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Obtaining macroscopic properties from a mesoscale thermomechanical model of concrete

Christoph Pohl[1]* and Jörg F. Unger[1]

Micro Abstract
A coupled thermomechanical mesoscale model for concrete under heating is presented. When considering the heterogeneous structure under coupled loads, complex macroscopic material properties can be modelled using simple constitutive relations. For instance, damage evolution is directly driven by the incompatibility of thermal strains between matrix and aggregates. Without prescribing $f_c = f(T)$, a decline in compressive strength with rising temperatures will be shown.

[1]Safety of Structures, Federal Institute for Materials Research and Testing, Berlin, Germany
***Corresponding author**: christoph.pohl@bam.de

Introduction

To assess the strength of concrete under high temperatures, a common experiment is the heat-then-load (HTL) steady-state test, where the specimen is first heated to a pre-defined temperature and then mechanically loaded. This way, a relation between temperature and compressive strength $f_c = f(T)$ can be obtained. For most test setups and concrete mixes, the strength decreases with rising temperatures [1].

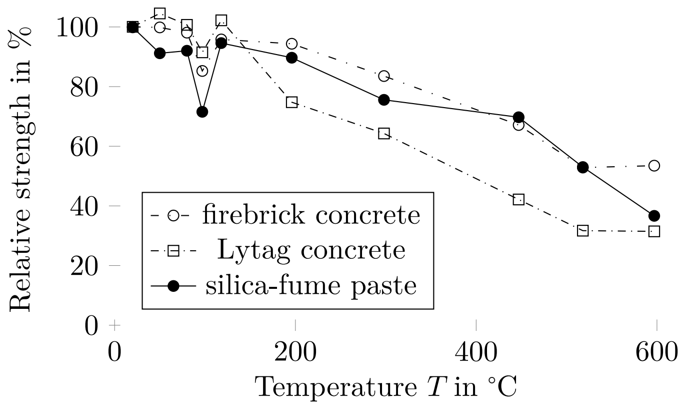

Figure 1. Residual strength of different concretes with temperature (adapted from [9])

The resulting curves can be used in material models for numeric simulations, but this comes with some disadvantages. The calibration of these curves is difficult and thermodynamic consistency can not be ensured. Additionally, there is an inherent size effect for concrete experiments that is laborious to quantify, making the curves limited in applicability.

Once the coupling between thermal behaviour and mechanical performance is taken into account, the resulting model is more accurate and more widely applicable. Here, a constitutive relation with only one value for the compressive strength $f_c|_{T_0}$ will be used, but the specimen will experience failure as if the strength reduced. Or to put it another way: the material has a constant compressive strength, but the specimen acts as if $f_c = f(T)$, yet without prescribing it.

In this contribution, the influence of thermal strains and material damage on the reduction in macroscopic strength will be shown. The damage is computed using the gradient enhanced damage model proposed by [7] see section 2. The whole model has been implemented in the finite element code NuTo.

Other work in this area often looks at more complex interactions, particularly taking the hygral component into account, yet often refrains from projecting the results back on the compressive strength. In [12], the authors use a coupled thermo-hygro-mechanical (THM) model for each constituent of the concrete, i.e. the aggregates, the hardened cement paste and the ITZ. The damage model used was proposed by [5] and is a strongly nonlocal model using a nonlocal equivalent strain as the driving variable behind the damage evolution. In addition, the B3 model [2] is used to describe creep and shrinkage strains as functions of loading and humidity. While the model is more comprehensive, it only investigated the mesoscale interactions without projecting the results back onto the macroscopic behaviour. Additionally, strongly nonlocal formulations can exhibit numerical difficulties.

Another THM model presented by [3] also takes the dehydration of the cement paste at higher temperatures into account. They apply a local isotropic damage model, which exhibits no permanent strain after unloading and is therefore only accurate for pre-peak and early post-peak stages [4]. The influence of the heterogeneous structure of concrete has not been investigated and no observations on the macroscopic mechanical behaviour that results from the model were made.

1 Nonlinear Thermal Expansion

As with most materials, concrete and its constituents expand as they are heated. The matrix material and the aggregates expand at different rates, incurring strains that drive damage growth. The resulting internal stresses than further reduce the load bearing capacity of the specimen.

