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EARLY-AGE EFFECTIVE ELASTIC PROPERTIES OF CEMENT-BASED COMPOSITES

V. V. Kravchenko

Candidate of Technical Sciences, Doctoral Student, Brest State Technical University, Brest, Belarus, e-mail: vvkravchenko@g.bstu.by

Abstract

The problem of the prediction the early age effective elastic properties of cement-based composites is one of the most important and at the same time complicated problems of concrete technology. Cement-based composites consist of a large number of randomly distributed phases with different geometric shapes and sizes at each structural level.

Currently, there are two common approaches to modeling the effective elastic properties of cement-based composites – analytical and numerical homogenization. Most of the researches of the effective properties of cement-based composites focused their attention on the effective medium theory as a part of analytical homogenization, in which all composite phases are considered as spherical inclusions leading to relatively simple computational models for prediction. This significant assumption affects the accuracy of predicting the effective properties, since it is a well-known fact that the real geometric shape of most phases of cement-based composites differs from spherical. One of the drawbacks of the effective medium theory is that solutions for non-spherical inclusions can only be received for a regular geometric shape representing an ellipsoid.

At the same time, one of the advantages of numerical homogenization based on finite element analysis is the possibility of calculating elastic properties for an arbitrary geometric shape of inclusions.

The purpose of the study is multiscale modelling the effective elastic properties of cement-based composites, using a combination of analytical and numerical homogenization, considering the geometric shape of the phases at each heterogeneous level, close to their real shape in the structure of composites.

Keywords: cement paste, concrete, analytical and numerical homogenization, multiscale structure, geometric shape.

ЭФФЕКТИВНЫЕ УПРУГИЕ СВОЙСТВА ЦЕМЕНТНЫХ КОМПОЗИТОВ В РАННЕМ ВОЗРАСТЕ

В. В. Кравченко

Реферат

Проблема оценки эффективных упругих свойств цементных композитов в раннем возрасте является одной из важнейших и в то же время сложных проблем технологии бетона. Цементные композиты состоят из большого количества случайно распределенных фаз различной геометрической формы и размеров на каждом из элементарных уровней строения их структуры.

В настоящее время существуют два распространенных подхода к моделированию эффективных упругих свойств цементных композитов – аналитическая и численная гомогенизация. Большинство проведенных исследований эффективных свойств цементных композитов основаны на положениях теории эффективной среды, относящейся к аналитической гомогенизации, в которых все фазы композита рассматривают как сферические включения, что позволяет получить относительно простые расчетные модели для их оценки. Это существенное допущение оказывает влияние на точность прогнозирования свойств, поскольку хорошо известно, что реальная геометрическая форма большинства фаз цементных композитов отличается от сферической. Одним из недостатков теории эффективной среды является то, что решения для несферических включений, могут быть получены только для правильной геометрической формы в виде эллипсоида.

В тоже время одним из преимуществ численной гомогенизации на основе конечно-элементного анализа является возможность определения упругих свойств для произвольной геометрической формы включений.

Данное исследование ориентировано на моделирование эффективных упругих свойств цементных композитов на основе многоуровневой схемы их структуры, используя для их оценки комбинацию аналитической и численной гомогенизации, рассматривая геометрическую форму фаз на каждом элементарном гетерогенном уровне, близкую к их реальной форме в структуре цементных композитов.

Ключевые слова: цементный камень, бетон, аналитическая и численная гомогенизация, многоуровневая структура, геометрическая форма.

Introduction

The elastic properties are crucial parameters, along with the compressive and tensile strengths, for describing the mechanical behavior of cement-based composites at an early age.

Modeling the elastic properties is the most complicated task in concrete technology. The reason is that, cement-based materials are three-phase composites consisting of a porous cement paste, the interfacial transition zone (ITZ), and aggregates [1]. In turn, cement paste itself is a composite with an extremely complex and heterogeneous structure formed during the hydration process.

It causes the fact, that modern approaches to modelling the elastic properties of cement-based composites involve a multiscale technique. This technique includes separate modelling the elastic properties at different scales depending on the microstructural morphology and sequential upscaling of properties from the underlying level to the upper one. A homogenization scheme is implemented at each level for predicting the effective elastic properties.

The key parameter of the homogenization is a representative element volume (REV), which is defined as the smallest volume element that has the same behaviour as the full-scale material [2]. Two scales can be well identified in the REV: the microscopic scale (or local scale) which represents the scale of inclusions, and the macroscopic scale (or overall scale) which represents the scale of the REV itself.

There are two principal ways for homogenization the elastic properties of composites:

1. Analytical homogenization (also called mean-field homogenization) based on the continuum mechanics, involving two class of effective theories: effective medium theory (EMT) and differential effective medium theory (DEMT) [3].
2. Numerical homogenization based on the finite element analysis (FEA)[1] [4].

[1] The numerical homogenization also involves the Fourier transform approach, which is not discussed here.

