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Porous media modeling and micro-structurally motivated material moduli determination via the micro-dilatation theory

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Abstract. In the present contribution, the porous material modeling and micro-structural material parameters determination are scrutinized via the micro-dilatation theory. The main goal is to take advantage of the micro-dilatation theory which belongs to the generalized continuum media. In the first stage, the thermodynamic laws are entirely revised to reach the energy balance relation using three variables, deformation, porosity change and its gradient underlying the porous media as described in the micro-dilatation theory or so-called void elasticity. Two experiments over cement mortar specimens are performed in order to highlight the material parameters related to the pore structure. The shrinkage due to CO_2 carbonation, porosity and its gradient are calculated. The extracted values are verified via ^{14}C-PMMA radiographic image method. The modeling of swelling phenomenon of Delayed Ettringite Formation (DEF) is studied later on. This issue is performed via the crystallization pressure application using the micro-dilatation theory.

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1 Introduction

1.1 Scientific motivation

The study of the materials with the micro-structure is of great importance in the physics of solids. Basically, the chemical reactions across the porous media, e.g. cement-based materials and concrete, yield the micro-structural changes. These changes can be obviously seen at macro-scale and they would affect the durability issue of the above-indicated materials.

Some of these drawbacks which stem from the chemically-driven porosity change are well known as concrete pathologies. One of the most harsh pathologies in the concrete society would be CO_2 carbonation and Delayed Ettringite Formation (DEF). The concrete pathology is affected by the porosity and micro-structure modification at micro-scale where the chemical reaction happens. The main question in conjunction with the deformable porous materials and chemical deformations is how one can link them. Clearly, these effects go altogether and the key point is to link them properly. The main link can be obtained by means of the Duhamel-Neumann additive deformation principle. This deformation decomposition rule indicates that the total deformation can be divided into the mechanical deformation and the other deformations. There is a bunch of applications of this method in the literature [4–8]. By taking advantage of the mentioned method, the stress tensor due to the chemically-motivated actions can be accounted for and the stress distribution can be found out.

Evidently, these stresses come up from the chemical reactions and the micro-cracking would be expected at pore scale. This micro-cracking at pore scale can be taken into account as the micro-damage herein. It is well worth noting that the micro-cracking or micro-damage can be observed at pore scale, whereas the material still turns to be linear. To pursue this goal, it is necessary to consider the damage variable at the pore-scale moduli and bring the appropriate formulation to achieve this assignment. In the present paper, the theoretical issues of the micro-dilatation theory is primarily presented [9–15] and the use of the generalized continuum mechanics is justified. The main fresh issues pertaining to the micro-dilatation theory comparing to the original theory can be summarized as below:

1. The micro-dilatation theory description underlying the current porosity as the additional state field variable.
2. The application of this theory to the concrete pathologies and pore-scale material parameters.
3. The micro-damage concept based on the first and second thermodynamic laws.

1.2 Theoretical background

The classical continuum mechanics known as Cauchy-Boltzmann's theory is widely applied to investigate the material's behavior [16]. Unfortunately, the classical theory does not take into account the micro-structure features. The generalized continuum mechanics make possible to scrutinize these issues in a subtle manner[1]. Therefore, there are additional kinematical variables in describing the continuum micro-structure

[1] The generalized continuum mechanics is more likely addressed to the continuum mechanics containing the additional kinematical relations and state field variables. This theory can be categorized to the Cosserat theory [17,18], indeterminate couple stress theory [19,20], micro-dilatation theory or so-called void elasticity [9,10,21–23], micro-stretch theory [18,24], micro-strain theory [25] and micro-morphic theory [18].

features, e.g. the micro-rotation, micro-dilatation and so on. This issue provides several micro-macro coupled constitutive laws and material parameters. The main benefit of this matter is to define the micro-structure state comparing to the homogenization techniques. However, the main challenge is the additional material moduli determination and the possible way out under the experimental points of view. Among the generalized continuum theory family, one can readily distinguish the **micro-dilatation theory** or so-called **void elasticity** theory due to the particular view about the porosity and the induced stress distribution for the porous body modeling. The most well-known theory in conjunction with the classical theory and porous media has been suggested by Biot [26,27] in the early fifties. This makes possible to use the available finite element method implementations and to describe the porous media using the global porosity definition. One major drawback of the Biot's theory is that it coincides with the classical theory excluding the pore-fluid pressure. Furthermore, it provides the rigid pore system and sustains only the total porosity description.

Consequently, the main goal is to understand the additional parameters related to the porous structure through two pathologies of concrete, i.e. CO_2 carbonation and DEF. The paper is organized as following. The original micro-dilatation theory is presented in Sect. 2. The enhancement of the micro-dilatation theory including the thermodynamic laws, total strain energy density concept for the micro-dilatation and porous-damage model is discussed in Sect. 3. Afterwards, the micro-dilatation theory material moduli identification as well as the numerical experiments have been brought in Sect. 4. Some conclusions and outlooks are described and discussed in the last section.

