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SIMULATION AND MATHEMATICAL OPTIMIZATION OF THE HYDRATION OF CONCRETE FOR AVOIDING THERMAL CRACKS

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Abstract. *After mixing of concrete, the hardening starts by an exothermic chemical reaction known as hydration. As the reaction rate depends on the temperature $y(t,x)$, the time in the description of the hydration is replaced by the maturity $\int_0^t g(y(\vartheta,x))\mathrm{d}\vartheta$ with a certain function $g(\cdot)$ according to Freiesleben-Hansen (see e.g. [6]). The temperature y is governed by the heat equation with a right hand side depending on the maturity and the temperature y itself, see [6]. We compare of the performance of different time integration schemes of higher order with an automatic time step control.*

The simulation of the heat distribution is of importance as the development of mechanical properties is driven by the hydration. During this process it is possible that the tensile stresses exceed the tensile strength and cracks occur. The goal is to produce cheap concrete without cracks. Simple criteria use only temperature differences between two specified points. More involved criteria are based on thermal stresses. If the criterion predicts cracks some kind of changes in the input data are needed.

Optimization is a concept which sometimes has a completely different meaning to engineers and to mathematicians. In engineering literature optimization is often understood as a variation of the input data (by hand) and a following simulation. The optimization is stopped if some criterion is fulfilled, never mind whether it is really the cheapest possible solution [13, Figure 1.3]. The target of mathematical optimization is the computation of this cheapest possible solution, or at least a good approximation of it.

The final goal will be to adopt mathematical optimization to the problem of the hydration of young concrete and the avoidance of cracks. The first step is the simulation of the hydration, which we focus in this paper, further steps are results about the mathematical background (proof of existence and uniqueness of the solution of the optimal control problem) which will follow in the upcoming paper [1].

1 INTRODUCTION

Modern civil engineering and architecture would not be possible without concrete. So measurement and simulation of all the different aspects of concrete is a wide field of activity in (civil) engineering. Our aim is not the overall simulation of all aspects of concrete, but the simulation of the temperature distribution and a prediction of thermal cracks during hydration.

The simulation of hydration is needed as input for the calculation of material properties, strengths and stresses and therefore also for the calculation of a crack criterion [20]. Some crack criteria consider only the temperature but generally a criterion would be preferred which also accounts for the development of stresses [18, 19]. We summarize the modeling of the hydration, the thermo-mechanical properties and crack criteria in section 2.

Then we discuss the numerical solution of the heat distribution in young concrete in section 3. If, after the simulation of the hydration, the crack criterion indicates that there will be thermal cracks, some changes in the input data are required. The variation of the input data can be interpreted as optimization. We discuss simulation based optimization and model based optimization in section 4. Further we introduce a family of abstract optimal control problems for the hydration of concrete in this section. One problem of this family is introduced in deeper detail. Finally conclusions and an outlook are given.

2 MODELING OF THE HYDRATION OF CONCRETE

2.1 General idea

Concrete is produced from the mixing of cement, aggregate, admixtures and water. By varying the ratio and kind of the ingredients a wide range of concrete for different purposes can be composed. After mixing, the hardening of the concrete starts by an exothermic chemical reaction known as hydration. During this reaction the liquid or plastic viscous mass develops the solid properties of the concrete. The specific solid properties of the concrete are determined by the ratio of the ingredients.

The hydration can be studied on different scales. Studies on microscopic scales inspect the chemical reaction on a molecular scale. On the other hand studies on the macroscopic scale investigate the development of heat, mechanical properties and cracks. Therefore the molecular processes are hidden in an averaged description. We want to introduce and simulate such a model.

The basis of this description is the degree of hydration which defines the fraction of the reaction which has been occurred until a specific point in time. As this ratio can not be measured directly different indirect definitions are in use. We use a common definition of the degree of hydration based on the heat development

$$\alpha(t,x) = \frac{Q(t,x)}{Q_\infty}, \tag{1}$$

where Q_∞ is the overall heat that is produced by hydration and $Q(t,x)$ is the heat produced until the time t. Note, that the degree of hydration can assume different values in different points of the same concrete structure.

A model for the degree of hydration is one of the two main ingredients of a description of concrete. On the other hand the reaction rate of this reaction depends on the temperature $y = y(t,x)$ measured in °C. Therefore time in the description of the hydration is replaced by

the maturity (effective age). A common form for the maturity is $\tau(t, y(\cdot,\cdot)) = \int_0^t g\left(y(\vartheta, x)\right) \mathrm{d}\,\vartheta$ with an appropriate function $g(\cdot)$.