The analytical homogenization assumes that the microscopic strain fields are linked to the macroscopic ones throw the following linear dependency [5, 6]:

$$\boldsymbol{\varepsilon}_r = \mathbb{A}_r : \langle \boldsymbol{\varepsilon}_r \rangle_V; r = 1,2,\ldots,n, \tag{1}$$

where $\boldsymbol{\varepsilon}_r$ – is the second-order strain tensor of the phase *r*;

$\mathbb{A}_r$ – is the fourth-order strain concentration tensor of the phase *r*;

$\langle \boldsymbol{\varepsilon}_r \rangle_V$ – is the second-order macroscopic strain tensor;

V – is the REV;

$\langle * \rangle_V$ – is the average of a field $\boldsymbol{f}$ over the REV, $\langle \boldsymbol{f} \rangle_V = \frac{1}{V}\int_V \boldsymbol{f}(\boldsymbol{x})dV$;

$\boldsymbol{x}$ – is the position of an arbitrary point in the REV;

n – is the number of phases;

«:» – is the double dot product.

The equation (1) describes the so-called localization problem in the homogenization theory.

Following the Hill-Mandel lemma, it leads to the macroscopic constitutive elastic law $\langle \boldsymbol{\sigma}_r \rangle_V = \mathbb{C}_{hom} : \langle \boldsymbol{\varepsilon}_r \rangle_V$, which along with the equation (1) brings out the next expression:

$$\langle \boldsymbol{\sigma}_r \rangle_V = \langle \mathbb{C}_r : \boldsymbol{\varepsilon}_r \rangle_V = \langle \mathbb{C}_r : \mathbb{A}_r : \langle \boldsymbol{\varepsilon}_r \rangle_V \rangle_V = \\ = \langle \mathbb{C}_r : \mathbb{A}_r \rangle_V : \langle \boldsymbol{\varepsilon}_r \rangle_V , \tag{2}$$

where $\langle \boldsymbol{\sigma}_r \rangle_V$ – is the second-order macroscopic stress tensor;

$\mathbb{C}_{hom}$ – is the fourth-order effective elasticity tensor;

$\mathbb{C}_r$ – is the fourth-order elasticity tensor of the phase *r*.

This in turn, yields the EMT homogenization model [5, 6]:

$$\mathbb{C}_{hom} = \sum_r f_r\, (\mathbb{C}_r : \mathbb{A}_r) , \tag{3}$$

where f_r – is the volume fraction of the phase *r*.

The most common solution of the localization problem, widely applied to cement-based composites, is the ellipsoidal inhomogeneity inclusion (also called the Eshelby's inclusion) embedded in a reference medium subjected to some uniform strain at infinity ($\boldsymbol{\varepsilon}_\infty$) [5]:

$$\boldsymbol{\varepsilon}_r = \mathbb{A}_r : \boldsymbol{\varepsilon}_\infty \tag{4}$$

$$\mathbb{A}_r = \left[\mathbb{I} + \mathbb{S}_r : \left({\mathbb{C}_0}^{-1} : \mathbb{C}_r - \mathbb{I}\right)\right]^{-1}, \tag{5}$$

where $\mathbb{I}$ – is the fourth-order unit tensor;

$\mathbb{C}_0$ – is the fourth-order elasticity tensor of a reference medium;

$\mathbb{C}_r$ – is the fourth-order elasticity tensor of the phase *r*;

$\mathbb{S}_r$ – is the Eshelby tensor of the phase *r*, which depends on its geometric shape and elastic properties of a reference medium.

Taking the average of (4), we have:

$$\langle \boldsymbol{\varepsilon}_r \rangle_V = \langle \mathbb{A}_r : \boldsymbol{\varepsilon}_\infty \rangle_V = \langle \mathbb{A}_r \rangle_V : \boldsymbol{\varepsilon}_\infty = \left(\sum_r f_r\, \mathbb{A}_r\right) : \boldsymbol{\varepsilon}_\infty . \tag{6}$$

Finally, combining (3), (4), and (6) is given the following homogenization equation [3, 5]:

$$\mathbb{C}_{hom} = \sum_r f_r\, \mathbb{C}_r : [\mathbb{A}_r : (\sum_r f_r\, \mathbb{A}_r)^{-1}]. \tag{7}$$

The elasticity tensor $\mathbb{C}_0$ should be chosen depending on specific morphology of the composite material. At the same time, there are several classical estimates for $\mathbb{C}_0$: the Mori-Tanaka (MT) scheme $\mathbb{C}_0 = \mathbb{C}_m$ ($\mathbb{C}_m$ – is the fourth-order elasticity tensor of a matrix phase), and the Self-Consistent (SC) scheme $\mathbb{C}_0 = \mathbb{C}_{hom}$ [5].

The DEMT deals with a two-phase composite characterized by matrix-inclusion morphology. Its homogenization model brings out from an iterative starting from a step where a dilute concentration of inclusions is randomly dispersed throughout a continuous matrix phase. At each step a differential volume element dV is replaced with the same volume of new inclusions randomly dispersed throughout the effective medium. Replacement inclusions are always an order of magnitude greater in size than those at the previous step. The effective elasticity tensor at each step is expressed by [3, 7]:

$$\mathbb{C}_{hom}(c + \Delta c) = \mathbb{C}_{hom}(c) + [(\mathbb{C}_{inc} - \mathbb{C}_{hom}) : \mathbb{A}_{inc}]\frac{dV}{V} , \tag{8}$$

where $\mathbb{C}_{inc}$ – is the fourth-order elasticity tensor of an inclusion;

$\mathbb{A}_{inc}$ – is the fourth-order strain concentration tensor of an inclusion;

c – is the volume fraction of an inclusion;

Δc – is the incremental volume concentration of an inclusion.

