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COUPLED ANALYSIS OF TRANSPORT PROCESSES AND MECHANICAL BEHAVIOUR OF CONCRETE AT HIGH TEMPERATURES

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Abstract. A model for the numerical analysis of hygro-thermal and mechanical behaviour of concrete at high temperatures including transport, reaction and deformation processes is presented. For the description of transport and material behaviour the model comprises the balance equations for mass and enthalpy and the constitutive equations for concrete at high temperatures. The degradation of the cement minerals C-S-H and portlandite is described by two chemical reactions. The consideration of thermo-chemical damage in the classical non-local damage theory is discussed. Finally, the finite element formulation for solving the coupled balance equations regarding the primary variables displacement, temperature and relative humidity is presented and numerical results of a 3-D frame corner are discussed.

1 INTRODUCTION

Several serious fires in multi-story buildings and tunnels have been leading to increased research interest in material behaviour under extremely high temperatures. Especially in buildings made of concrete, the most frequently reported building material, fire may effect the strength of construction and reduces the load-carrying capacity.

Concrete is a composite material and consists of several phases. The solid phase comprises of aggregates and cement paste. Here, the cement paste is composed of Calcium-Silicate-Hydrates (C-S-H) and portlandite (CH) and the aggregates are made up of siliceous sand and gravel. The liquid phase consists of capillary water and physically bounded water, dry air and vapour provide the gas phase. High temperatures rising up to 1000 K in the case of fire lead to evaporation of capillaries and absorbed water with concurrent increase of the pore pressure in areas close to surfaces. Above the critical temperature of water, $T_{cr} = 647.3\ K$, water only exists in form of gas, i.e. vapour.

Additionally a chemical reaction in the cement paste leads to degradation of the cement minerals, vapour is released and the porosity of the cement stone increases. As the result of evaporation and dehydration the rising pore pressure and thermal strains lead to damage which often manifests in the form of spalling.

2 BALANCE EQUATION

For the description of transport and reaction phenomena the balance equations of vapour and water and the conservation of energy are taken into account. In the proposed model the effect of dry air is neglected, thence for the gas phase only a vapour balance is necessary. The following balance equations are formulated for the volume average on macroscopic level

$$\frac{\partial}{\partial t}\left(S_g\, n\, \rho_v\right) + \nabla \cdot \boldsymbol{q}_v = s_{v \leftrightarrow w} + s_{v,deh} \quad . \tag{1}$$

The first term of the vapour balance covers the local mass and depends on the porosity n, the saturation of the gas phase S_g and the density of vapour ρ_v. The source terms $s_{v \leftrightarrow w}$ and $s_{v,deh}$ represent sources from phase changes between liquid and gas and the freed vapour from the dehydration reaction. The water balance equation is formulated equivalently with saturation of the liquid phase S_w, density of water ρ_w and the phase change $s_{w \leftrightarrow v}$. The second term in equation (1) represents the pressure driven flow. Here a Darcy law is used for water and vapour. With the assumption of an instant phase change of water and vapour, the summation of water and vapour balances leads to the general water balance equation

$$\frac{\partial}{\partial t}\left(S_g\, n\, \rho_v\right) + \nabla \cdot \boldsymbol{q}_v + \frac{\partial}{\partial t}\left(S_w\, n\, \rho_w\right) + \nabla \cdot \boldsymbol{q}_w = s_{v,deh} \quad . \tag{2}$$

In context of modelling concrete under high temperatures the formulation of the conservation equation of energy leads to the conservation of heat which depends on the heat capacities C_i of each phase, flows, the source terms for evaporation or condensation and the heat of dehydration

$$\left(\sum C_i \overline{\rho}_i\right) \frac{\partial T}{\partial t} + \nabla \cdot \boldsymbol{q}_T = s_{v \leftrightarrow w} \cdot \Delta H_{v \leftrightarrow w} + \Delta H_{deh} \quad . \tag{3}$$

The first term of Equation (3), the local change of heat, depends on temperature T and density of the components related to the concrete volume $\overline{\rho}_i$. The next term describes the heat flow which is divided in a convective and a conductive flow following the Fourier law. The convective part of heat flow is described by the product of the respective flow velocity, density and heat capacity. The heat of evaporation and condensation is the product of change of pore water and latent heat of water which depends on temperature. The last term gives the heat of chemical reaction and may be determined as the product of dehydration rate multiplied by the specific reaction heat. For coupling heat and mass transfer with mechanical behaviour in addition the balance of linear momentum

$$\nabla \cdot \boldsymbol{\sigma} + \rho_c \, \boldsymbol{g} = 0 \tag{4}$$

with Cauchy stress $\boldsymbol{\sigma}$, density of concrete ρ_c and gravitation $\boldsymbol{g}$ is formulated. The density of concrete ensues from the density of the components in consideration of their volume contents.

