Awesome Article Title

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Abstract

The abstract serves both as a general introduction to the topic and as a brief, non-technical summary of the main results and their implications. Authors are advised to check the author instructions for the journal they are submitting to for word limits and if structural elements like subheadings, citations, or equations are permitted.

Keywords: keyword1, Keyword2, Keyword3, Keyword4

1 Introduction

The Introduction section, of referenced text Campbell and Gear (1995) expands on the background of the work (some overlap with the Abstract is acceptable). The introduction should not include subheadings.

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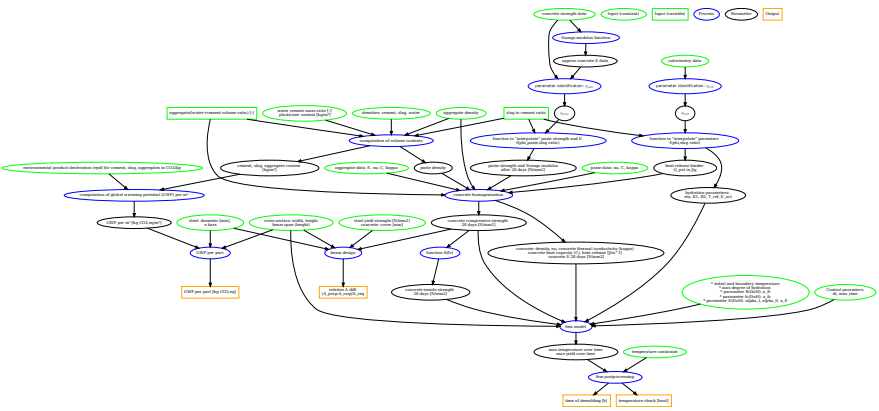

Fig. 1 Testing doit workflow. Figure is created by script. Macro for path is created by other script

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,

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

where $\boldsymbol{I}_{\mathrm{V}}$ and $\boldsymbol{I}_{\mathrm{D}}$ 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 $\boldsymbol{L}_{\mathrm{eff}}$ as a volumetric sum over the constituents weighted by the concentration factor

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

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

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

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

are based on the dilute concentration factors $\boldsymbol{A}_{\mathrm{dil}}^{(r)}$, 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 $\boldsymbol{\varepsilon}^{(0)}$.

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

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

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

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 uncloated inclusion r are

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

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

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 Dilute concentration factors for coated inclusions

The formulation for the coated phases is more complex. The derivation for multi-layered inclusions presented in **?**, where this example is given for a single coat. The application for our example is a single coating describing the interaction of an aggregate surrounded by an ITZ embedded in the cement matrix. This requires three materials and with that three indices. These are defined in the vector $\boldsymbol{i} = \left[i_1, i_2, i_3\right]^{\mathrm{T}}$, where i_1 refers to the index of the inclusion, i_2 to the coat and i_3 to the matrix, therefore $i_3 = 0$.

The effect of the coating is considered with the auxiliary factors Q^k, A^k and B^k, which are given in the following subsection. We need to distinguish between the index related to the phase (k) and the index related to the auxiliary values k with $k = 1, 2$, for this single-layered inclusion. In addition the index (k) is given with the local numbering $i = [i_1, i_2, i_3]^{\mathrm{T}}$,

$$A^{(i_1)}_{\mathrm{dil,V}} = \frac{1}{Q^2_{11}} \quad \text{and} \quad A^{(i_1)}_{\mathrm{dil,D}} = A_1 - \frac{21}{5}\frac{R^{(i_1)2}}{1 - 2\nu^{(i_1)}}B_1, \tag{12}$$

$$A^{(i_2)}_{\mathrm{dil,V}} = \frac{Q^1_{11}}{Q^2_{11}} \quad \text{and} \quad A^{(i_2)}_{\mathrm{dil,D}} = A_2 - \frac{21}{5}\frac{R^{(i_2)5} - R^{(i_1)5}}{(1 - 2\nu^{(i_2)})(R^{(i_2)3} - R^{(i_1)3})}B_2. \tag{13}$$

The amount of sub- and superscripts as indices in theses and the following formulations is at times confusing and can possibly be improved. When in doubt, it is an index not a exponential. Exponential only appear in combination with superscripts in parentheses, they are therefore clearly distinguishable. In addition the index k, here noted as a superscript, only takes values of 1 and 2.