Which leads to the following generalized differential form [3, 7]:

$$\frac{d\boldsymbol{C}_{hom}}{dc} = \frac{1}{1-c}(\mathbb{C}_{inc} - \mathbb{C}_{hom}) : \mathbb{A}_{inc} , \tag{9}$$

with initial condition $\mathbb{C}_{hom} = \mathbb{C}_m$ at $c = 0$.

To sum up, analytical homogenization is most suitable for composites with spherical inclusions providing fairly simple models for calculating the effective elastic moduli. The considerable drawback is that analytical solutions to the Eshelby's inclusion are expressed for ellipsoidal inclusions, which restricts the geometric shape of composite inclusions to a sphere or spheroid.

The numerical homogenization assumes that the REV is subjected to a homogeneous strain field, where the equilibrium conditions for the microscopic stress field ($\boldsymbol{\sigma}(\boldsymbol{x})$) read as [4, 8]:

$$\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{x}) = 0\ \forall \boldsymbol{x} \in V \tag{10}$$

with the linear elastic constitutive law:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{x})\ \forall \boldsymbol{x} \in V, \tag{11}$$

where $\mathbb{C}(\boldsymbol{x})$ – is the fourth-order elasticity tensor.

The microscopic strain field $\boldsymbol{\varepsilon}(\boldsymbol{x})$ can be split into the macroscopic strain $\bar{\boldsymbol{\varepsilon}}$ which would be the actual strain field in the REV if it were homogeneous, and the periodic fluctuation strain $\tilde{\boldsymbol{\varepsilon}}$ which accounts for the presence of heterogeneities [4, 8]:

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}\big(\tilde{\boldsymbol{u}}(\boldsymbol{x})\big) , \tag{12}$$

where $\tilde{\boldsymbol{u}}(\boldsymbol{x})$ – is the periodic fluctuating displacement field.

Taking into consideration the condition $\langle \boldsymbol{\varepsilon} \rangle_V = \bar{\boldsymbol{\varepsilon}}$, it follows that $\langle \tilde{\boldsymbol{\varepsilon}} \rangle_V = 0$.

Generalizing (9), (10), and (11), the following variational formulation can be applied.

Find $\tilde{\boldsymbol{u}} \in V$ such that:

$$\int_V \big(\bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\tilde{\boldsymbol{u}})\big) : \mathbb{C}(\boldsymbol{x}) : \tilde{\boldsymbol{\varepsilon}}(\tilde{\boldsymbol{v}})dV = 0\ \forall \tilde{\boldsymbol{v}} \in V, \tag{13}$$

$$\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) , \tag{14}$$

where $\tilde{\boldsymbol{v}}$ – is the test displacement function.

The above formulation is not well-posed due to the existence of the constraint $\langle \tilde{\boldsymbol{\varepsilon}} \rangle_V = 0$. One way to circumvent this is introducing a vectoral Lagrange multiplier $\boldsymbol{\lambda}$ as an additional unknown and reformulate the problem [9].

Find $(\tilde{\boldsymbol{u}}, \boldsymbol{\lambda}) \in V$ such that:

$$\int_V \big(\bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\tilde{\boldsymbol{u}})\big) : \mathbb{C}(\boldsymbol{x}) : \tilde{\boldsymbol{\varepsilon}}(\tilde{\boldsymbol{v}})dV + \int_V \boldsymbol{\lambda} \cdot \tilde{\boldsymbol{v}}dV + \int_V \boldsymbol{\theta} \cdot \tilde{\boldsymbol{u}}\,dV = \\ = 0\ \forall (\tilde{\boldsymbol{v}}, \boldsymbol{\theta}) \in V , \tag{15}$$

where «·» – is the dot product.

The solution of above problem is performed for six elementary load cases consisting of uniaxial strain and pure shear solicitations by assigning unit values of the corresponding $\bar{\varepsilon}_{ij}$. The value $\bar{\varepsilon}_{ij}$ is usually taken to be 1 and 1/2 for uniaxial strain and shear, respectively. For example:

$$\bar{\varepsilon}_{11} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \bar{\varepsilon}_{12} = \begin{bmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{16}$$

For each load case, the average stress $\bar{\sigma}_{ij}$ is computed and then the components of the elasticity tensor $\boldsymbol{C}_{hom}$ are evaluated (see Figure 1).

Unlike the analytical homogenization, the numerical homogenization makes it possible to evaluate the effective elastic moduli of composites with inclusions of arbitrary geometrical shapes. The crucial disadvantages are significant difficulties related to generating a mesh for arbitrary geometry, and high computational complexity, which heavily depends on the mesh resolution and the finite elements used.

