From concrete mixture to structural design - a holistic optimization procedure

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Abstract

Concrete is a highly complex heterogeneous material. Not only are the effective mechanical properties highly dependent on various factors, as for example aggregate type, water content or additives, but the properties change over time and the evolution of properties is in turn dependent on the specific mix design of the concrete. This is already a challenge in it self when only dealing with concrete properties. To ... something about structural design... connecting them... 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 main cause of GWP is connected to the cement. Some explanation and citation... There are three obvious ways to reduce the amount of cement. First, replace the cement with a substitute, as for example ground granulated slag. This can change mechanical properties, but does not necessarily mean a reduction in strength. Second, increase the amount of aggregates. This is certainly only possible op to a limit, as the matrix is required to glue the inclusions together. In addition, the workability can suffer when the amount and size of the aggregates is exagerated. Third, use less volume of concrete. This must be optimized on a structural level. Reducing cross sections of parts, will usually require imporved material properties, liked to an increase in cement in the mix design. Finding the optimum within these three methods is not trivial. This publication will focus, as a first step in the first two options (?????????). However evaluating constrains at the structural level, making th extension to topology optimization possible without a change in procedure.

For the specific application, an extension to coated inclusions has been used, based on Herve and Zaoui (1993).

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.

There are many parameters affecting the effective properties of concrete, as aggregate type, water amount, cement type, admixtures, additives or temperature. To run a completely data driven optimization scheme would require a vast amount of data as most parameters are interdependent. This means, that the number of required data point increases exponetially with the number of paramters. Therefore we apply established modeling assumptions to reduce the amount of required experiments, to a realistic level.

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.

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

Section 5 then goes into detail about the optimzation scheme applied in this work.

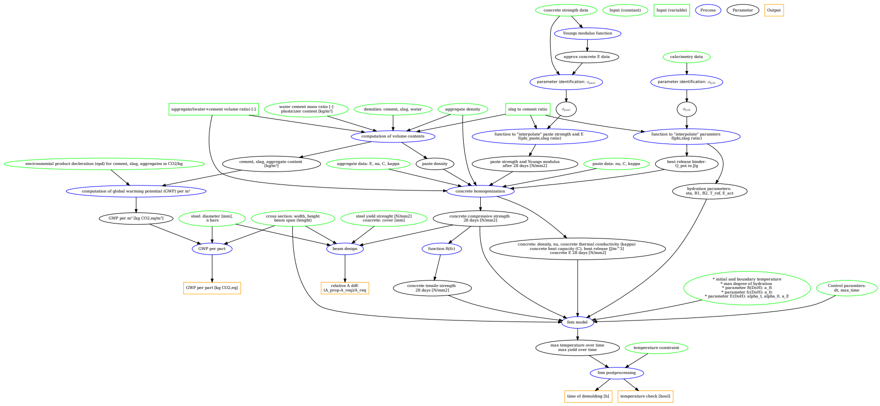

Fig. 1 Testing doit workflow. Figure is created by script. Macro for path is created by other script

2 Experimental data

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

3 Models

3.1 Micromechanics based concrete homogenization

The homogenization method approximates concrete material properties, based on the properties of the cement paste and the aggregates. This step is necessary for two reasons. First, there are some properties like the heat release during hydration, that are more easily measured on the cement paste. Second, the homogenization method allows for a continuous optimization of the aggregate amount, requiring few experimental data points. The properties in question, are the Young's modulus E, the Poission's ratio ν, the compressive strength f_{c}, the density ρ, the thermal conductivity χ, the heat capacity C and the total heat release Q_∞. Depending on the physical meaning, these properties need different methods to estimate the effective concrete properties.