Auxiliary factors

The formulation for the auxiliary factors A^k, B^k and $\boldsymbol{Q}^k$ is not difficult, just long. For easy implementation they have been broken down into further auxiliary variables. The formulation of $\boldsymbol{Q}^k$ is based on $\boldsymbol{N}^k$, both are 2×2 matrices. Scalars A^k and B^k are based on the vector $\boldsymbol{W}^k$ and the 4×4 matrices $\boldsymbol{P}^k$ and $\boldsymbol{M}^k$. $\boldsymbol{M}^k$ is further defined by variables $a^k, b^k, c^k, d^k, e^k, f^k$ and α^k. The formulations are taken from **?**, however there are mistakes in a^k through α^k as well as $\boldsymbol{N}^k$ and $\boldsymbol{M}^k$. The correct formulations are found within the source **?**. The auxiliary factor are defined as follows

$$\boldsymbol{N}^k = \frac{1}{3K^{(i_{k+1})} + 4G^{(i_{k+1})}} \begin{bmatrix} 3K^{(i_k)} + 4G^{(i_{k+1})} & \frac{4}{R^{(i_k)^3}}(G^{(i_{k+1})} - G^{(i_k)}) \\ 3R^{(i_k)^3}(K^{(i_{k+1})} - K^{(i_k)}) & 3K^{(i_{k+1})} + 4G^{(i_k)} \end{bmatrix} \tag{14}$$

$$\boldsymbol{Q}^1 = \boldsymbol{N}^1 \quad \text{and} \quad \boldsymbol{Q}^2 = \boldsymbol{N}^2\boldsymbol{Q}^1 \tag{15}$$

$$a^k = \frac{G^{(i_k)}}{G^{(i_{k+1})}}(7 + 5\nu^{(i_k)})(7 - 10\nu^{(i_{k+1})}) - (7 - 10\nu^{(i_k)})(7 + 5\nu^{(i_{k+1})}) \tag{16}$$

$$b^k = \frac{G^{(i_k)}}{G^{(i_{k+1})}}(7 + 5\nu^{(i_k)}) + 4(7 - 10\nu^{(i_k)}) \tag{17}$$

$$c^k = 2\frac{G^{(i_k)}}{G^{(i_{k+1})}}(4 - 5\nu^{(i_{k+1})}) + (7 - 5\nu^{(i_{k+1})}) \tag{18}$$

$$d^k = 4\frac{G^{(i_k)}}{G^{(i_{k+1})}}(7 - 10\nu^{(i_{k+1})}) + (7 + 5\nu^{(i_{k+1})}) \tag{19}$$

$$e^k = \frac{G^{(i_k)}}{G^{(i_{k+1})}}(7 - 5\nu^{(i_k)}) + 2(4 - 5\nu^{(i_k)}) \tag{20}$$

$$f^k = -\frac{G^{(i_k)}}{G^{(i_{k+1})}}(7 - 5\nu^{(i_k)})(4 - 5\nu^{(i_{k+1})}) + (4 - 5\nu^{(i_k)})(7 - 5\nu^{(i_{k+1})}) \tag{21}$$

$$\alpha^k = \frac{G^{(i_k)}}{G^{(i_{k+1})}} - 1 \tag{22}$$

$$\boldsymbol{M}^k = \frac{1}{5(1 - \nu^{(i_{k+1})})}\widetilde{\boldsymbol{M}} \tag{23}$$