Cement-based composites consist of a large number of randomly distributed phases of different shapes and sizes, so to evaluate the effective elastic moduli it is most appropriate to use a combination of presented approaches, applying them primarily depending on the morphology of the phases at each elementary level. The geometric shape of phases plays important role in homogenization of effective properties along with their elastic properties and concentration, and is underestimated in the most existing models.

This paper presents the linear model of elastic properties of cement-based composites at early age based on the combination of these two approaches to provide a solution considering phase shapes close to the real ones, in contrast to existing approaches where they are mostly represented as spherical.

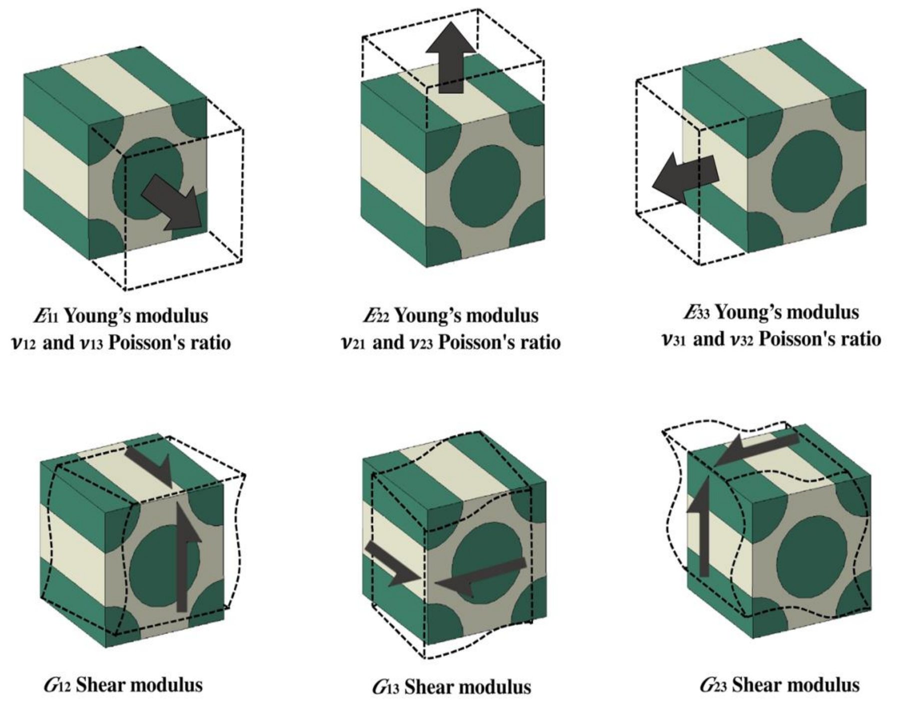

Figure 1 – Schematic representation of six elementary load cases required to estimate the effective elastic properties, according to [10]

Representation of multiscale microstructure

The microstructure of cement-based composites is divided into three elementary levels:

1. Level 1: Unhydrated cement consists of the C_3S[2], C_2S, C_3A, and C_4AF minerals, and hydration products consists of the CSH, CH, $C_6A\bar{S}_3H_{32}$, $C_4A\bar{S}H_{12}$, C_3AH_6, and FH_3 compounds;
2. Level 2: Cement paste consists of homogenous unhydrated cement, homogenous solid of hydration products, and porosity;
3. Level 3: Concrete consists of homogenous cement paste, the ITZ, and aggregates.

Microstructure development

One of the key features of modeling the effective elastic properties of cement-based composites is change over time in the volume fractions of the constitutive phases of cement paste.

The modeling of the microstructure development is a complex approach that includes two parts:

1) A hydration kinetics model for evaluating the hydration degree α at an arbitrary time step;

2) Predicting the volume fractions of cement paste phases corresponding hydration degree $f_r(\alpha)$ and associated with each hydration reaction.

The present model involves the kinetics model of Parrot and Killoh [11] and predicting the volume fractions using the stoichiometry of hydration reactions of clinker phases. To carry out the stoichiometry calculations, the sets of most well-known hydration reactions of Portland cement were taken from the model of Tennis and Jennings [12].

Another aspect of modeling is related to the fact that numerical homogenization requires spatial distribution cement paste phases over REV, which changes with time.

The most appropriate for these purposes is the discrete approach based on splitting up of REV into cubic cells with a certain edge length, typically 1 μm, called voxels. Each voxel represents part of a specific phase of REV at an arbitrary time step according to the stoichiometry of hydration reactions and the rules of handle individual voxels. The discrete approach can significantly simplify mesh generation.

One the well-known discrete models is CEMHYD3D [13]. However, the considered model uses a computationally simpler model presented in [14].

Multiscale homogenization

Level 1

The most suitable scheme at that level is the SC scheme, in which the reference medium coincides with the homogenized medium:

– for unhydrated cement: $\mathbb{C}_0 = \mathbb{C}_{uc}$;

– for hydration products: $\mathbb{C}_0 = \mathbb{C}_{hp}$;

where $\mathbb{C}_{uc}$ – is the fourth-order effective elasticity tensor of homogenous unhydrated cement;

$\mathbb{C}_{hp}$ – is the fourth-order effective elasticity tensor of homogenous solid of hydration products.