3.1.1 Approximation of elastic properties

The chosen method to homogenize the elastic, isotropic properties E and ν is the Mori-Tanaka homogenization scheme, Mori and Tanaka (1973) It is a well-established, analytical homogenization method. The formulation uses bulk and shear moduli K and G. They are related to E and ν as $K = \frac{E}{3(1-2\nu)}$ and $G = \frac{E}{2(1+\nu)}$. The used Mori-Tanaka method assumes sphecial inclusions in an infinite matrix and considers the interactions of multiple inclusions. The applied formulations follow the notation published in Nežerka and Zeman (2012), where this method is applied to successfully model the effective concrete stiffness for multiple types of inclusions. The full formulation of the method is given in Appendix A. Here the final equation is simplified for the single inclusion material considered in this application. The effective bulk and shear modului are computed as the volume average of its constituents, while considering a reduction factor $\boldsymbol{A}_{\mathrm{dil}}^{(\mathrm{i})}$ for the inclusions, here split in to a volumetric and deviatoric part,

$$K_{\mathrm{eff}} = \frac{c^{(\mathrm{m})} K^{(\mathrm{m})} + c^{(\mathrm{i})} K^{(\mathrm{i})} A_{\mathrm{dil,V}}^{(\mathrm{i})}}{c^{(\mathrm{m})} + c^{(\mathrm{i})} A_{\mathrm{dil,V}}^{(\mathrm{i})}}, \tag{1}$$

$$G_{\mathrm{eff}} = \frac{c^{(\mathrm{m})} G^{(\mathrm{m})} + c^{(\mathrm{i})} G^{(\mathrm{i})} A_{\mathrm{dil,D}}^{(\mathrm{i})}}{c^{(\mathrm{m})} + c^{(\mathrm{i})} A_{\mathrm{dil,D}}^{(\mathrm{i})}}. \tag{2}$$

The superscript (m) denotes quantities associated with the matrix material and (i) quantities associated with the inclusion material, in our case respectively the cement paste and the aggregates.

3.1.2 Approximation of compressive strength

The estimation of the concrete compressive strength $f_{\mathrm{c,eff}}$ follows the ideas of Nežerka et al (2018). The assumption is that a failure in the cement paste will cause the concrete crack. The approach is based on two main assumptions. First, the Mori-Tanaka method is used to estimate the average stress within the matrix material $\boldsymbol{\sigma}^{(\mathrm{m})}$. The formulation is given in Appendix A in (A14). Second, the von Mises failure criterion of the average matrix stress is used to estimate the uniaxial compressive strength

$$f_{\mathrm{c}} = \sqrt{3J_2}, \tag{3}$$

with $J_2(\boldsymbol{\sigma}) = \frac{1}{2}\boldsymbol{\sigma}_{\mathrm{D}} : \boldsymbol{\sigma}_{\mathrm{D}}$ and $\boldsymbol{\sigma}_{\mathrm{D}} = \boldsymbol{\sigma} - \frac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})\boldsymbol{I}$. It is achieved by finding a uniaxial macroscopic stress $\boldsymbol{\sigma} = \begin{bmatrix} -f_{\mathrm{c,eff}} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$, which exactly fulfills the von Mises failure criterion (3) for the average stress within the matrix $\boldsymbol{\sigma}^{(\mathrm{m})}$. The procedure here is taken from the code provided in the link in Nežerka and Zeman (2012). First a J_2^{test} is computed for a uniaxial test stress $\boldsymbol{\sigma}^{\mathrm{test}} = \begin{bmatrix} f^{\mathrm{test}} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$. Then the matrix stress $\boldsymbol{\sigma}^{(\mathrm{m})}$ is computed based on the test stress following (A14). This is used to compute the second deviatoric stress invariant $J_2^{(\mathrm{m})}$ for the average matrix stress. Finally the effective compressive strength is estimated as

$$f_{\mathrm{c,eff}} = \frac{J_2^{\mathrm{test}}}{J_2^{(\mathrm{m})}} f^{\mathrm{test}}. \tag{4}$$