$$\widetilde{M}^k_{11} = \frac{c^k}{3} \tag{24}$$

$$\widetilde{M}^k_{12} = \frac{R^{(i_k)2}(3b^k - 7c^k)}{5(1 - 2\nu^{(i_k)})} \tag{25}$$

$$\widetilde{M}_{13}^{k} = \frac{-12\alpha^{k}}{R^{(i_k)5}} \tag{26}$$

$$\widetilde{M}_{14}^{k} = \frac{4(f^{k} - 27\alpha^{k})}{15R^{(i_k)3}(1 - 2\nu^{(i_k)})} \tag{27}$$

$$\widetilde{M}_{21}^{k} = 0 \tag{28}$$

$$\widetilde{M}_{22}^{k} = \frac{b^{k}(1 - 2\nu^{(i_{k+1})})}{7(1 - 2\nu^{(i_k)})} \tag{29}$$

$$\widetilde{M}_{23}^{k} = \frac{-20\alpha^{k}(1 - 2\nu^{(i_{k+1})})}{7R^{(i_k)7}} \tag{30}$$

$$\widetilde{M}_{24}^{k} = \frac{-12\alpha^{k}(1 - 2\nu^{(i_{k+1})})}{7R^{(i_k)5}(1 - 2\nu^{(i_k)})} \tag{31}$$

$$\widetilde{M}_{31}^{k} = \frac{R^{(i_k)5}\alpha^{k}}{2} \tag{32}$$

$$\widetilde{M}_{32}^{k} = \frac{-R^{(i_k)7}(2a^{k} + 147\alpha^{k})}{70(1 - 2\nu^{(i_k)})} \tag{33}$$

$$\widetilde{M}_{33}^{k} = \frac{d^{k}}{7} \tag{34}$$

$$\widetilde{M}_{34}^{k} = \frac{R^{(i_k)2}(105(1 - \nu^{(i_{k+1})}) + 12\alpha^{k}(7 - 10\nu^{(i_{k+1})}) - 7e^{k})}{35(1 - 2\nu^{(i_k)})} \tag{35}$$

$$\widetilde{M}_{41}^{k} = \frac{-5\alpha^{k}R^{(i_k)3}(1 - 2\nu^{(i_{k+1})})}{6} \tag{36}$$

$$\widetilde{M}_{42}^{k} = \frac{7\alpha^{k}R^{(i_k)5}(1 - 2\nu^{(i_{k+1})})}{2(1 - 2\nu^{(i_k)})} \tag{37}$$

$$\widetilde{M}_{43}^{k} = 0 \tag{38}$$

$$\widetilde{M}_{44}^{k} = \frac{e^{k}(1 - 2\nu^{(i_{k+1})})}{3(1 - 2\nu^{(i_k)})} \tag{39}$$

$$\boldsymbol{P}^{1} = \boldsymbol{M}^{1} \quad \text{and} \quad \boldsymbol{P}^{2} = \boldsymbol{M}^{2}\boldsymbol{P}^{1} \tag{40}$$

The variable $\boldsymbol{W}^{k}$ is special, as only $\boldsymbol{W}^{2}$ is required

$$\boldsymbol{W}^{2} = \frac{1}{P_{22}^{2}P_{11}^{2} - P_{12}^{2}P_{21}^{2}}\boldsymbol{P}^{1}\begin{bmatrix} P_{22}^{2} & -P_{21}^{2} & 0 & 0 \end{bmatrix}^{\mathrm{T}} \tag{41}$$

and finally

$$\boldsymbol{A}^{1} = \frac{P_{22}^{2}}{P_{11}^{2}P_{22}^{2} - P_{12}^{2}P_{21}^{2}} \quad \text{and} \quad \boldsymbol{A}^{2} = W_{1}^{2} \tag{42}$$

$$\boldsymbol{B}^{1} = \frac{-P_{21}^{2}}{P_{11}^{2}P_{22}^{2} - P_{12}^{2}P_{21}^{2}} \quad \text{and} \quad \boldsymbol{B}^{2} = W_{2}^{2} \tag{43}$$