The SC scheme is classically used to homogenize a polycrystalline structure consists of an agglomeration of individual crystallites (grains), that accurately reflects both the structure of unhydrated cement and the solid of hydration products.

The main problem here is the choice of geometrical shape of phases. A spherical shape is a classical choice in most existing models. This is considerable assumption, since a lot of SEM analyses of the microstructure of cement paste identify that the shape of most hydration products is not spherical [15].

Meanwhile, as it has been noted, the analytical homogenization imposes restrictions that non-spherical inclusions can be approximated by one of the spheroidal shapes: oblate or prolate, i. e. homogenous solid of hydration products is represented by a set of spheroids, which differ in orientation. In this way, the problem is reduced to choosing the appropriate spheroid shape for each hydration product by determining its aspect ratio.

Assuming that spheroidal phases are isotropically oriented (i. e. in all directions) in the REV, the average strain concentration tensor is defined as [16, 17]:

$$\langle \mathbb{A}_r \rangle = \frac{1}{4\pi}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \widetilde{\mathbb{A}}_r \sin\theta \, d\theta \, d\phi, \qquad (17)$$

where $\widetilde{\mathbb{A}}_r$ – is the strain concentration tensor of the spheroidal phase *r* in the spherical coordinates, calculated as:

$$\widetilde{\mathbb{A}}_r = R_{im}R_{jn}R_{kp}R_{lq}A_{mnpq},$$

$$\text{and} = \begin{bmatrix} cos\theta & -sin\theta & 0 \\ sin\theta cos\phi & cos\theta cos\phi & -sin\phi \\ sin\theta sin\phi & cos\theta sin\phi & cos\phi \end{bmatrix}, \qquad (18)$$

[2] The cement chemist notation is used.

where ϕ and θ – are the azimuthal and polar angle, respectively.

The average strain concentration tensor now should be taken for calculating the effective elasticity tensor in the homogenization equation (7), since the original tensor (5) assumes to axis-aligned orientation.

It is worth noting, that the above solution significantly increases computational costs, since the SC scheme is a system of nonlinear equations with respect to the components of the effective tensor, involving the above complex transformation of the fourth-order strain concentration tensor in solving it.

Regarding the morphology of Portland cement, it is not known with any certainty. Nevertheless, in this paper is assumed that it is close to spherical.

Level 2

The most frequent scheme at that level is the MT scheme, in which porosity is considered as spherical inclusions. However, pores cannot be completely characterized by a single geometric shape, the morphology of pores is complex and has a wide range of both pore shapes and sizes (from the nanometer to micrometer scale). In order to account the realistic pore characteristics, it is more suitable to use the FEA-based homogenization.

Besides, the pure MT scheme is not well-posed at that level since, the porosity of cement paste is partially saturated with water during the hydration process. Consequently, a combination of the MT scheme and poromechanics is required for predicting the effective moduli [18].

The FEA-based homogenization taken in conjunction with a discrete REV of cement paste provides more flexible solution not restricted by porosity shape, and can be effectively implemented without involving poromechanics.

The discrete REV represents the set of voxels each of which has stiffness depending on the phase it belongs to. And in addition, a voxel is cubic element that can be easily transformed into a hexahedral finite element.

The presented model uses a hexahedral mesh which is generated based on the discrete REV obtained from the microstructural model [14], and consists of the following finite elements:

– for strain field: a trilinear 8 nodes hexahedron with 3 degree-of-freedom (DOF) per node;

– for stress field: a trilinear 8 nodes hexahedron with 1 DOF per node.

The mesh has four subdomains related to the phases of unhydrated cement, hydration products, and porosity, represented by water and air subdomains. Each finite element has the same elasticity tensor within a subdomain.

The global stiffness matrix and nodal load vector are assembled by applying the variational formulation (15), where:

$$\mathbb{C}(\boldsymbol{x}) = \begin{cases} \mathbb{C}_{uc}\ \forall \boldsymbol{x} \in V_{uc} \\ \mathbb{C}_{hp}\ \forall \boldsymbol{x} \in V_{hp} \\ \mathbb{C}_{w}\ \forall \boldsymbol{x} \in V_{w} \\ \mathbb{C}_{air}\ \forall \boldsymbol{x} \in V_{air} \end{cases}, \quad (19)$$

where $\mathbb{C}_w$, $\mathbb{C}_{air}$ – is the fourth-order elasticity tensor of water and air, respectively;

V_{uc}, V_{hp}, V_w, V_{air} – are the subdomains of the REV referring to the phases of unhydrated cement, hydration products, water, and air, respectively.

One more important aspect of the FEA-based homogenization is boundary condition. Typical boundary condition for approximating a solution over a REV are periodic boundary conditions under which each node experiences the same periodic displacement as the opposite node.

This approach is characterized by high computational complexity associated with the assembly of the stiffness matrix and nodal load vector as well as solving the linear system, and the regeneration of the mesh at each time step.

