From concrete mixture to structural design - a holistic optimization procedure

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Abstract

Amazing introduction to this topic, talking about problemes with local optimization on mix and strucutre. We are ... By applying .... stochastic methods, the quality of the data can be estimated. Automated workflow to simplify addition of additional data points and general reproducibility.

Keywords: performance oriented design, stochastic optimization, precast concrete, mix design

1 Introduction

General introduction. Giving background, motivation and state of the art. I would focus on example with reduction of GWP, as this is a good example where the optimum is difficult to find by local optimization. Improving GWP usually reduces material properties. Reduced properties usually increases GWP, as mor ematerial is required, therefore this is an insteresting problem.

The focus of this paper is not on the model applied, these are not newly developed on their own. The added value of this manuscript is on the one hand

showing a method that is able to automatically compute relevant KPI on the structural level, based on input values, including parameters relevant for the concrete mix design. On the other hand this paper gives details on numerical methods to run a robust (?) optimization method which takes into account uncertainties based on the raw experimental data.

In Figure 1 an overview of the workflow is given which is used to compute the KPIs and is the heart of the optimization scheme.

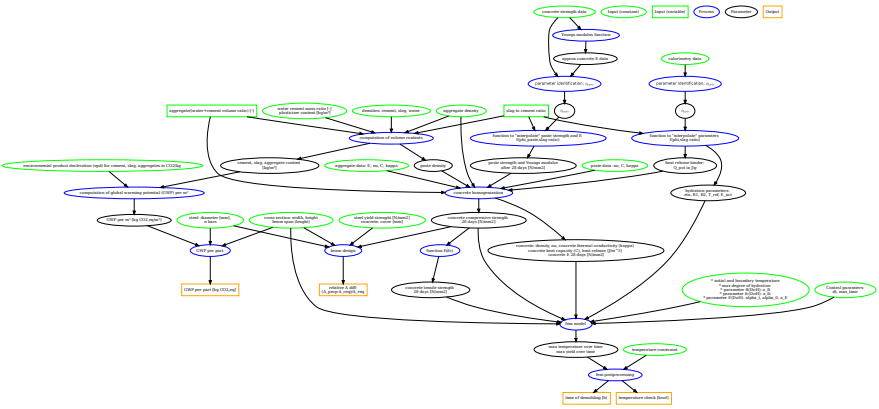

Fig. 1 Testing doit workflow. Figure is created by script. Macro for path is created by other script

Section 2 gives an overview of the material models and approximations used to ... the concrete properties. This section is not ... as curtting edge but rather a ... for each deterministic model applied, there are more advanced and usually more complex .. model can de found in the literature. The aim here is to show the applicability of the overall method with a sufficient level of sophistication. More in debth derivation of the models are found in the appendix

Section 3 gives insight in the the calibration methods used to identify material parameters and their uncertainties.

Section 4 then goes into detail about the optimzation scheme applied in this work.

2 Models

2.1 Notes on micromechanic based concrete homogenization

This manuscript gives an overview of the implementation used within my concrete simulation. The goal is to compute effective concrete parameters based on information of the micro constituents. In particular the cement paste and aggregates are considered. It is possible to consider air pores as well as the influence of the interfacial transition zone (IFZ) as a coat surrounding aggregates

with reduced stiffness. First the estimation of the effective Young's modulus E_{eff} and Poisson's ratio ν_{eff} is given. It is based on the classical analytical Mori-Tanaka homogenization formulation **?** for spherical inclusions in a matrix. This is extended to the case of a coated inclusions, following **?**. In general the implementation of the stiffness homogenization is following the formulations presented in **?**, however the appendix includes some errors, where the original paper **?** should be consulted. Subsequently the estimation of the effective compressive strength $f_{\text{c,eff}}$ is given, following the ideas of **?**.