3.1.3 Approximation of thermal conductivity

Homogenization the thermal conductivity is also based on the Mori-Tanaka method. The formulation is similar to (A12) and (A13). The expressions are taken from Stránský et al (2011). The thermal conductivity χ_{eff} is computed as

$$\chi_{\text{eff}} = \frac{c^{(\text{m})}\chi^{(\text{m})} + c^{(\text{i})}\chi^{(\text{i})}A_\chi^{(\text{i})}}{c^{(\text{m})} + c^{(\text{i})}A_\chi^{(\text{i})}} \quad \text{and} \quad A_\chi^{(\text{i})} = \frac{3\chi^{(\text{m})}}{2\chi^{(\text{m})} + \chi^{(\text{i})}}. \tag{5}$$

3.2 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.

3.3 Modeling of the temperature field

Temperature is generally described as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \frac{\partial Q}{\partial t} \tag{6}$$

λ is the effective thermal conductivity in $\text{Wm}^{-1}\text{K}^{-1}$. C is the specific heat capacity. ρ is the density. ρC is the volumetric heat capacity in $\text{Jm}^{-3}\text{K}^{-1}$. Q is the volumetric heat, due to hydration, it is also called the latent heat of hydration, or the heat source in 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.

3.3.1 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_∞,

$$\alpha(t) = \frac{Q(t)}{Q_\infty}, \tag{7}$$

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,

$$\frac{\partial Q}{\partial t} = \frac{\partial \alpha}{\partial t} Q_\infty. \tag{8}$$

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.

3.3.2 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

$$\dot{\alpha} = \tilde{A}(\alpha)a(T) \tag{9}$$

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

$$\tilde{A}(\alpha) = B_1 \left(\frac{B_2}{\alpha_{\max}} + \alpha \right) (\alpha_{\max} - \alpha) \exp \left(-\eta \frac{\alpha}{\alpha_{\max}} \right) \tag{10}$$

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

$$a = \exp \left(-\frac{E_\mathrm{a}}{R} \left(\frac{1}{T} - \frac{1}{T_\mathrm{ref}} \right) \right) \tag{11}$$

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

$$\alpha_{\max} = \frac{1.031 r_\mathrm{wc}}{0.194 + r_\mathrm{wc}}, \tag{12}$$

this refers to Portland cement. Looking at this function this does not seem to be a good expproximation. Need to find better!!! This is a simple but probably better option. Pichler and Hellmich (2011) also includes lot of other wc dependencies...

$$\alpha_{\max} = \frac{r_\mathrm{wc}}{0.42} \quad \text{for} \quad r_\mathrm{wc} < 0.42 \tag{13}$$

$$\alpha_{\max} = 1 \quad \text{for} \quad r_\mathrm{wc} \geq 0.42 \tag{14}$$

3.3.3 Time derivative

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

$$\dot{T} = \frac{T^{n+1} - T^n}{\Delta t} \quad \text{and} \tag{15}$$

$$\dot{\alpha} = \frac{\Delta \alpha}{\Delta t} \quad \text{with} \quad \Delta \alpha = \alpha^{n+1} - \alpha^n \tag{16}$$

3.3.4 Formulation

Using (8) in (6) the heat equation is given as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q_\infty \frac{\partial \alpha}{\partial t} \tag{17}$$

Now we apply the time discretizations (15) and (16) and drop the index $n+1$ for readability (15)

$$\rho C T - \Delta t \nabla \cdot (\lambda \nabla T) - Q_\infty \Delta\alpha = \rho C T^n \tag{18}$$

Now, we use (16) and (9) to get a formulation for $\Delta\alpha$

$$\Delta\alpha = \Delta t \tilde{A}(\alpha) a(T) \tag{19}$$

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

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

3.3.6 Solving for $\Delta\alpha$

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

$$\tilde{A} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha^n}{\alpha_{\max}}\right)\left(\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha^n\right)(\alpha_{\max} - \Delta\alpha - \alpha^n). \tag{20}$$