3 CONSTITUTIVE EQUATIONS

In addition to the balance equations constitutive models for transport, chemical reactions and the mechanical behaviour are necessary which relate the primary variables relative humidity φ, temperature T and displacement vector $\boldsymbol{u}$ with other variables. They are assembled in the next section.

3.1 Heat and mass transport

The transport processes in general may be divided into convection and diffusion. The convective transport is described by Darcy's law and reads for the liquid phase as

$$\mathbf{q}_w = \rho_w \cdot \frac{\mathbf{k} \cdot k_{rw}}{\mu_w} \cdot \left(-\nabla p_w + \rho_w \, \boldsymbol{g}\right). \tag{5}$$

The water pressure p_w which can be expressed in terms of the gas pressure and the capillary pressure $p_w = p_g - p_c$ is the driving force for the transport in the liquid phase, thence the last term is significantly smaller. Further parameters are the intrinsic permeability tensor $\mathbf{k}$, which is depending on the degree of dehydration and the grade of damage, the relative permeability k_{rw} and the dynamic viscosity of water μ_w which is a function of temperature. Analogously the vapour flow is determined by respective parameters. The relative permeabilities k_{rw} and k_{rg} depend only on saturation [1] and are given in Figure 1. As a result of evaporation of pore water and dehydration vapour is generated, what locally leads to an increase of vapour pressure and therewith a higher vapour concentration. The resulting diffusion is described by the diffusion model after Fick

$$\mathbf{q}_v = -\mathbf{D} \cdot \nabla \rho_v. \tag{6}$$

The diffusion coefficient tensor $\mathbf{D}$ incorporates the influence of pore structure and depends on the saturation, temperature and pressure as well.

The saturation of water described by p_c-S_w-relation is received from experimental results [1]. Furthermore, saturation depends on temperature which influences the surface tension of water. Above the critical temperature only vapour exists which is described by the ideal gas law.

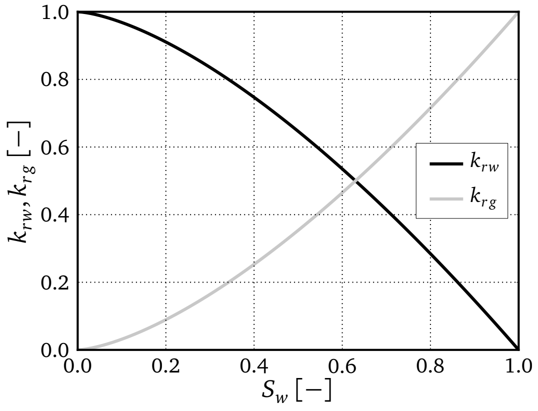

Figure 1: Relative permeability of liquid and gas phase

3.2 Chemical reaction

Besides the transport dehydration is a determining process at high temperatures. During dehydration water, which the concrete contains in form of pore water or chemically bounded water in the crystals, is released and the cement paste is decomposed. Figure 2 shows the degree of dehydration. Here, degradation of portlandite and C-S-H phases may be considered by two chemical reactions, which are leading to additional sources in the heat balance and in the vapour balance [6]. Due to the decomposed cement paste the porosity n increases, see Figure 2, which leads to a significant change in permeability. The enormous ascent of the curves in the temperature range 800-850 K is due to the reaction of the portlandite phase.

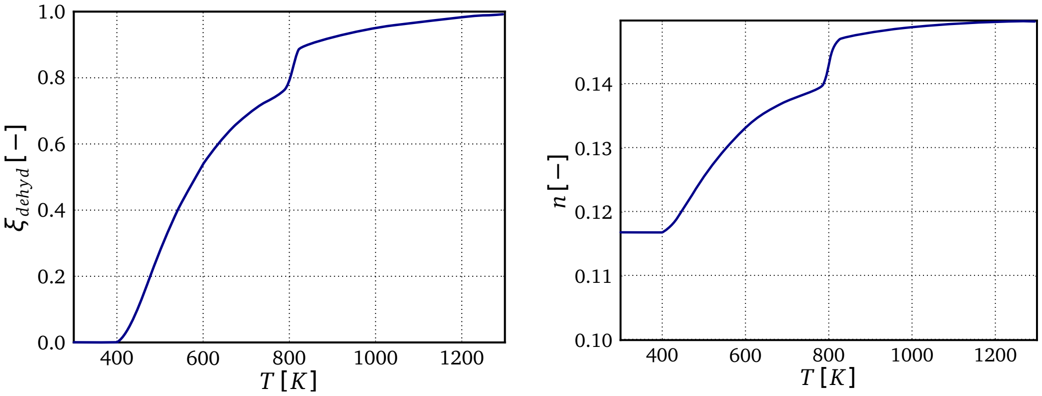

Figure 2: Degree of dehydration and porosity

After the dehydration process the micro structure is not destructed completely, therefore the scalar chemical damage D_{chem} is defined with the linear relationship $D_{chem} = 0.5 \cdot \xi_{dehyd}$.