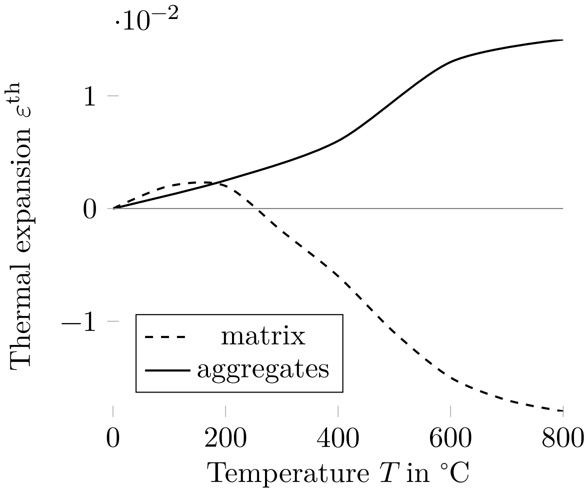

Figure 2. Thermal expansion of concrete constituents (adapted from [8])

As can be seen in fig. 2, the expansion of aggregates and hardened cement paste are similar up to temperatures of about 200 °C. Beyond that, the matrix materials undergoes a substantial contraction. This phenomenon is called shrinkage and is caused by the reduction of water in the specimen at higher temperatures. The influence of the moisture distribution will not be explicitly considered here. Using a nonlinear $\varepsilon^{\mathrm{th}} = g(T)$ will approximate the behaviour described here, but is unable to capture any hysteresis should the specimen undergo cyclic heating.

2 Gradient Enhanced Damage Model

Concrete failure happens in a quasi-brittle fashion, which leads to strain softening. This mechanism incurs the local loss of ellipticity of the governing PDE, making the resulting problem ill-posed. Most models for concrete damage deal with this by considering the vicinity of the material point under consideration. Strongly nonlocal approaches, which integrate over a finite neighbourhood, suffer from certain disadvantages, such as difficulties when dealing with edges and requiring drastic changes to finite element codes.

The Gradient Enhanced Damage Model is a weakly nonlocal model proposed by [7]. By using a Taylor series expansion, the governing differential equation is derived from the nonlocal model. Damage is assumed to be isotropic and is represented by the scalar quantity $D \in [0,1]$, so that the stress-strain relation becomes $\boldsymbol{\sigma} = (1-D)\,\mathbf{C} : \boldsymbol{\varepsilon}$. With growing damage, the load bearing capacity of the material is reduced. This damage variable is a function of a scalar history parameter κ, which is governed by the Karush-Kuhn-Tucker conditions

$$\dot{\kappa} \geq 0, \qquad \bar{\varepsilon}_{\mathrm{eq}} - \kappa \leq 0, \qquad \dot{\kappa}(\bar{\varepsilon}_{\mathrm{eq}} - \kappa) = 0,$$

i.e. κ can only grow, the nonlocal equivalent strain is always smaller or equal to the history parameter, and κ grows only when $\bar{\varepsilon}_{\mathrm{eq}} = \kappa$.

The use of the gradient enhanced damage model will result in an additional independent variable: the nonlocal equivalent strains $\bar{\varepsilon}_{\mathrm{eq}}$. The associated PDE

$$\bar{\varepsilon}_{\mathrm{eq}} - c\nabla^2 \bar{\varepsilon}_{\mathrm{eq}} = \varepsilon_{\mathrm{eq}}.$$

connects this new degree of freedom with the equivalent strains $\varepsilon_{\mathrm{eq}}$, a norm of the strain tensor. The parameter c is the nonlocal radius and relates to the length scale of the nonlocal zone being approximated.

Naturally, there is a need for additional boundary conditions. Imposing either $\bar{\varepsilon}_{\mathrm{eq}}$ or $\nabla\bar{\varepsilon}_{\mathrm{eq}} \cdot \mathbf{n}$ is possible, but the physical interpretation of both these additional conditions is difficult. Often, simply $\nabla\bar{\varepsilon}_{\mathrm{eq}} \cdot \mathbf{n} = 0$ is used.

3 Concretes Mesoscale Structure

Concrete is a composite material with complex internal structure that influences its behaviour. In numerics of concrete, a common approach is to use a homogenized model that smears individual components to a homogeneous material. This necessarily leads to complex constitutive models to capture the observed behaviour. Additional parameters without physical meaning are introduced and experimental data are fitted to them, restricting the validity of these constitutive relations to certain load cases or specimen sizes. This complexity also makes discerning the influences and interactions of the different simultaneous phenomena more difficult.