Now we can solve the nonlinear function

$$f(\Delta\alpha) = \Delta\alpha - \Delta t \tilde{A}(\Delta\alpha) a(T) = 0 \tag{21}$$

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

$$\frac{\partial f}{\partial \Delta\alpha} = 1 - \Delta t a(T) \frac{\partial \tilde{A}}{\partial \Delta\alpha} \quad \text{with} \tag{22}$$

$$\begin{aligned}\frac{\partial \tilde{A}}{\partial \Delta\alpha} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha^n}{\alpha_{\max}}\right)\Big[\alpha_{\max} - \tfrac{B_2}{\alpha_{\max}} - 2\Delta\alpha - 2\alpha^n \\ + (\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha^n)(\Delta\alpha + \alpha^n - \alpha_{\max})(\tfrac{\eta}{\alpha_{\max}})\Big]\end{aligned} \tag{23}$$

3.3.7 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 $\dfrac{\partial \Delta\alpha}{\partial T}$

$$\frac{\partial \Delta\alpha}{\partial T} = \Delta t \tilde{A}(\alpha) \frac{\partial a(T)}{\partial T}, \text{ with} \tag{24}$$

$$\frac{\partial a(T)}{\partial T} = a(T) \frac{E_\mathrm{a}}{RT^2} \tag{25}$$

3.4 Coupling Material Properties to Degree of Hydration

3.4.1 Compressive and tensile strength

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

$$X(\alpha) = \alpha(t)^{a_X} X_\infty. \tag{26}$$

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 (26) in terms of the compressive strength f_c and the tensile strength f_t

$$f_\mathrm{c}(\alpha) = \alpha(t)^{a_{f_\mathrm{c}}} f_{\mathrm{c}\infty} \tag{27}$$

$$f_\mathrm{t}(\alpha) = \alpha(t)^{a_{f_\mathrm{t}}} f_{\mathrm{t}\infty} \tag{28}$$

$$\tag{29}$$

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 , $a_{f_\mathrm{t}} = 1.0$.

3.4.2 Young's Modulus

The publication proposes a new model for the evolution of the Young's modulus. Instead of the generalized model (26), the model assumes an initial linear increase of the Young's modulus up to a degree of hydration α_t.

$$E(\alpha < \alpha_\mathrm{t}) = E_\infty \frac{\alpha(t)}{\alpha_\mathrm{t}} \left(\frac{\alpha_\mathrm{t} - \alpha_0}{1 - \alpha_0} \right)^{a_E} \tag{30}$$

$$E(\alpha \geq \alpha_\mathrm{t}) = E_\infty \left(\frac{\alpha(t) - \alpha_0}{1 - \alpha_0} \right)^{a_E} \tag{31}$$

Values of α_{t} are assumed to be between 0.1 and 0.2. For the mix "C1" $\alpha_{\mathrm{t}} = 0.09$, $\alpha_0 = 0.06$, $E_\infty = 54.2$ MPa, $a_E = 0.4$.

3.5 Approximate concrete tensile strength based on compressive strenght

To reduce the number of required experiments, the tensile strength of concrete is approximated by a simple linear relationsship

$$f_{\mathrm{t}} = \frac{fc}{10} \tag{32}$$

3.6 α_{max} based on r_{wc}

...

3.7 Young's modulus E based on f_{c}

... maybe more to calibration part or description of data?

3.8 Beam design

...