Level 3

This level is characterized by fairly clear morphology: a cement matrix and aggregate particles of different sizes embedded into it. The ITZ around each aggregate particle separates them from a cement matrix. This area differs structurally and mechanically from both the cement matrix and aggregates.

One of possible approaches to modelling such a composite structure is reduce it to a two-phase morphology: a matrix with composite particles embedded into it, consisting of aggregate particles surrounded by an ITZ layer. It means, the original problem is divided into two subproblems:

1. Homogenization of a composite particle (also called effective particle mapping);
2. Homogenization of a concrete microstructure.

According to [19], the effective particle mapping for a spherical particle surrounded by a matrix shell, effectively can be done using the Generalized Self-Consistent (GSC) scheme:

$$\mathbb{C}_p = \mathbb{C}\left(\mathbb{C}_{ITZ}, \mathbb{C}_{agg}, \left(\frac{r_{agg}}{r_{agg}+\delta_{itz}}\right)^3\right), \quad (20)$$

where $\mathbb{C}_p$ – is the fourth-order effective elasticity tensor of a composite particle;

$\mathbb{C}_{ITZ}$ – is the fourth-order elasticity tensor of a matrix shell (in this case, it is the ITZ);

$\mathbb{C}_{agg}$ – is the fourth-order elasticity tensor of a representative aggregate particle;

r_{agg} – is the radius of a representative aggregate particle;

δ_{itz} – is the thickness of the ITZ around aggregate particles.

The presented scheme is certainly realizable for rounded fine aggregates and cubic coarse aggregates, since their shape can be approximated as spherical with relatively small error. On the contrary, the shape of flaky and elongated coarse aggregates is closer to a prolate spheroid, which reduces the accuracy of the scheme in relation to them.

In this way, for effective particle mapping of coarse aggregates preference is given to MT scheme:

$$\mathbb{C}_p = f_{agg}\left(\mathbb{C}_{agg} : \mathbb{A}_{agg}\right) + f_{ITZ}\mathbb{C}_{ITZ}, \quad (21)$$

where $\mathbb{A}_{agg}$ – is the strain concentration tensor of a representative aggregate particle, which is calculated according to (5);

f_{agg} – is the volume fraction of a representative aggregate particle inside a composite particle, which is calculated as:

$$f_{agg} = \frac{V_{agg}}{V_p}, \quad (22)$$

V_{agg} – is the volume of a representative aggregate particle;

V_p – is the volume of a composite particle;

f_{ITZ} – is the volume fraction of the ITZ in a composite particle, $f_{ITZ} = 1 - f_{agg}$.

The aggregates are a huge mass of particles of different sizes characterized by a particle size distribution. So, the following question arises, what a representative aggregate particle is in this case? The simplest answer to this is to take any type of averages, for instance, weighted average. However, it is obvious, simple averaging is not appropriate for estimating the entire population of aggregate particles.

Here, a more flexible iterative process is used, where at each step a composite consisting of a representative aggregate particle of the i-th fraction surrounded by a uniform matrix shell is considered. At each step, the thickness of a matrix shell remains constant. A number of steps is equal to a number of aggregate fractions.

The effective elasticity tensor calculated by (20) or (21) from the previous step is the matrix elasticity tensor for the current step. At the first step, the matrix elasticity tensor is $\mathbb{C}_{ITZ}$. Finaly, the effective elasticity tensor of a composite particle will be reached in the last step.

The analyzes of the concrete morphology indicates that the DEMT is probably the best choice for the homogenization its microstructure, since a well match is observed between a concept of the DEMT and the concrete microstructure. So, the effective elasticity tensor of concrete ($\mathbb{C}_c$) computes according to (9):

$$\frac{d\mathbb{C}_c}{dc} = \frac{1}{1-c}\left(\mathbb{C}_p - \mathbb{C}_c\right) : \langle\mathbb{A}_p\rangle, \quad (23)$$

with initial condition $\mathbb{C}_c = \mathbb{C}_{cp}$ at $c = 0$.

where $:\langle\mathbb{A}_p\rangle$ – is the average fourth-order strain concentration tensor of a composite particle, calculated using (17) for non-spherical particles, otherwise $\langle\mathbb{A}_p\rangle = \mathbb{A}_p$;

$\mathbb{C}_{cp}$ – is the fourth-order effective elasticity tensor of homogenous cement paste.

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Nevertheless, it is impossible to directly solve the above differential equation, since the composite contains composite particles of two types – fine and coarse. To get around this problem, one of the possible solutions is to use an iterative process similar to described one earlier: first the equation is solved for the fine composite particles, then this solution is the initial condition for the equation solving with respect to coarse composite particles.

Percolation threshold

Percolation threshold of the solid phase of cement paste plays key role from the point of view of its mechanical behavior. It describes a state of cement paste corresponding to the setting process during which the initial stiffness of the cement system is formed, i.e. below which elastic moduli can be neglected.

According to percolation theory any mechanical characteristic will be proportional to the volume of connected (percolated) clusters in the system. This means that it is necessary to determine the percolation clusters each time step in the discrete REV and the stiffness matrix and nodal vector must be assembled only from finite elements related to these clusters, that is a rather complex computational problem.