2.2 Maturity

In the literature different choices for the maturity are known. We present maturities which are widely used in engineering literature. Freiesleben-Hansen introduced a formula which can be motivated by chemical reaction kinetics (see Eierle [6])

$$\tau(t, y(x,\cdot)) = \int_0^t \exp\left(\frac{A}{R}\left(\frac{1}{293} - \frac{1}{273 + y(x,\vartheta)}\right)\right) \mathrm{d}\,\vartheta. \tag{2}$$

where R is the universal gas constant and the activation energy A is a material parameter. In general A may depend on the temperature but according to [13, (5.22)] an activation energy which is independent of the temperature is applicable to a large class of cements.

Another simpler maturity was introduced by Saul as

$$\tau(t, y(x,\cdot)) = \int_0^t \frac{y(x,\vartheta) + 10}{30} \mathrm{d}\,\vartheta. \tag{3}$$

This maturity is independent of the concrete in use. Therefore it seems very logical that the maturity of Freisleben-Hansen (2) will produce more realistic simulations. Finally we mention Röhling [17] who uses

$$\tau(t, y(x,\cdot)) = \int_0^t \left(\frac{y(x,\vartheta) + 15}{35}\right)^d \mathrm{d}\,\vartheta, \qquad d \approx 2 \tag{4}$$

as approximation of the maturity of Freiesleben-Hansen for some specific cements.

But nevertheless all the maturities have the abstract form

$$\tau(t, y(x,\cdot)) = \int_0^t g\left(y(x,\vartheta)\right) \mathrm{d}\,\vartheta. \tag{5}$$

In our analysis we will use this abstract notation and assume only the characteristics which we need for a specific result.

2.3 Adiabatic heat development

As mentioned in section 2.1 the basis of the description of hydration is the degree of hydration. Even if there is a wide range of applications and compositions of concretes, they all share the basic shape of the development of the degree of hydration (see Figure 1). Eierle [6] compares different approaches the modeling of this shape. A well-known approach was introduced by Wesche [25]

$$\alpha = \alpha(\tau) = \mathrm{e}^{a\tau^b} \qquad a, b < 0. \tag{6}$$

Another very common approach is the model of Jonasson (see e.g. [6])

$$\alpha = \alpha(\tau) = \mathrm{e}^{a\left[\log\left(1+\frac{\tau}{\tau_k}\right)\right]^b} \qquad a,\ b < 0,\ \tau_k > 0. \tag{7}$$

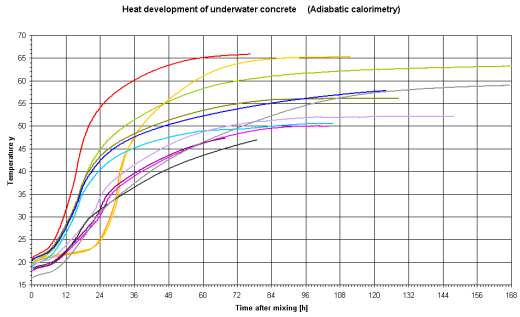

Figure 1: Adiabatic heat development of different concrete recipes according to experimental data from Prof. Dr.-Ing. Manfred Keuser and Dr.-Ing. Eugen Hiller, Professur für Massivbau, Universität der Bundeswehr München. In adiabatic experiments the temperature y is directly proportional to the degree of hydration $\alpha = \frac{Q(t,x)}{Q_\infty}$ as there is no heat conduction and therefore $c\rho y(t,x) = Q(t,x)$.

The parameters $a,\ b,\ \tau_k$ in the models by Jonasson (7) and Wesche (6) are obtained by measurement of the adiabatic heat development and a parameter fit. In the model of Jonasson (7) a is often set to -1.

Actually we present the different approaches but we do not want to evaluate them. In our mathematical setting we hide the model for the adiabatic heat development with the formula

$$\alpha(\tau) = \int_0^\tau h(\vartheta)\,\mathrm{d}\,\vartheta. \tag{8}$$

2.4 Heat conduction

As the development of the mechanical properties of concrete in every point is driven by the hydration the simulation of the progress of hydration is an important task. As the degree of hydration is measured by the heat development, the heat distribution must be calculated.

For a new concrete structure Ω the heat distribution is governed by the heat equation with the hydration rate as heat source. Therefore the temperature $y = y(t,x)$ is determined by the heat equation

$$c\rho y_t - \nabla\cdot(\lambda\nabla y) = Q_\infty\dot{\alpha} = Q_\infty\frac{\partial\alpha}{\partial\tau}\frac{\partial\tau}{\partial t} = Q_\infty h(\tau)g(y). \tag{9}$$

We assume that the material parameter $c,\ \rho$ and λ are independent of space, time, temperature and degree of hydration [13, chapter 5.1].