Concrete is a composite material of multiple phases. These are the hardened cement paste, the coarse and fine aggregates, and—in a sense—the interfacial transition zone (ITZ). This thin layer of matrix material around the aggregates has a lower density and higher permeability [6]. It is the weakest region in the concrete, with experiments having shown that the Young's modulus of concrete is strictly related to the Young's modulus and volume fraction of the ITZ.

Mesoscale modeling allows resolution of this inner structure [11], allowing the use of simpler constitutive models for each component. Together with the resulting complex geometry, the macroscopic behaviour can be represented. In addition, small scale information, such as stress concentration around aggregates and microcrack distribution, can be resolved. The main disadvantages are the high computational costs and memory consumption, due to the fact that the discretization needs to capture the mesoscopic structure.

The mesoscale geometries in this work have been generated using the algorithm from [10].

4 Results

4.1 Size Effect

The temperature distribution inside a specimen during heating is heterogeneous, causing thermal stresses. The magnitude of these stresses depend on material parameters, such as diffusivity and expansion coefficient, but also on the specimen size and heating rates. One advantage of numerical simulations is the possibility of easily ”turning off” the different influences. To look closer at the influence of the size effect on thermal stresses, a homogeneous, macroscale model has been used.

For cylindrical specimen, the thermal stresses on the outer surface are tensile stresses quickly leading to concrete damage. As the stresses rise with higher radii, the remaining strength decreases, which is corroborated by the results seen in fig. 3.

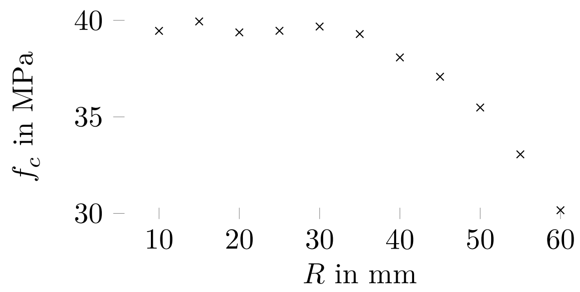

Figure 3. Compressive strength at 500 °C for varying radii

4.2 Influence of Mesoscale Structure

While the size effect is an important phenomenon that should not be neglected, it does not explain the large decline in load bearing capacity seen in experiments. The incompatible thermal expansions of matrix and aggregates lead to further stresses and damage; for typical setups often an order of magnitude larger than those caused by the heterogeneous temperature field. Modeling the mesoscale structure explicitly, with nonlinear expansion functions as seen in section 1, the computations show a much larger decrease in macroscopic compressive strength (fig. 4).

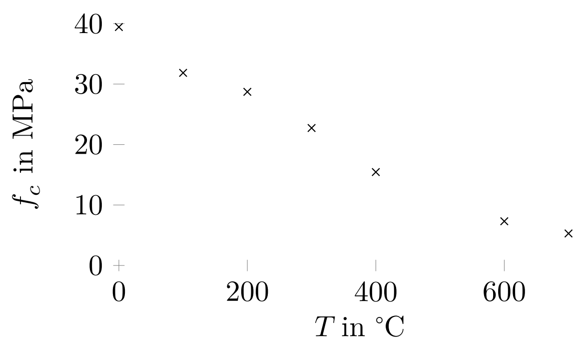

Figure 4. Remaining compressive strength of specimens after being heated to temperature T

The reduction of compressive strength that the specimen exhibits has been obtained with a damage model that is temperature-independent. This result demonstrates the usefulness of numerical calculations in general, and specifically coupled approaches, in the prediction of concrete performance.

Conclusions

The approaches presented here reduces the number of necessary experiments to characterize a concrete mix. Particularly, there is no need to supply a time-dependent strength function for each concrete anymore. Sensitivity calculations and checks for thermodynamic consistency are simplified by avoiding an unnecessarily complex material model. This comes, however, at the price of having to explicitly consider the interactions between thermodynamics and mechanics.

While this model omits important phenomena, most notably the moisture changes during heating, it is an important step towards solving more complicated problems. As the number of additional phenomena under consideration rises, for example water content, shrinkage and creep, the need to apply simpler material laws, while handling the intricacies numerically, increases.

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