2.2 Stiffness homogenization as presented in ?

The general idea of this analytical homogenization procedure is to describe the overall stiffness of a body Ω, based on the properties of the individual phases, i.e. the matrix and the inclusions. Each of the n phases is denoted by the index r, where $r = 0$ is defined as the matrix phase. The volume fraction of each phase is defined as

$$c^{(r)} = \frac{\left\|\Omega^{(r)}\right\|}{\|\Omega\|} \quad \text{for } r = 0, ..., n. \tag{1}$$

The inclusions are assumed to be spheres, defined by their radius $R^{(r)}$. The shells are defined by their outer radius, their thickness follows as the difference to the inner inclusions. The elastic properties of each homogeneous and isotropic phase is given by the material stiffness matrix $\boldsymbol{L}^{(r)}$, here written in terms of the bulk and shear moduli K and G,

$$\boldsymbol{L}^{(r)} = 3K^{(r)}\boldsymbol{I}_{\text{V}} + 2G^{(r)}\boldsymbol{I}_{\text{D}} \quad \text{for } r = 0, ..., n, \tag{2}$$

where $\boldsymbol{I}_{\text{V}}$ and $\boldsymbol{I}_{\text{D}}$ are the orthogonal projections of the volumetric and deviatoric components.
The methods assumes that the micro-heterogeneous body Ω is subjected to a macroscale strain $\boldsymbol{\varepsilon}$. It is assumed that for each phase concentration factor $\boldsymbol{A}^{(r)}$ can be defined such that

$$\boldsymbol{\varepsilon}^{(r)} = \boldsymbol{A}^{(r)}\boldsymbol{\varepsilon} \quad \text{for } r = 0, ..., n, \tag{3}$$

which computes the average strain $\boldsymbol{\varepsilon}^{(r)}$ based on the overall strains. This can then be used to compute the effective stiffness matrix $\boldsymbol{L}_{\text{eff}}$ as a volumetric sum over the constituents weighted by the concentration factor

$$\boldsymbol{L}_{\text{eff}} = \sum_{r=0}^{n} c^{(r)}\boldsymbol{L}^{(r)}\boldsymbol{A}^{(r)} \quad \text{for } r = 0, ..., n. \tag{4}$$

The concentration factors $\boldsymbol{A}^{(r)}$,

$$\boldsymbol{A}^{(0)} = \left(c^{(0)}\boldsymbol{I} + \sum_{r=1}^{n} c^{(r)}\boldsymbol{A}_{\text{dil}}^{(r)} \right)^{-1} \tag{5}$$

$$\boldsymbol{A}^{(r)} = \boldsymbol{A}_{\text{dil}}^{(r)}\boldsymbol{A}^{(0)} \quad \text{for } r = 1, ..., n, \tag{6}$$

are based on the dilute concentration factors $\boldsymbol{A}_{\text{dil}}^{(r)}$, which need to be obtained first. The dilute concentration factors are based on the assumption that each inclusion is subjected to the average strain in the matrix $\boldsymbol{\varepsilon}^{(0)}$.

$$\boldsymbol{\varepsilon}^{(r)} = \boldsymbol{A}_{\text{dil}}^{(r)}\boldsymbol{\varepsilon}^{(0)} \quad \text{for } r = 1, ..., n. \tag{7}$$

The dilute concentration factors neglect the interaction among phases and are only defined for the inclusion phases $r = 1, ..., n$. The applied formulation uses an additive volumetric-deviatoric split. where

$$\boldsymbol{A}_{\text{dil}}^{(r)} = A_{\text{dil,V}}^{(r)}\boldsymbol{I}_{\text{V}} + A_{\text{dil,D}}^{(r)}\boldsymbol{I}_{\text{D}} \quad \text{for } r = 1, ..., n, \tag{8}$$

This chosen method extends the basic Mori-Tanaka method the coated inclusions, following **?**, therefore two different formulations for the dilute concentration factors are given for the uncoated and coated inclusion.

2.2.1 Dilute concentration factors for uncoated inclusions

The formulations of the dilute concentration factors for an uncoated inclusion r are

$$A_{\text{dil,V}}^{(r)} = \frac{K^{(0)}}{K^{(0)} + \alpha^{(0)}(K^{(r)} - K^{(0)})}, \tag{9}$$

$$A_{\text{dil,D}}^{(r)} = \frac{G^{(0)}}{G^{(0)} + \beta^{(0)}(G^{(r)} - G^{(0)})}, \tag{10}$$

with the auxiliary factors following from the Eshelby solution as

$$\alpha^{(0)} = \frac{1 + \nu^{(0)}}{3(1 + \nu^{(0)})} \quad \text{and} \quad \beta^{(0)} = \frac{2(4 - 5\nu^{(0)})}{15(1 - \nu^{(0)})} \tag{11}$$

where $\nu^{(0)}$ refers to the Poission's ratio of the matrix phase.