As the maturity τ is defined in (5) as some integral over y the heat equation (9) is a integrodifferential equation. For the analysis and numerical analysis of this equation we prefer to compute τ as additional function [7, Chapter II.17, p.351f], so we have as additional equation

$$\tau_t = g(y) = \frac{\partial\tau}{\partial t} \tag{10}$$

Therefore we can use for the discretization in time any discretization method for ordinary differential equations and do not need method specialized for integrodifferential equations as in [5].

To complete the system of equation we still need to specify boundary and initial conditions. As initial condition for the equation for the maturity (10) we choose zero initial data with respect to the definition of the maturity (5). For the temperature y the initial condition is the temperature

y_0 of the concrete after mixing and installation.On the boundary we assume Robin conditions (boundary conditions of 3rd kind)

$$\frac{\partial y(t,x)}{\partial \nu} = \sigma(t,x)\left(y_{\text{BND}}(t,x) - y(t,x)\right).$$

This boundary condition describes the heat transfer through the formwork. Typically the coefficient σ is not any $L^2\left((0,T]\times\partial\Omega\right)\cap L^\infty\left((0,T]\times\partial\Omega\right)$ function but (piecewise) constant in space and has only finitely many jumps between discrete values in time. These jumps occur when the formwork is removed or changed. With these Robin boundary conditions it is also possible to simulate Neumann boundary conditions for symmetry axes ($\sigma = 0$ on Γ_N).

For the ambient temperature we assume the smooth distribution

$$y_{\text{BND}}(t) = y_{\text{med}} + \frac{1}{2} y_{\text{Delta}} \cos\left(\frac{2\cdot\pi}{24}\cdot t\right),$$

where t is measured in hours and the values y_{med} and y_{Delta} are chosen according to the values summarized in the German code DIN 4710.

Altogether the temperature distribution during hydration is described by

$$\begin{aligned}
\tau_t &= g(y) && \text{in } (0,T]\times\Omega && (11)\\
c\rho y_t - \lambda\,\Delta\, y &= Q_\infty h(\tau) g(y) && \text{in } (0,T]\times\Omega && (12)\\
\frac{\partial y(t,x)}{\partial \nu} &= \sigma(t,x)\left(y_{\text{BND}}(t,x) - y(t,x)\right) && \text{on } (0,T]\times\partial\Omega && (13)\\
\tau(0,x) &= 0 && \text{in } \{0\}\times\Omega && (14)\\
y(0,x) &= y_0(x) && \text{in } \{0\}\times\Omega. && (15)
\end{aligned}$$

2.5 Mechanical properties

The heat distribution influences the development of the mechanical properties of concrete. We consider Young Modulus E, tensile strength f_{ct} and compressive strength f_{cc}. The Poisson ratio ν is assumed to be constant. These quantities develop during hydration, and therefore commonly used models (see e.g. [13]) describe them depending on the degree of hydration α. We use the following model (see also [13, 18, 19])

$$E(\alpha) = E_\infty \left(\frac{\alpha-\alpha_0}{1-\alpha_0}\right)^{\gamma_1} \tag{16}$$

$$f_{ct}(\alpha) = f_{ct,\infty} \left(\frac{\alpha-\alpha_0}{1-\alpha_0}\right)^{\gamma_2} \tag{17}$$

$$f_{cc}(\alpha) = f_{cc,\infty} \left(\frac{\alpha-\alpha_0}{1-\alpha_0}\right)^{\gamma_3}. \tag{18}$$

The final values $E_\infty,\ f_{ct,\infty}$ and $f_{cc,\infty}$ and the exponents $\gamma_1,\ \gamma_2$ and γ_3 are material parameters, typical values for γ_i are $\gamma_1 = \frac{1}{2},\ \gamma_2 = 1$ and $\gamma_3 = \frac{3}{2}$. Further the value α_0 marks the degree of hydration above which solid body properties can be measured. This value can also depend on the concrete in use.

With this material properties it is possible to compute the thermoelastic stresses. In thermoelasticity it is assumed that temperature changes induce thermal strains of the form

$$\varepsilon_{\text{therm}}(y) = \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix} \alpha_{\text{therm}} \Delta y \tag{19}$$

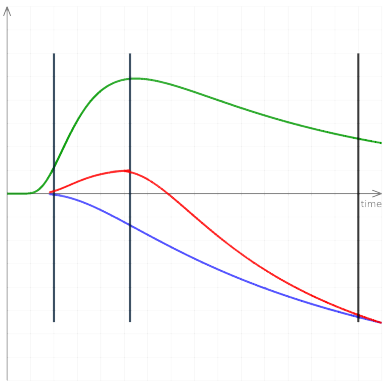

Figure 2: Development of temperature (green), stresses (red) and strength (blue) over time t in a specific point of the concrete

where no shear strains are introduced [2]. Further these thermal strains are additive to the elastic strains.