3.3 Mechanical behaviour

The stress state at a material point is bounded by a failure surface consisting of a Rankine criterion for tensile principal stresses and of a Drucker-Prager criterion for compressive stresses. Due to the composite failure surface, Koiter's flow rule for multi-surface plasticity [5] with the internal variables λ_R and λ_{DP} is used to compute the inelastic strain tensor for stress states at the surface.

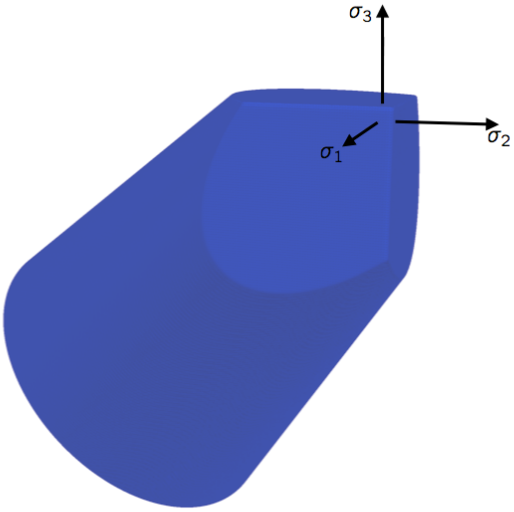

Figure 3: Segmented failure surface for tension and compression

Due to the fact that in classical damage models the results depends on the discretisation parameters the non-local damage theory is used. The isotropic damage parameters D_R and D_{DP} are described with an exponential approach by Peerlings [7] and are affected by the non-local variables $\overline{\lambda}_R$ for tension and $\overline{\lambda}_{DP}$ for compression.
The total mechanical damage which is defined by

$$D_{mech} = 1 - (1 - D_R) \cdot (1 - D_{DP}) \tag{7}$$

allows an individual damage evolution for concrete in uniaxial and multiaxial stress states.

3.4 Coupling of heat and mass transport with the mechanical behaviour

For the coupling of heat and mass transport with the mechanical behaviour it is essential to consider the pore pressure. Often an effective stress tensor

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + b \, p_{pore} \, \boldsymbol{I} \tag{8}$$

is employed, which is the sum of the Cauchy stress tensor and the product of effective pore pressure time the Biot number b times the unit tenor [4]. Baroghel-Bouny et al. define the effective pore pressure as the of the sum of the pressures of liquid and gas phase [1]. Against this Gawin et al. propose a definition of the effective pore pressure as the difference of gas pressure and the capillary pressure [2]. On the other hand pore pressure can be considered by using an equivalent strain

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{el} + \boldsymbol{\varepsilon}^{in} + \boldsymbol{\varepsilon}^{hom} \quad . \tag{9}$$

The elastic strain $\boldsymbol{\varepsilon}^{el}$ and the inelastic strain $\boldsymbol{\varepsilon}^{in}$ result from external load or displacement constraints, whereas the homogenised strain $\boldsymbol{\varepsilon}^{hom}$ is effected by pore pressure within the cement paste, thermal strain of aggregates and cement, and chemical and hygral shrinkage of the cement paste.

Furthermore a combination of mechanical damage D_{mech} and thermo-chemical damage D_{chem} for the description of the total damage D is necessary. Therefore the product approach

$$D = 1 - (1 - D_{chem}) \cdot (1 - D_{mech}) \tag{10}$$

is used. The total damage D is included by the effective stress concept in the material model.

4 STRUCTURAL ANALYSIS

The balance equations are discretised in space by a finite element formulation. The primary variables relative humidity, temperature and displacement are expressed by their nodal values. The discretised form of the model equations reads as the non-linear coupled equations system

$$\mathbf{C}_{ij}(\mathbf{x})\frac{\partial \mathbf{x}}{\partial t} + \mathbf{K}_{ij}(\mathbf{x})\mathbf{x} = \mathbf{f}_i(\mathbf{x}). \tag{11}$$

The non-linear coefficient matrix $\mathbf{C}$ describes the local changes of variables with respect to time, $\mathbf{K}$ the fluxes. For the discretisation in time an implicit Euler scheme is used. The system of non-linear equations is solved by the Newton-Raphson procedure.