At the same time, the percolation theory provides a simple analytical solution represented by a power law in the following normalized form:

$$\mathbb{C}_{cp} = \mathbb{C}_{cp}^{FEA}\left(\frac{\alpha-\alpha_{per}}{1-\alpha_{per}}\right)^{\gamma}, \tag{24}$$

where $\mathbb{C}_{cp}^{FEA}$ – is the is the effective fourth-order elasticity tensor of cement paste according to the FEA-based homogenization;

α – is the hydration degree of cement;

α_{per} – is the hydration degree of cement corresponding to the percolation threshold of the solid phase;

γ – is the exponent.

Modelling results

Concrete with parameters reported in Table 1 was used for the simulation.

The parameters of the constitutive phases of cement paste report in Table 2. The elastic properties of the phases in Table 2 were taken according to [20].

The analyzed hydration period is 28 days.

The predicted phase composition of cement paste during hydration period is shown in Figure 2.

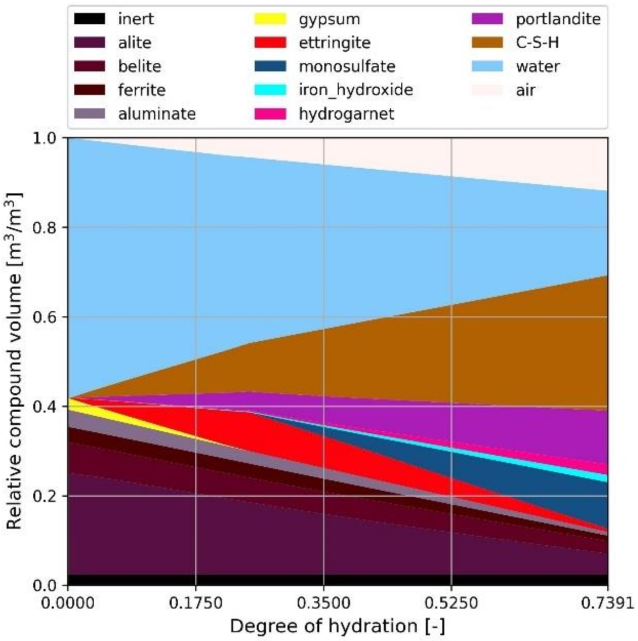

Figure 2 – The predicted phase composition of cement paste during hydration period

The REV resolution was considered in the range from 10 voxels/edge to 20 voxels/edge to reduce the computational cost (1 voxel = 1 μm^3).

The Eshelby's tensor was computed according to [21].

Table 1 – Parameters of concrete

Mix proportions, kg/m^3				Water to cement ratio	Density, kg/m^3			Fineness of cement, m^2/kg	Mineral composition of cement (mass %)
Portland Cement	Water	Aggregate			Portland Cement	Aggregate			
		fine	coarse			fine	coarse		
370	185	754	969	0,5	3150	2510	2640	345	C_3S: 54,5; C_2S: 17,3; C_3A: 8,9; C_4AF: 7,6; Gypsum: 5

Table 2 – Parameters of the constitutive phases of cement paste

Parameter	Phase										
	C_3S	C_2S	C_3A	C_4AF	CSH	CH	$C_6A\bar{S}_3H_{32}$	$C_4A\bar{S}H_{12}$	C_3AH_6	FH_3	Gypsum
Young's modulus, GPa	137,4	135,5	145,2	150,8	23,8	43,5	24,1	43,2	93,8	22,4	44,5
Poisson's ratio	0,299	0,297	0,278	0,318	0,24	0,294	0,321	0,292	0,32	0,25	0,33
Aspect ratio	1,0	1,0	1,0	1,0	0,01	0,1	100	10	1,0	1,0	1,0

The elastic properties of water: the bulk modulus is 2,2 GPa, the Poisson's ratio is 0,499. The elastic properties of air were taken to be close to zero.

The particle size distribution of aggregates is provided by Gates-Gaudin-Schuhman distribution. Characteristic particle diameter was taken for fine aggregate 8 mm, for coarse aggregate 31,5 mm. Particle size distribution exponent is equal to 1,5 for both cases.

The average particle size for each fraction of aggregates was determined as the volume-weighted mean diameter (also called De Brouckere mean diameter).

The parameters of aggregates report in Table 3.

The elastic properties of the ITZ were considered as 1/3 of the effective elastic properties of cement paste. The thickness of the ITZ is equal to 50 μm.

The exponent in the equation (24) is equal to 1.

The modeling results are presented in Figures 3, 4, and 5.

