); \qquad \lambda_i = \frac{\tau_i}{\Delta t}(1-\beta_i)$$

The first equation calculates the strain increment $\Delta\varepsilon''$ due to creep in dependency of the history variables $\gamma_i^n$. The result is used to obtain the stress increment caused by strain variations and creep. $\mathbf{D}_\nu$ is the linear elastic stiffness matrix calculated with a Young's Modulus of value 1. $\bar{\mathrm{E}}$ is the effective stiffness of the Kelvin-Chain.

After the global system converged, the history variables are updated as given in eq. (7) before proceeding with the next timestep.

$$\gamma_i^{n+1} = \frac{\lambda_i \bar{\mathrm{E}}}{\mathrm{E}_i}\left(\Delta\varepsilon - \Delta\varepsilon''\right) + \beta_i \gamma 1^n \tag{7}$$

## Numerical investigations

### Mesoscale and shrinkage

The described moisture transport model and shrinkage model were used in combination with a linear elastic constitutive law and a rectangular, two dimensional mesh. Starting with 100% relative water content, the atmospheric relative humidity at the boundaries was reduced to 40% to start the drying process. The moisture gradient between the boundaries and the center results in higher shrinkage strains close to the surface. This causes tensile stresses close to the boundaries and compressive stresses at the center. While the stress distribution is symmetric in case of a homogeneous material, the consideration of the mesostructure of concrete causes local variations. As shown in fig. 2 the moisture transport is influenced by the position and sizes of the aggregates. The varying moisture content further enhances the development of stress concentrations caused by the aggregates (fig. 3). In comparison to the homogeneous calculation, the observed maximum tensile stresses are three times higher.

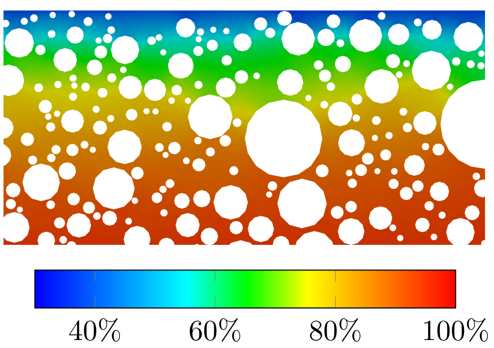


**Figure 2.** Relative water content

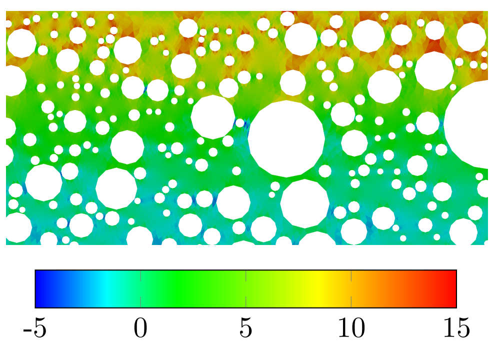


**Figure 3.** Axial stresses [MPa]

### Mesoscale and creep

A linear, viscoelastic creep law as described in section 1.4 will always converge towards the linear elastic solution for $t \to \infty$.

If a constant, uniaxial load is applied to a mesoscale specimen, the stress distribution does not change during the whole simulation. Like the linear elastic case, stress concentrations arise close to the aggregates. The strains in the cement paste grow in accordance with the calibrated creep curve and the local stresses. But the overall shape of the strain field does not change from one timestep to another. In case of a constant uniaxial displacement applied to the boundary the opposite case can be observed. The strain distribution remains constant and the initially high stresses decrease while the shape of the stress field remains constant.

However, in case of varying constraints and loads (for example caused by shrinkage or damage), the situations are different. The previous timestep's load case is partially "conserved" inside the Kelvin-Chains and therefore influences the stress and strain distribution of all further timesteps. Because the aggregates have a significant impact on the internal stress distribution, they also intensify the resulting creep deformations.

## Conclusions

The heterogeneous material structure of concrete effects phenomena like moisture transport, creep, shrinkage and damage. They are also interacting with each other which further enhances the effect of the mesostructure. Some macroscopically observable effects like drying creep or irreversible shrinkage might be direct results of those mesoscale interactions. Further numerical investigations on this subject are necessary to verify this assumption.

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