2.2.3 Effective stiffness

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

$$K_{\text{eff}} = \frac{c^{(0)}K^{(0)} + \sum_{r=1}^{n} c^{(r)}K^{(r)}A^{(r)}_{\text{dil,V}}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A^{(r)}_{\text{dil,V}}}, \tag{44}$$

$$G_{\text{eff}} = \frac{c^{(0)}G^{(0)} + \sum_{r=1}^{n} c^{(r)}G^{(r)}A^{(r)}_{\text{dil,D}}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A^{(r)}_{\text{dil,D}}}. \tag{45}$$

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

$$\boldsymbol{\sigma}^{(0)} = \boldsymbol{L}^{(0)}\boldsymbol{A}^{(0)}{\boldsymbol{L}_{\text{eff}}}^{-1}\boldsymbol{\sigma}. \tag{46}$$

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

$$\sqrt{3J_2} - f_c = 0. \tag{47}$$

The second deviatoric stress invariant is defined as

$$J_2 = \frac{1}{2}\boldsymbol{\sigma}_{\text{D}} : \boldsymbol{\sigma}_{\text{D}}, \quad \text{with} \quad \boldsymbol{\sigma}_{\text{D}} = \boldsymbol{\sigma} - \frac{1}{3}\,\text{tr}(\boldsymbol{\sigma})\boldsymbol{I}. \tag{48}$$

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 (47) 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 (46). 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

$$f_{\text{c,eff}} = \frac{J_2^{\text{test}}}{J_2^{(0)}} f^{\text{test}}. \tag{49}$$

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. (44) and (45). 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

$$\chi_{\text{eff}} = \frac{c^{(0)}\chi^{(0)} + \sum_{r=1}^{n} c^{(r)}\chi^{(r)}A_{\chi}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\chi}^{(r)}} \quad \text{and} \quad A_{\chi}^{(r)} = \frac{3\chi^{(0)}}{2\chi^{(0)} + \chi^{(r)}}. \tag{50}$$

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

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \frac{\partial Q}{\partial t} \tag{51}$$

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_∞,

$$\alpha(t) = \frac{Q(t)}{Q_\infty}, \tag{52}$$

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,

$$\frac{\partial Q}{\partial t} = \frac{\partial \alpha}{\partial t} Q_\infty. \tag{53}$$

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

$$\dot{\alpha} = \tilde{A}(\alpha) a(T) \tag{54}$$

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

$$\tilde{A}(\alpha) = B_1 \left(\frac{B_2}{\alpha_{\max}} + \alpha \right) (\alpha_{\max} - \alpha) \exp\left(-\eta \frac{\alpha}{\alpha_{\max}} \right) \tag{55}$$

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

$$a = \exp\left(-\frac{E_\mathrm{a}}{R} \left(\frac{1}{T} - \frac{1}{T_\mathrm{ref}} \right) \right) \tag{56}$$

An example function to approximate the maximum degree of hydration based on w/c ratio, by Mills (1966)

$$\alpha_{\max} = \frac{1.031 w/c}{0.194 + w/c}, \tag{57}$$

this refers to Portland cement.

2.6.3 Time derivative

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

$$\dot{T} = \frac{T^{n+1} - T^n}{\Delta t} \quad \text{and} \tag{58}$$

$$\dot{\alpha} = \frac{\Delta \alpha}{\Delta t} \quad \text{with} \quad \Delta \alpha = \alpha^{n+1} - \alpha^n \tag{59}$$

2.6.4 Formulation

Using (53) in (51) the heat equation is given as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q_\infty \frac{\partial \alpha}{\partial t} \tag{60}$$

Now we apply the time discretizations (58) and (59) and drop the index $n+1$ for readability (58)

$$\rho C T - \Delta t \nabla \cdot (\lambda \nabla T) - Q_\infty \Delta \alpha = \rho C T^n \tag{61}$$