If we choose a material model, either a linear elastic material law with time dependent Young modulus or a viscoelastic model according to [17], the mechanical properties and thermal stresses can be calculated in a post processing step after simulation of the hydration.

2.6 Crack criteria

The computation of the mechanical properties is the base of the decision whether thermal cracks in the concrete occur or not. The qualitative development of temperature, tensile strength and thermal stresses is drafted in Figure 2. In the first phase of hydration the concrete is still liquid and has no rigid body properties. At some point in time, when the degree of hydration reaches α_0, rigid body properties are measurable for the first time, then the temperature still rises and therefore small compressive stresses establish as Young modulus is still small. After the temperature maximum is reached larger tensile stresses can be observed as Young modulus is already larger. Cracks occur when the tensile stress is larger than the tensile strength.

After this short discussion it is clear that no cracks will occur because of tensile stresses if

$$|\min(0, \sigma(t,x))| \leq |f_{\text{ct}}(t,x)| \qquad \forall (t,x) \in (0,T] \times \Omega. \tag{20}$$

In engineering practice one would even add some safety factor so that

$$\frac{|\min(0, \sigma(t,x))|}{|f_{\text{ct}}(t,x)|} \leq k \qquad \forall (t,x) \in (0,T] \times \Omega \tag{21}$$

with some $k < 1$ must hold [18, 19].

Crack criteria of this kind need the computation of mechanical properties which is more expensive than the computation of the heat distribution (2 or 3 degree of freedom in every node in contrast to only one degree of freedom for the heat distribution). As the prediction of cracks in young concrete has a long history in civil engineering there are temperature criteria which predict cracks only with the information on the heat distribution. These criteria are computable with less computational effort and ignore solid mechanical properties of the young concrete so they must be less accurate. But they are exact enough for the assessment of the crack risk.

If we consider a new concrete wall on a old bottom plate as in Figure 3, a temperature criterion would read as

$$|y(t,x_1) - y(t,x_2)| \leq 15K \qquad \forall t \in (0,T], \tag{22}$$

where x_1 and x_2 denote the midpoints of the new wall and the bottom plate.

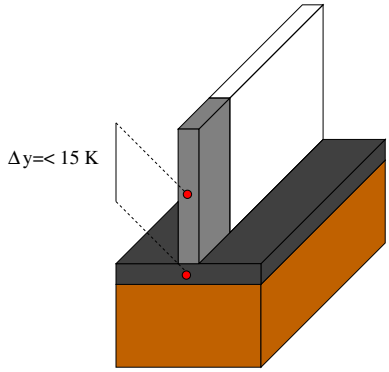

Figure 3: Geometry for the temperature criterion: Old bottom plate (black), old wall(gray), a new wall (white) and substrate (brown). The temperature difference along the middle points in x_2-direction is observed.

3 ANALYSIS AN NUMERICAL ANALYSIS OF THE MODEL

3.1 Existence and uniqueness of solutions

Theorem 3.1. *For any combination of the maturities of Freisleben-Hansen (2) or Saul (3) with the model for the degree of hydration of Wesche (6) or Jonasson (7), a unique solution (τ, y) for the nonlinear heat equation (11)–(15) exists.*

Proof. The existence can be proven by the use of the Schauder fixed point theorem. The uniqueness follows by contradiction and appropriate and realistic assumptions on g and h. For details we refer to [1]. □

3.2 Numerical analysis

For the numerical simulation we consider a method of lines. First we discretize in space with finite elements. This leads to the semidiscrete system of ordinary differential equations

$$\tau_{h,t} = g(y_h) \tag{23}$$

$$My_{h,t} = -(\lambda K + \sigma R)y_h + \sigma R y_{\text{BND}} + Q_\infty M h(\tau_h) g(y_h), \tag{24}$$

where M is the mass matrix, K the stiffness matrix and R the matrix which implements the Robin boundary conditions. For the discretization in time we choose Matlab's time integration schemes for stiff ordinary differential equations.

In particular we study the performance of the following integration schemes. The routine `ode23t` implements a midpoint rule with step size control [22]. The performance of this time integration scheme is of interest as the midpoint rule can be interpreted as a continuous Galerkin scheme. For optimal control problems with parabolic partial differential equations Galerkin schemes in time are often used as the commutation of discretization and optimization result in the same discrete scheme (see e.g. [14, 15]).