4 Calibration Method

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5 Optimization Method

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6 Results

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7 Conclusion and Outlook

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Appendix A Mori-Tanaka Homogenization

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

$$c^{(r)} = \frac{\left\|\Omega^{(r)}\right\|}{\|\Omega\|} \quad \text{for } r = 0, ..., n. \tag{A1}$$

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,

$$\boldsymbol{L}^{(r)} = 3K^{(r)}\boldsymbol{I}_{\mathrm{V}} + 2G^{(r)}\boldsymbol{I}_{\mathrm{D}} \quad \text{for } r = 0, ..., n, \tag{A2}$$

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

$$\boldsymbol{\varepsilon}^{(r)} = \boldsymbol{A}^{(r)}\boldsymbol{\varepsilon} \quad \text{for } r = 0, ..., n, \tag{A3}$$

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

$$\boldsymbol{L}_{\mathrm{eff}} = \sum_{r=0}^{n} c^{(r)}\boldsymbol{L}^{(r)}\boldsymbol{A}^{(r)} \quad \text{for } r = 0, ..., n. \tag{A4}$$

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

$$\boldsymbol{A}^{(0)} = \left(c^{(0)}\boldsymbol{I} + \sum_{r=1}^{n} c^{(r)}\boldsymbol{A}_{\mathrm{dil}}^{(r)}\right)^{-1} \tag{A5}$$

$$\boldsymbol{A}^{(r)} = \boldsymbol{A}_{\mathrm{dil}}^{(r)}\boldsymbol{A}^{(0)} \quad \text{for } r = 1, ..., n, \tag{A6}$$

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 $\boldsymbol{\varepsilon}^{(0)}$.

$$\boldsymbol{\varepsilon}^{(r)} = \boldsymbol{A}_{\mathrm{dil}}^{(r)}\boldsymbol{\varepsilon}^{(0)} \quad \text{for } r = 1, ..., n. \tag{A7}$$

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

$$\boldsymbol{A}_{\mathrm{dil}}^{(r)} = A_{\mathrm{dil,V}}^{(r)}\boldsymbol{I}_{\mathrm{V}} + A_{\mathrm{dil,D}}^{(r)}\boldsymbol{I}_{\mathrm{D}} \quad \text{for } r = 1, ..., n, \tag{A8}$$

This chosen method extends the basic Mori-Tanaka method the coated inclusions, following Herve and Zaoui (1993), therefore two different formulations for the dilute concentration factors are given for the uncoated and coated inclusion.

Dilute concentration factors for uncoated inclusions

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

$$A_{\mathrm{dil,V}}^{(r)} = \frac{K^{(0)}}{K^{(0)} + \alpha^{(0)}(K^{(r)} - K^{(0)})}, \tag{A9}$$

$$A_{\mathrm{dil,D}}^{(r)} = \frac{G^{(0)}}{G^{(0)} + \beta^{(0)}(G^{(r)} - G^{(0)})}, \tag{A10}$$

with the auxiliary factors following from the Eshelby solution as

$$\alpha^{(0)} = \frac{1 + \nu^{(0)}}{3(1 + \nu^{(0)})} \quad \text{and} \quad \beta^{(0)} = \frac{2(4 - 5\nu^{(0)})}{15(1 - \nu^{(0)})} \tag{A11}$$

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

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

$$K_{\mathrm{eff}} = \frac{c^{(0)}K^{(0)} + \sum_{r=1}^{n} c^{(r)}K^{(r)}A_{\mathrm{dil,V}}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\mathrm{dil,V}}^{(r)}}, \tag{A12}$$

$$G_{\mathrm{eff}} = \frac{c^{(0)}G^{(0)} + \sum_{r=1}^{n} c^{(r)}G^{(r)}A_{\mathrm{dil,D}}^{(r)}}{c^{(0)} + \sum_{r=1}^{n} c^{(r)}A_{\mathrm{dil,D}}^{(r)}}. \tag{A13}$$

Average stress in matrix

Based on the concept of (A3), with the formulations (A2),(A4) and (A5), the average matrix stress is defined as

$$\boldsymbol{\sigma}^{(0)} = \boldsymbol{L}^{(0)}\boldsymbol{A}^{(0)}\boldsymbol{L}_{\mathrm{eff}}{}^{-1}\boldsymbol{\sigma}. \tag{A14}$$

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