Now, we use (59) and (54) to get a formulation for $\Delta\alpha$

$$\Delta \alpha = \Delta t \tilde{A}(\alpha) a(T) \tag{62}$$

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 $\Delta\alpha$

$$\tilde{A} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha_n}{\alpha_{\max}}\right) \left(\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha_n\right) (\alpha_{\max} - \Delta\alpha - \alpha_n). \tag{63}$$

Now we can solve the nonlinear function

$$f(\Delta\alpha) = \Delta\alpha - \Delta t \tilde{A}(\Delta\alpha) a(T) = 0 \tag{64}$$

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

$$\frac{\partial f}{\partial \Delta\alpha} = 1 - \Delta t a(T) \frac{\partial \tilde{A}}{\partial \Delta\alpha} \quad \text{with} \tag{65}$$

$$\begin{aligned} \frac{\partial \tilde{A}}{\partial \Delta\alpha} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha_n}{\alpha_{\max}}\right) \Big[& \alpha_{\max} - \tfrac{B_2}{\alpha_{\max}} - 2\Delta\alpha - 2\alpha_n \\ & + (\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha_n)(\Delta\alpha + \alpha_n - \alpha_{\max})(\tfrac{\eta}{\alpha_{\max}}) \Big] \end{aligned} \tag{66}$$

The choice of a good starting value for the iteration seems to be critical. For some reason values close to zero can make to algorithm not converge, or to find negative values, which is non physical. When a starting values of eg. 0.2 is chosen, it seem to be stable. There is room for improvement here.

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 $\frac{\partial \Delta\alpha}{\partial T}$

$$\frac{\partial \Delta\alpha}{\partial T} = \Delta t \tilde{A}(\alpha) \frac{\partial a(T)}{\partial T}, \text{ with} \tag{67}$$

$$\frac{\partial a(T)}{\partial T} = a(T) \frac{E_\mathrm{a}}{RT^2} \tag{68}$$

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,

$$X(\alpha) = \alpha(t)^{a_x} X_\infty. \tag{69}$$

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 $X_2 8$ values and the ultimate value can be approximated. To write (69) in terms of the compressive strength f_c and the tensile strength f_t

$$f_\mathrm{c}(\alpha) = \alpha(t)^{a_\mathrm{c}} f_{\mathrm{c}\infty} \tag{70}$$

$$f_\mathrm{t}(\alpha) = \alpha(t)^{a_\mathrm{t}} f_{\mathrm{t}\infty} \tag{71}$$

$$\tag{72}$$

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

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 (69), the model assumes an initial linear increase of the Young's modulus up to a degree of hydration α_t.

$$E(\alpha < \alpha_t) = E_\infty \frac{\alpha(t)}{\alpha_t} \left(\frac{\alpha_t - \alpha_0}{1 - \alpha_0} \right)^{a_E} \tag{73}$$

$$E(\alpha \geq \alpha_t) = E_\infty \left(\frac{\alpha(t) - \alpha_0}{1 - \alpha_0} \right)^{a_E} \tag{74}$$

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, $a_E = 0.4$.

2.8 Fitting of model parameters

As an initial example I will use the concrete applied in the "Cost Action TU1404".

2.8.1 Task 1 Adiabatic temperature

Vol therm al capacity 2.4 x 10^6 in J/()m3 K)
therm conductivity 1.75 w/(mK)
Initial temperature 20 degree C
Temperature data given for two initial values (temp and time/hours) Fig 2
results: activation energy 4029-5402 K**-1

2.8.2 Task 2 temperature development in a massive cube

400 mm edge cube
20 degree ambient temp
CEM I (table 4) 52.5R and other stuff...
isothermal calorimetry data 20,30,40,50,60 degree c (fig 5)
Values used by team 2 for massive cube: q pot 500 J/g
Ea/R= 5653 1/K
B1 = 0.0002916 1/s
B2 = 0.0024229
alpha max = 0.875
eta = 5.554

3 Calibration

Here is an empty file as example to start the calibration section. Feel free to create as many sections as necessary :D.