We compare `ode23t` with the other integrators for stiff differential equations (`ode15s`, `ode23s` and `ode23tb`). The routine `ode15s` is the Matlab implementation of numerical differentiation formulas (NDF), a variant of Gear's backward differentiation formulas (BDF) [21]. But `ode15s` can also be configured to use the BDF integration scheme. And finally `ode23s` and `ode23tb` are implicit Runge-Kutta methods, whereas `ode23s` is a Rosenbrock method , and `ode23tb` is a diagonally implicit Runge-Kutta (DIRK) method [10, 21].

For the numerical tests we use a two dimensional cross section of the geometry which we used to introduce a temperature criterion without the substrate (see Figure 3). For the maturity

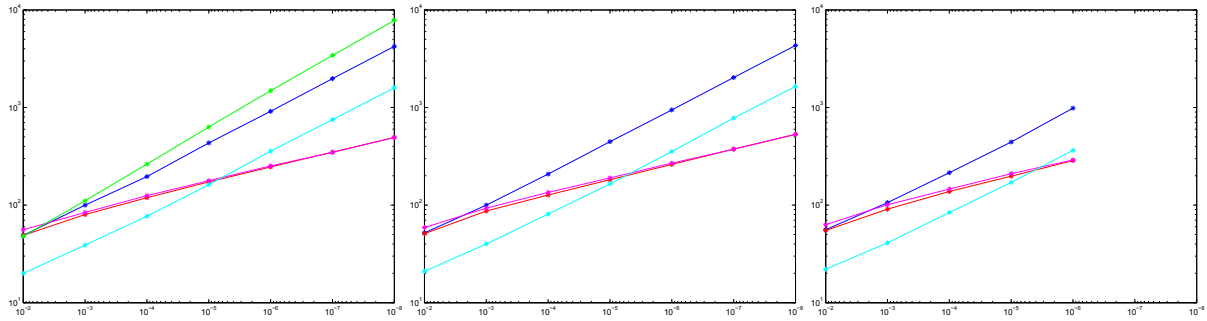

Figure 4: Number of time steps for different space discretization levels (from left to right 300, 1100 and 4200 nodes) which are needed to fulfill the error estimator of the time integration scheme with $ATOL = RTOL = 10^{-2} \cdots 10^{-8}$ respectively $RTOL = ATOL = 10^{-2} \cdots 10^{-6}$ in the last case. Red NDF, magenta BDF, blue midpoint rule, cyan `ode23tb`, green `ode23s`

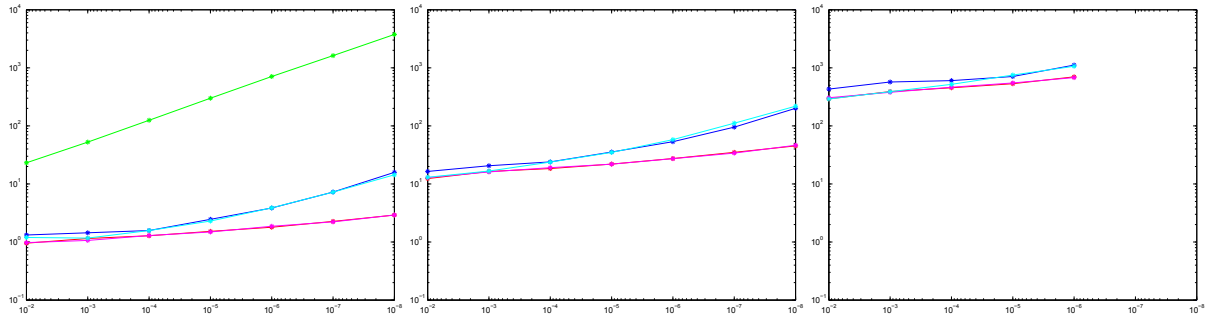

Figure 5: Work-precision diagrams for different space discretization levels (from left to right 300, 1100 and 4200 nodes) which are needed to fulfill the error estimator of the time integration scheme with $ATOL = RTOL = 10^{-2} \cdots 10^{-8}$ respectively $RTOL = ATOL = 10^{-2} \cdots 10^{-6}$ in the last case. Red NDF, magenta BDF, blue midpoint rule, cyan `ode23tb`, green `ode23s`

we use the formula of Freiesleben-Hansen (2) and for the hydration the model of Jonasson (7). The post processing step for the calculation of strength and stresses was not part of the performance test.

The discretization in space is done with triangular linear finite elements with a uniform mesh and about 500, 2000 and 4200 elements (300, 1100 and 4200 nodes). The time stepsize was adaptively chosen by Matlab's ODE integrators.

As first indication for the performance of a time integration scheme is the number of time steps which is needed to satisfy the error estimator to fulfill a given tolerances. This number is given for the different methods in Figure 4. First it is obvious that `ode23s` needs the most time steps, especially on small tolerances for the time integration. The number of timesteps is even nearly two times the number of time steps of the midpoint rule which needs most timestep of the other methods. Therefore we did not plot the number of time steps of `ode23s` on the finer meshes.