Table 3 – Parameters of aggregates

Parameter	Aggregate	
	fine	coarse
Young's modulus, GPa	59,5	63,5
Poisson's ratio	0,25	0,31
Aspect ratio	1,0	3,0
Sieve size, mm	0,5; 1; 2; 4; 8	4; 8; 16; 31,5

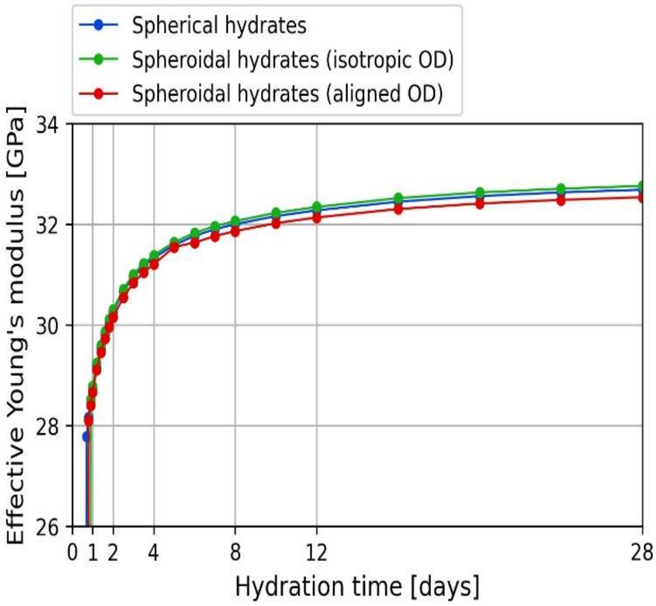

Figure 3 – Comparison of the effective Young's modulus of hydration products computed by using the SCS scheme, depending on their shape and orientation (OD – orientation distribution)

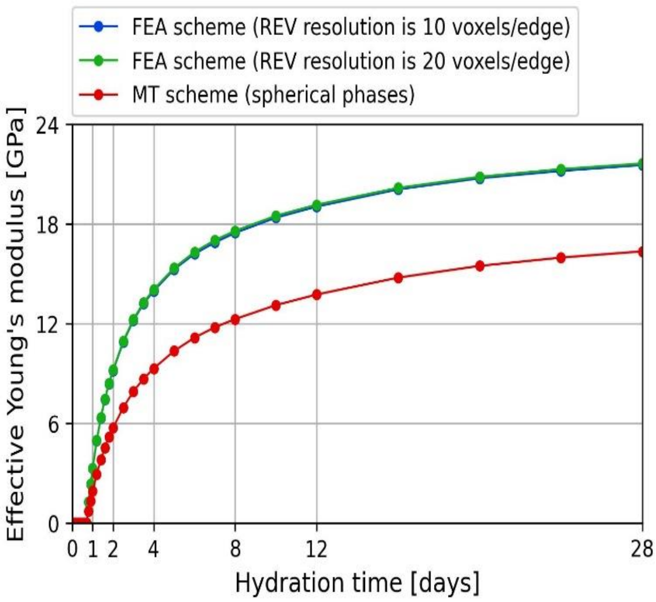

Figure 4 – Comparison of the effective Young's modulus of cement paste computed by using the FEA and MT schemes (the effective Young's modulus of hydration products and clinker phases were computed by using the SC scheme)

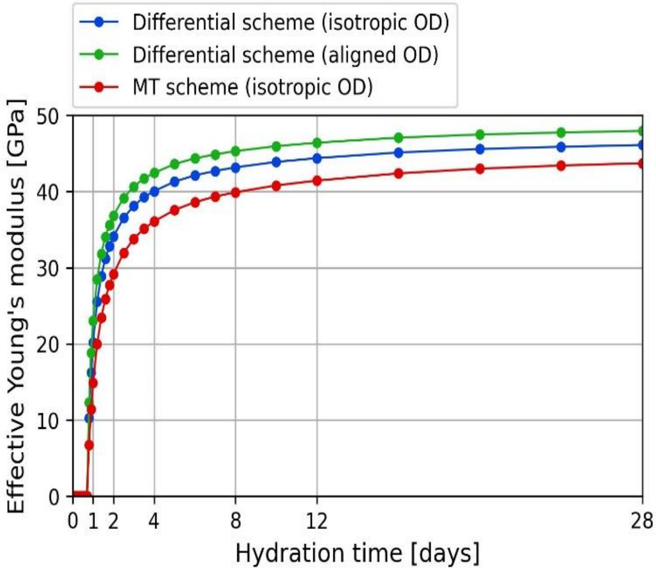

Figure 5 – Comparison of the effective Young's modulus of concrete computed by using the Differential and MT schemes (the effective Young's modulus of hydration products and clinker phases were computed by using the SC scheme, the effective Young's modulus of cement paste using the FEA scheme at a REV resolution of 10 voxels/edge)

Conclusions

1. Cement-based composites consist of a large number of phases of different shapes and sizes, so an approach to predicting effective elastic properties considering all phases as spherical inclusions, is not an effective solution that may reduce the accuracy of predicting.
2. The structure of cement-based composites and morphology of phases differ significantly at each scale level preventing the use of only one specific way for homogenization elastic properties.
3. The most preferable approach is to use both analytical and numerical homogenization, which leads to achieving acceptable accuracy in predicting effective characteristics.
4. The limitation of as such approach is the high computational complexity.
5. Analysis of the microstructure of cement-based composites cement-based composites indicates that the SC scheme is the best possible way to predict the effective elastic properties of hydration products and clinker phases, for a cement paste – the FEA scheme, and for concrete – Differential scheme.

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