4 Example code from template

4.1 Tables

Tables can be inserted via the normal table and tabular environment.

In case of double column layout, tables which do not fit in single column width should be set to full text width. For this, you need to use `\begin{table*} ... \end{table*}` instead of `\begin{table} ... \end{table}` environment. Lengthy tables which do not fit in textwidth should be set as rotated table. For this, you need to use `\begin{sidewaystable} ...`

Table 1 Caption text

Column 1	Column 2	Column 3	Column 4
row 1	data 1	data 2	data 3
row 2	data 4	data 5[1]	data 6
row 3	data 7	data 8	data 9[2]

Source: This is an example of table footnote. This is an example of table footnote.

[1]Example for a first table footnote. This is an example of table footnote.

[2]Example for a second table footnote. This is an example of table footnote.

Table 2 Example of a lengthy table which is set to full textwidth

	Element 1[1]			Element 2[2]		
Project	Energy	σ_{calc}	σ_{expt}	Energy	σ_{calc}	σ_{expt}
Element 3	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 4	500 A	961	922 ± 10	900 A	1268	1092 ± 40

Note: This is an example of table footnote. This is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote.

[1]Example for a first table footnote.

[2]Example for a second table footnote.

`\end{sidewaystable}` instead of `\begin{table*} ... \end{table*}` environment. This environment puts tables rotated to single column width. For tables rotated to double column width, use `\begin{sidewaystable*} ... \end{sidewaystable*}`.

4.2 Algorithms

Packages `algorithm`, `algorithmicx` and `algpseudocode` are used for setting algorithms in LaTeX using the format:

```
\begin{algorithm}
\caption{<alg-caption>}\label{<alg-label>}
\begin{algorithmic}[1]
. . .
\end{algorithmic}
\end{algorithm}
```

You may refer above listed package documentations for more details before setting `algorithm` environment. For program codes, the "program" package is required and the command to be used is `\begin{program} ... \end{program}`. A fast exponentiation procedure:

Table 3 Tables which are too long to fit, should be written using the "sidewaystable" environment as shown here

	Element 1[1]			Element[2]		
Projectile	Energy	σ_{calc}	σ_{expt}	Energy	σ_{calc}	σ_{expt}
Element 3	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 4	500 A	961	922 ± 10	900 A	1268	1092 ± 40
Element 5	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 6	500 A	961	922 ± 10	900 A	1268	1092 ± 40

Note: This is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote.

[1]This is an example of table footnote.

```
begin
  for i := 1 to 10 step 1 do
      expt(2, i);
      newline() od                    Comments will be set flush to the right margin
where
proc expt(x, n) ≡
  z := 1;
  do if n = 0 then exit fi;
      do if odd(n) then exit fi;
          comment: This is a comment statement;
          n := n/2; x := x * x od;
      {n > 0};
      n := n − 1; z := z * x od;
  print(z).
end
```

Algorithm 1 Calculate $y = x^n$

Require: $n \geq 0 \vee x \neq 0$
Ensure: $y = x^n$

```
y ⇐ 1
if n < 0 then
    X ⇐ 1/x
    N ⇐ −n
else
    X ⇐ x
    N ⇐ n
end if
while N ≠ 0 do
    if N is even then
        X ⇐ X × X
        N ⇐ N/2
    else[N is odd]
        y ⇐ y × X
        N ⇐ N − 1
    end if
end while
```

Similarly, for `listings`, use the `listings` package. `\begin{lstlisting} ... \end{lstlisting}` is used to set environments similar to `verbatim` environment. Refer to the `lstlisting` package documentation for more details.

```
for i:=maxint to 0 do
begin
{ do nothing }
end;
Write('Case insensitive ');
Write('Pascal keywords.');
```

Supplementary information. If your article has accompanying supplementary file/s please state so here.

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Please refer to Journal-level guidance for any specific requirements.

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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