For small requirements on the time integration error all methods need a comparable number of time steps. On higher requirements the BDF and NDF scheme need the fewest timesteps and the number of time steps of the NDF and BDF schemes nearly coincide.

But a scheme with many very "cheap" time steps can be faster than another scheme with less, but more expensive time steps. Therefore one must also pay attention to the overall simulation time, see the work precision diagrams in Figure 5. Again `ode23s` needs the longest computation time. On small and middle requirements for the accuracy all other integration schemes

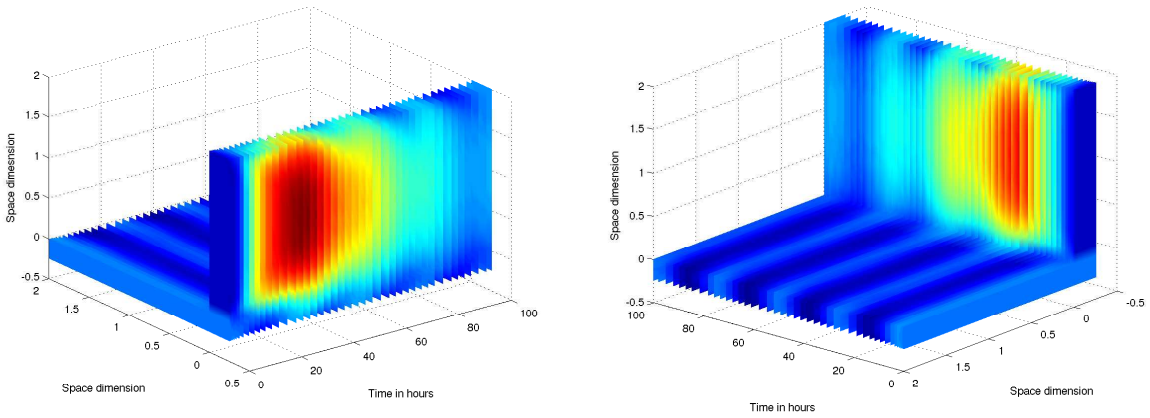

Figure 6: Numerical solution of the simulation of the situation of Figure 3. For symmetry reasons only the half half of the geometry was simulated. Midpoint rule `ode23t` with ATOL=RTOL=10^{-2} and 300 nodes.

have comparable computation times. On high requirements on the tolerance the NDF and BDF schemes perform best, again with nearly identical computation times.

Finally we present some figures of the computed solutions in Figure 6. As noted before we simulated two dimensional cross section of the geometry of Figure 3 without the substrate. Further we simulated only the left half of the geometry for symmetry reasons. The figure presents the temperature distributions for the cross section at the time steps of the midpoint rule in two points of view. The rising and decreasing of the temperature because of the hydration can be seen in the new wall. One can also observe the temperature variations because of the time dependent ambient temperature in the bottom plate.

4 OPTIMIZATION

4.1 Simulation based and model based optimization

Until now we have only simulated the heat distribution during hydration. But in engineering practice one is always interested in a solution which is (in some sense) “optimal”.

Optimization is a concept which sometimes has a completely different meaning to engineers and mathematicians. In engineering literature optimization is often understood as a variation of the input data (sometimes even by hand) and a following simulation. The optimization is stopped if some criterion is fulfilled, never mind whether it is really the cheapest possible solution (see Figure 7). This approach is also called simulation based optimization. So the solutions depends on the experience of the engineer who performs the simulation and on the way the input data are changed.

The target of mathematical optimization, also called model based optimization, is the computation of this cheapest possible solution, or at least a good approximation of it. Furthermore the effort for optimization (and simulation) should be less then n times effort for the only simulation, with n small [9], so that the effort of model based optimization is competitive to the effort of simulation based optimization. The optimal solutions depends only on the data (constraints, initial value, geometry) and discretization step sizes (k for the time discretization and h for the discretization in space) but not on the experience of the person who performs the optimization. A schematic sketch is provided in Figure 8.