For numerical analysis of the process of heating concrete, a 3-D frame corner with heat impact at three surfaces is considered taking the symmetry of the structure into account. The dimension of the cross-section area is 30x30 cm^2. The exposure of the structure to fire is modelled by means of the volume averaged flux boundary condition as described in [3]. The initial conditions of temperature and relative humidity are $T_0 = 293.15\,K$ and $\varphi_0 = 0.6$, the temperature of the fire T_∞ follows the Standard-Fire characteristics.

Figure 4 depicts results of numerical analysis after 10 min. for temperature, degree of dehydration, relative humidity and vapour pressure. During the heat impact the temperature increases and diffuses into the interior. The highest temperature and therefore the greatest damage occurs between the claimed surfaces. At the same time, water evaporates rapidly which induces enormous pressure increase in the gas phase and causes a moisture clog which can be identified by local increase in relative humidity. The highest vapour pressure from evaporation and dehydration appears behind the edges near to the surfaces. Here spalling occurs first.

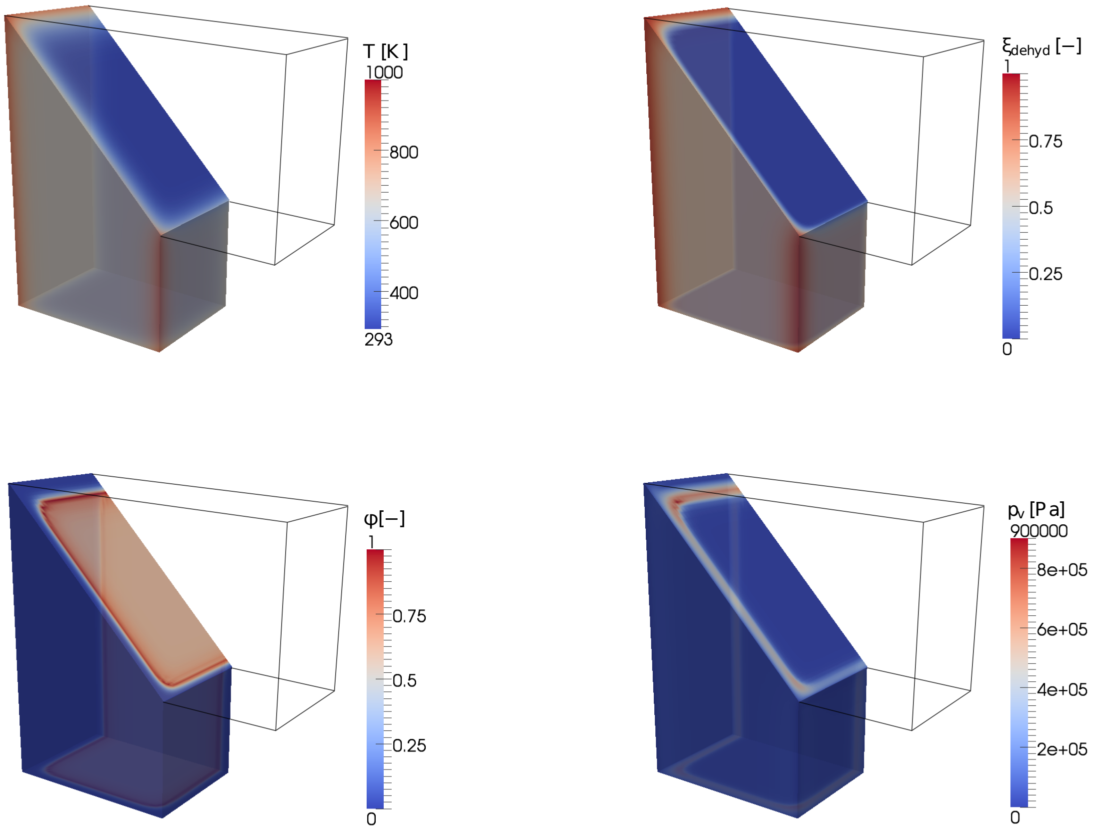

Figure 4: Numerical analysis of a 3-D frame corner - distributions of temperature, degree of dehydration, relative humidity and vapour pressure after 10 min.

5 CONCLUSIONS

A mathematical model for the numerical analysis of hygro-thermal behaviour of concrete structures subjected to high temperatures, including the developing of temperatures and vapour pressure and the damage evolution is presented. The macroscopic balance equations for the conservation of heat, mass of water and vapour and the linear momentum are formulated and important constitutive relations are proposed. The thermo-chemical damage in concrete under high temperatures is considered by non-local damage theory. Finally results of numerical analysis of a 3-D frame corner are discussed. The presented model allows a more detailed understanding of material degradation of concrete at high temperatures. The decrease of load-carrying capacity after fire events may be predicted more realistically.

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