2.2.2 Effective stiffness

Now that the formulation for the dilute concentration factor for inclusions are defined the effective bulk and shear modului can be computed based on a sum

over the phases

$$K_{\text{eff}} = \frac{c^{(0)}K^{(0)} + \sum_{r=1}^{n} c^{(r)}K^{(r)}A_{\text{dil,V}}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\text{dil,V}}^{(r)}}, \tag{12}$$

$$G_{\text{eff}} = \frac{c^{(0)}G^{(0)} + \sum_{r=1}^{n} c^{(r)}G^{(r)}A_{\text{dil,D}}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\text{dil,D}}^{(r)}}. \tag{13}$$

2.3 Strength homogenization as presented in ?

Based on the ideas of the previous section, a formulation is used to homogenize the effective strength of the composite. The strength estimation is based on two main assumptions. First assumptions, the Mori-Tanaka method is used to estimate the average stress within the matrix material, which is the indicator of overall failure. Based on the concept of (3), with the formulations (2),(4) and (5), the average matrix stress is defined as

$$\boldsymbol{\sigma}^{(0)} = \boldsymbol{L}^{(0)}\boldsymbol{A}^{(0)}\boldsymbol{L}_{\text{eff}}{}^{-1}\boldsymbol{\sigma}. \tag{14}$$

Second assumption, the von Mises failure criterion is used to estimate the uniaxial compressive strength

$$\sqrt{3J_2} - f_{\text{c}} = 0. \tag{15}$$

The second deviatoric stress invariant is defined as

$$J_2 = \frac{1}{2}\boldsymbol{\sigma}_{\text{D}} : \boldsymbol{\sigma}_{\text{D}}, \quad \text{with} \quad \boldsymbol{\sigma}_{\text{D}} = \boldsymbol{\sigma} - \frac{1}{3}\,\text{tr}(\boldsymbol{\sigma})\boldsymbol{I}. \tag{16}$$

The goal is to find a uniaxial macroscopic stress $\boldsymbol{\sigma} = \begin{bmatrix} -f_{\text{c,eff}} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{\text{T}}$ which exactly fulfills the von Mises failure criterion (15) for the average stress within the matrix $\boldsymbol{\sigma}^{(0)}$. The procedure here is taken from the code provided in the link in **?**.

First we compute the second deviatoric stress invariant J_2^{test} for a uniaxial test stress $\boldsymbol{\sigma}^{\text{test}} = \begin{bmatrix} f^{\text{test}} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{\text{T}}$. Then the matrix stress $\boldsymbol{\sigma}^{(0)}$ is computed based on the test stress following (14). This is used to compute the second deviatoric stress invariant $J_2^{(0)}$ for the average matrix stress. Now the effective compressive strength is estimated as

$$f_{\text{c,eff}} = \frac{J_2^{\text{test}}}{J_2^{(0)}} f^{\text{test}}. \tag{17}$$

2.4 Thermal conductivity homogenization as presented in ?

Homogenization the thermal conductivity is also based on the Mori-Tanaka method. The formulations are similar as for the stiffness homogenization, i.e. (12) and (13). Here only the implemented formulation is given, no further background. The expressions are taken from **?**, Section 2.2. The thermal conductivity χ_{eff} is given as

$$\chi_{\text{eff}} = \frac{c^{(0)}\chi + \sum_{r=1}^{n} c^{(r)}\chi^{(r)}A_{\chi}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\chi}^{(r)}} \quad \text{and} \quad A_{\chi}^{(r)} = \frac{3\chi^{(0)}}{2\chi^{(0)} + \chi^{(r)}}. \tag{18}$$

2.5 Notes on Early Age Concrete Model

Plan is do collect notes, information on the early age concrete model I am implementing. Currently the plan is to include temperature and humidity and couple them the respective mechanical fields. I will start with the temperature field.