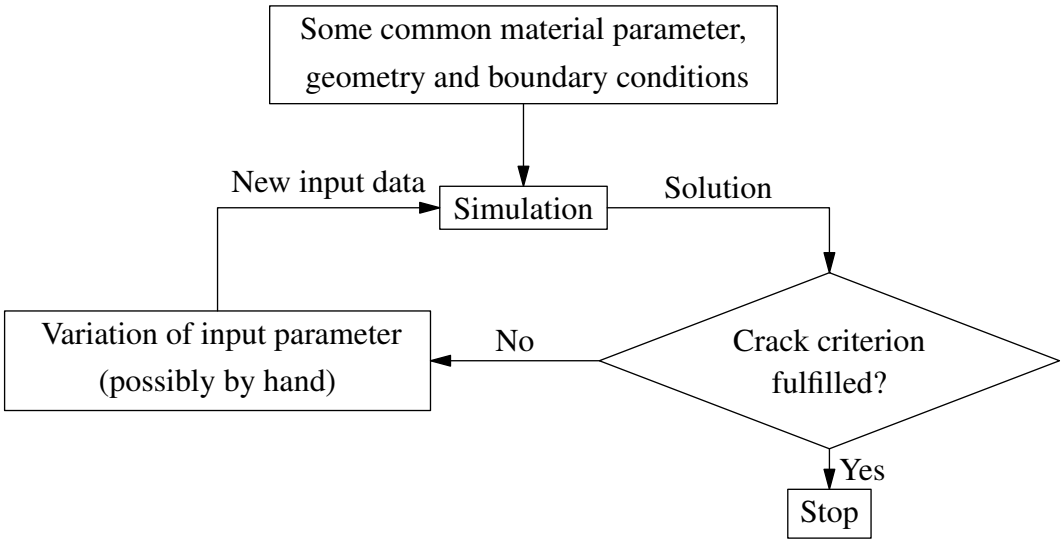

Figure 7: Optimization according to engineering literature (simplification of e.g. [13, Figure 1.3] or [8, Figure 4.2])

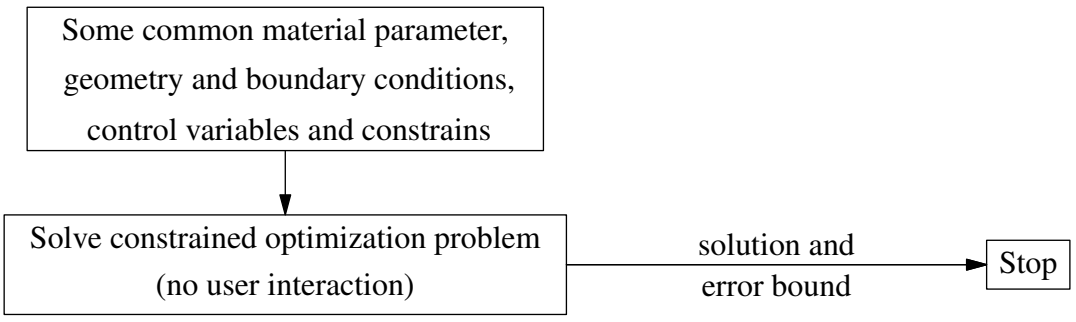

Figure 8: Mathematical optimization

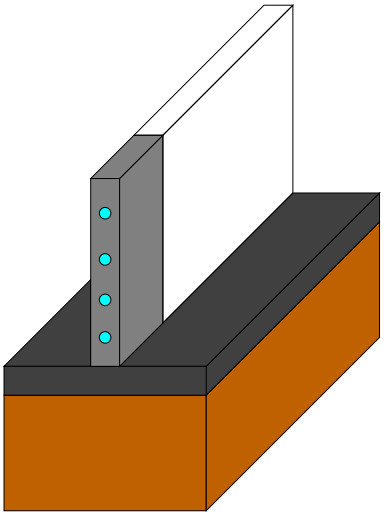

Figure 9: Geometry of Figure 3 with additional cooling pipes

4.2 A family of optimal control problems for the hydration of concrete

We introduce now a family of optimal control problems for the hydration of concrete. All these problems have the form

$$\min J(y, \tau, u) \tag{25}$$

$$\text{so that } y,\ \tau \text{ solve the equations (11)–(15)} \tag{26}$$

$$\text{where } u \text{ is a control variable and influences some input data of (26)} \tag{27}$$

$$\text{and a crack criterion is fulfilled.} \tag{28}$$

The cost functional (25) should represent realistic costs for the controls. There are different possibilities for controlling the state equation (26).

First the composition of the concrete may be controlled. With this kind of control we influence the heat development on the right hand side (and therefore the parameters a, b and τ_k in the model of Wesche (6) or Jonasson (7)) and all the material parameters. Further one could think about a modification of the fresh concrete temperature (see also [16] for a simulation based optimization), the installation of cooling pipes (see Figure 9 and [11] for a modeling of cooling pipes) or the the value of the heat transfer coefficient σ (e.g. variation of the formwork). For practical reasons the heat transfer coefficient should be piecewise constant in space and only change at specific points in time. All these controls have constraints by national or international codes, workability, technical possibilities or possible water flow rate. In specific control problems it is possible that not all mentioned controls are allowed. So one should specify which controls are possible.

Last, a crack criterion which we introduced in section 2.6 is an additional state constraint. Some of the examples of this family of optimization problems are discussed in [1] for the geometry which we introduced for the temperature crack criterion (see Figures 3 and 9).

4.3 A specific optimal control problem for the hydration of concrete

There are two ways for a mathematical treatment of the optimization problem (25)–(28). On the one hand one can first optimize and then discretize, i.e. calculate the first oder optimality conditions in appropriate function spaces and discretize the system [24]. On the other hand one

can first discretize the optimal control problem and afterwards solve the nonlinear optimization problem. For a discussion of both approaches see [9, Chapter 3]

Here we want to discuss the latter approach for an optimal control with the initial temperature and a temperature criterion. The problem is

$$\min \|u\|^2 \tag{29}$$

$$\tau_t = g(y) \qquad \text{in } (0,T] \times \Omega \tag{30}$$

$$c\rho y_t - \lambda \Delta y = Q_\infty h(\tau) g(y) \qquad \text{in } (0,T] \times \Omega \tag{31}$$

$$\frac{\partial y(t,x)}{\partial \nu} = \sigma(t,x)\left(y_{\text{BND}}(t,x) - y(t,x)\right) \qquad \text{on } (0,T] \times \partial\Omega \tag{32}$$

$$\tau(0,x) = 0 \qquad \text{in } \{0\} \times \Omega \tag{33}$$

$$y(0,x) = y_{o,1}(x) - u \qquad \text{in } \{0\} \times \Omega_1 \tag{34}$$

$$y(0,x) = y_{o,2}(x) \qquad \text{in } \{0\} \times \Omega_2 \tag{35}$$

$$|y(t,x_1) - y(t,x_2)| \leq 15K \qquad t \in [0,T]. \tag{36}$$

The control is performed by the initial condition (34). The initial temperature $y_{o,1}$ is cooled by the control u in the fresh concrete in Ω_1. The temperature in the bottom plate Ω_2 can not be controlled. For practical reasons $y_{o,1}$ would be the temperature at which the concrete can be produced without any additional costs for cooling. The cooling of the fresh concrete can be performed by the use of very cold water or even crashed ice.

As there are different ways to cool the fresh concrete down, the costs for the cooling are clearly nonlinear. We approximate these costs with a quadratic cost functional which can be motivated by the interpolation of the specific costs for the different cooling possibilities.

A discretization of this problem using finite elements in space and the Crank-Nicolson scheme in time is

$$\min u^T M u \tag{37}$$

$$\frac{\tau_{i+1} - \tau_i}{k} = \frac{g(y_{i+1}) + g(y_i)}{2} \tag{38}$$

$$M\frac{y_{i+1} - y_i}{k} + (\lambda K + \sigma R)\frac{y_{i+1} + y_i}{2} - \sigma R \frac{y_{\text{BND},i+1} - y_{\text{BND},i}}{2} = = Q_\infty \frac{h(\tau_{i+1})g(y_{i+1}) + h(\tau_i)g(y_i)}{2} \tag{39}$$

$$\tau_0 = 0 \tag{40}$$

$$y_0 = y_o - u \tag{41}$$

$$|y_i(x_1) - y_i(x_2)| \leq 15K, \tag{42}$$

if we assume that the fresh concrete can be produced and embedded with different temperatures in different places. Under the assumption that the temperature should be constant in the concrete the functional (37) can be replaced by $\min u^2$. This problems can be solved using solvers for nonlinear optimization problems.

5 CONCLUSIONS AND PERSPECTIVES

In this paper we presented a model for the hydration of concrete and have shown first numerical simulations of this model. Further we introduced the idea of model based optimization to

this class of problems. As earlier works on the model based optimization and optimal control for the hydration of concrete only one work is known to the authors. In 1986 Kalkowski discusses the optimal control for some special circumstances where the partial differential equation for the temperature distribution could be reduced to a system of ordinary differential equations [12]. But since this time the possibilities in scientific computing have dramatically changed. Today we can not only simulate partial differential equations but also simulate the optimal control for partial differential equations.

A first example of the approach first-discretize-then-optimize was presented. This very simple example shows that this approach is possible and should motivate the use of model based optimization in engineering practice. The existence of a solution of the (continuous) optimal control problems and further examples will be addressed in the forthcoming paper [1].

The numerical examples have been computed on a uniform mesh and with adaptive timestep control. For elliptic partial differential equations it is well known that on domains with reentrant corners mesh grading is essential for optimal convergence (see e.g. [26]). For the simulation of parabolic partial differential equations similar results exist [3, 23] but for the optimal control of parabolic differential equations such results are not proven yet.

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