2.6 Modeling of the temperature field

Temperature is generally described as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \frac{\partial Q}{\partial t} \tag{19}$$

λ is the effective thermal conductivity in $\mathrm{Wm^{-1}K^{-1}}$. C is the specific heat capacity. ρ is the density. ρC is the volumetric heat capacity in $\mathrm{Jm^{-3}K^{-1}}$. Q is the volumetric heat, due to hydration, it is also called the latent heat of hydration, or the heat source in $\mathrm{Jm^{-3}}$. For now we assume the density, the thermal conductivity and the volumetric heat capacity as constant, however there are models that make them dependent on the temperature, moisture and/or the hydration.

2.6.1 Degree of hydration α

The degree of hydration α is defined as the ratio between the cumulative heat Q at time t and the total theoretical volumetric heat by complete hydration Q_∞,

$$\alpha(t) = \frac{Q(t)}{Q_\infty}, \tag{20}$$

by assuming a linear relation between the degree of hydration and the heat development. Therefore the time derivative of the heat source $\dot{Q}$ can be

rewritten in terms of α,

$$\frac{\partial Q}{\partial t} = \frac{\partial \alpha}{\partial t} Q_\infty. \tag{21}$$

There are formulas to approximate total potential heat based on composition, approximated values range between 300 and 600 J/g of binder for different cement types, e.g. Ordinary Portland cement Q_∞ = 375–525 or Pozzolanic cement Q_∞ = 315–420.

2.6.2 Affinity

The heat release can be modeled based on the chemical affinity A of the binder. The hydration kinetics can be defined as a function of affinity at a reference temperature $\tilde{A}$ and a temperature dependent scale factor a

$$\dot{\alpha} = \tilde{A}(\alpha) a(T) \tag{22}$$

The reference affinity, based on the degree of hydration is approximated by

$$\tilde{A}(\alpha) = B_1 \left(\frac{B_2}{\alpha_{\max}} + \alpha \right) (\alpha_{\max} - \alpha) \exp\left(-\eta \frac{\alpha}{\alpha_{\max}} \right) \tag{23}$$

where B_1 and B_2 are coefficients depending on the binder. The scale function is given as

$$a = \exp\left(-\frac{E_\mathrm{a}}{R} \left(\frac{1}{T} - \frac{1}{T_\mathrm{ref}} \right) \right) \tag{24}$$

An example function to approximate the maximum degree of hydration based on the water to cement mass ratio r_wc, by Mills (1966)

$$\alpha_{\max} = \frac{1.031 r_\mathrm{wc}}{0.194 + r_\mathrm{wc}}, \tag{25}$$

this refers to Portland cement. Looking at this function this does not seem to be a good expproximation. Need to find better!!!

2.6.3 Time derivative

For a start I use a simple backward difference, backward Euler, implicit Euler method and approximate

$$\dot{T} = \frac{T^{n+1} - T^n}{\Delta t} \quad \text{and} \tag{26}$$

$$\dot{\alpha} = \frac{\Delta \alpha}{\Delta t} \quad \text{with} \quad \Delta \alpha = \alpha^{n+1} - \alpha^n \tag{27}$$

2.6.4 Formulation

Using (21) in (19) the heat equation is given as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q_\infty \frac{\partial \alpha}{\partial t} \tag{28}$$

Now we apply the time discretizations (26) and (27) and drop the index $n+1$ for readability (26)

$$\rho C T - \Delta t \nabla \cdot (\lambda \nabla T) - Q_\infty \Delta \alpha = \rho C T^n \tag{29}$$

Now, we use (27) and (22) to get a formulation for $\Delta\alpha$

$$\Delta \alpha = \Delta t \tilde{A}(\alpha) a(T) \tag{30}$$

2.6.5 Computing $\Delta\alpha$ at the Gauss-point

As $\Delta\alpha$ is not a global field, rather locally defined information.

2.6.6 Solving for $\Delta\alpha$

To solve for $\Delta\alpha$ we define the affinity in terms of α^n and $\Delta\alpha$

$$\tilde{A} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha^n}{\alpha_{\max}}\right) \left(\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha^n\right) (\alpha_{\max} - \Delta\alpha - \alpha^n). \tag{31}$$

Now we can solve the nonlinear function

$$f(\Delta\alpha) = \Delta\alpha - \Delta t \tilde{A}(\Delta\alpha) a(T) = 0 \tag{32}$$

using an iterative Newton-Raphson solver. For an effective algorithm we require the tangent of f with respect to $\Delta\alpha$

$$\frac{\partial f}{\partial \Delta\alpha} = 1 - \Delta t a(T) \frac{\partial \tilde{A}}{\partial \Delta\alpha} \quad \text{with} \tag{33}$$

$$\begin{aligned} \frac{\partial \tilde{A}}{\partial \Delta\alpha} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha^n}{\alpha_{\max}}\right) \Big[& \alpha_{\max} - \tfrac{B_2}{\alpha_{\max}} - 2\Delta\alpha - 2\alpha^n \\ & + (\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha^n)(\Delta\alpha + \alpha^n - \alpha_{\max})(\tfrac{\eta}{\alpha_{\max}}) \Big] \end{aligned} \tag{34}$$

2.6.7 Macroscopic tangent

To incorporate the heat term in the this in the global temperature field, we need to compute to tangent of the term $Q_\infty \Delta\alpha$. Therefore the sensitivity of

$\Delta\alpha$ with respect to the temperature T needs to be computed $\dfrac{\partial\Delta\alpha}{\partial T}$

$$\frac{\partial\Delta\alpha}{\partial T} = \Delta t\tilde{A}(\alpha)\frac{\partial a(T)}{\partial T}, \text{ with} \tag{35}$$

$$\frac{\partial a(T)}{\partial T} = a(T)\frac{E_\mathrm{a}}{RT^2} \tag{36}$$

2.7 Coupling Material Properties to Degree of Hydration

2.7.1 Compressive and tensile strength

Both compressive and tensile strength can be approximated using an generalized exponential function,

$$X(\alpha) = \alpha(t)^{a_X} X_\infty. \tag{37}$$

This model has two parameter, X_∞, the value of the parameter at full hydration, $\alpha = 1$ and a_X the exponent, which is a purely numerical parameter, difficult to estimate directly from a mix design, as the mechanisms are quite complex. The first parameter could theoretically be obtained through experiments. However the total hydration can take years, therefore usually only the value after 28 days is obtained. For now we will assume X_∞ to be a fitting parameter as well. Hopefully a functional relation of the standardized X_{28} values and the ultimate value can be approximated. To write (37) in terms of the compressive strength f_c and the tensile strength f_t

$$f_\mathrm{c}(\alpha) = \alpha(t)^{a_{f_\mathrm{c}}} f_{\mathrm{c}\infty} \tag{38}$$

$$f_\mathrm{t}(\alpha) = \alpha(t)^{a_{f_\mathrm{t}}} f_{\mathrm{t}\infty} \tag{39}$$

$$\tag{40}$$

The publication assumes for their "C1" mix values of $f_{\mathrm{c}\infty} = 62.1$ MPa , $a_{f_\mathrm{c}} = 1.2$,$f_{\mathrm{t}\infty} = 4.67$ MPa , $a_{f_\mathrm{t}} = 1.0$.

2.7.2 Young's Modulus

The publication proposes a new model for the evolution of the Young's modulus. Instead of the generalized model (37), the model assumes an initial linear increase of the Young's modulus up to a degree of hydration α_t.

$$E(\alpha < \alpha_\mathrm{t}) = E_\infty \frac{\alpha(t)}{\alpha_\mathrm{t}} \left(\frac{\alpha_\mathrm{t} - \alpha_0}{1 - \alpha_0}\right)^{a_E} \tag{41}$$

$$E(\alpha \geq \alpha_\mathrm{t}) = E_\infty \left(\frac{\alpha(t) - \alpha_0}{1 - \alpha_0}\right)^{a_E} \tag{42}$$

Values of α_t are assumed to be between 0.1 and 0.2. For the mix "C1" $\alpha_t = 0.09$, $\alpha_0 = 0.06$, $E_\infty = 54.2$ MPa, $a_E = 0.4$.

3 Calibration Method

Here is an empty file as example to start the calibration section.

4 Optimization Method

Here is an empty file as example to start the optimization section.

5 Results

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6 Conclusion and Outlook

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Appendix A Section title of first appendix

An appendix contains supplementary information that is not an essential part of the text itself but which may be helpful in providing a more comprehensive understanding of the research problem or it is information that is too cumbersome to be included in the body of the paper.

References

Campbell SL, Gear CW (1995) The index of general nonlinear DAES. Numer Math 72(2):173–196