2 Brief overview of the micro-dilatation theory

The additional kinematical variable in the micro-dilatation is called micro-dilatation variable written by φ and it can be denoted as the subtraction of the matrix volume fraction at the current configuration Λ and reference configuration Λ_{R} as below [28]:

$$\varphi := \Lambda - \Lambda_{\mathrm{R}} \quad \text{where} \quad \Lambda := \frac{\Omega_{\mathrm{matrix}}}{\Omega} \quad \text{and} \quad \Lambda_{\mathrm{R}} := \frac{\Omega_{\mathrm{matrix,R}}}{\Omega_{\mathrm{R}}} \tag{1}$$

where $\Omega_{\mathrm{matrix}}, \Omega, \Omega_{\mathrm{matrix,R}}, \Omega_{\mathrm{R}}$ are the matrix volume and total volume at current configuration and at reference configuration, respectively. Equation (1) can be again written in function of the current porosity P and reference porosity P_{R} as following:

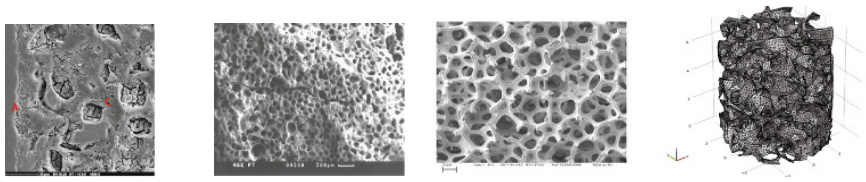
$$\varphi := -(\mathrm{P} - \mathrm{P}_{\mathrm{R}}). \tag{2}$$

The kinematical relations can be inferred in the micro-dilatation as follows:

$$\varepsilon := \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \hat{e}_i \otimes \hat{e}_j \quad \text{where} \quad \nabla u := (\nabla \otimes u)^T = u_{i,j}\, \hat{e}_i \otimes \hat{e}_j \quad \text{for} \quad i,j = 1,2,3 \tag{3a}$$

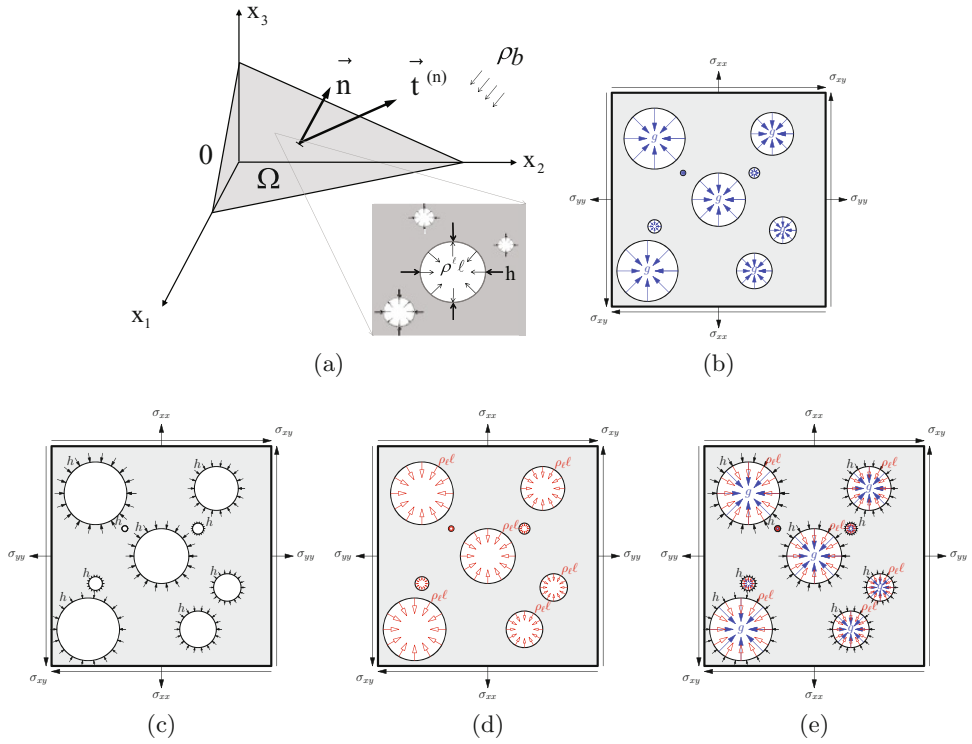
$$\Phi := \nabla\varphi = \varphi_{,i}\hat{e}_i \quad \text{for} \quad i = 1,2,3 \tag{3b}$$

where, ε and Φ are the infinitesimal deformation tensor and gradient of the micro-dilatation variable, respectively. This gets more important while one deals with the deformable porous media [29]. Therefore, it would be feasible to obtain the spatial distribution of porosity at every single node of the continuum media. This matter lies in the fact that the continuum point is small enough to be deemed as a point and it is large enough to contain the porosity in a statistical manner [30,31] (see Fig. 2 for more details). As discussed earlier, the outstanding point in dealing with



(a) (b) (c) (d)

Fig. 1. Some examples of the heterogeneous and porous materials, a) cement mortar [1], b) porous limestone, c) nickel-foam [2] and d) 3D reconstruction of human bone [3].



(a) (b) (c) (d) (e)

Fig. 2. Constitutive parameters illustration in the micro-dilatation theory [37], a) surface traction or stress vector, $t^{(n)}$ in the micro-dilatation theory, b) stress tensor, σ and micro-body force g, c) stress tensor, σ and equilibrated force or so-called hyper-stress, h, d) stress tensor, σ and $\rho_\ell \ell$ and e) illustration of all constitutive parameters, σ, g, h and $\rho_\ell \ell$.

the generalized continuum mechanics is that these theories take into account the micro-structural issues in an inherent manner. Consequently, there is no need to the up-scaling, homogenization and averaging issues [32–36].

According to the original study, there are three constitutive laws for the linear centro-symmetrical isotropic micro-dilatation elasticity as below (see Fig. 2):

$$\sigma_{ij} = \lambda \delta_{ij} u_{k,k} + \mu(u_{i,j} + u_{j,i}) + \beta \varphi \delta_{ij} \quad \text{for} \quad \text{i,j,k} = 1,2,3 \tag{4a}$$

$$h_i = \alpha \varphi_{,i} \quad \text{for} \quad \text{i} = 1,2,3 \tag{4b}$$

$$-g = \xi \varphi + \omega \dot{\varphi} + \beta u_{k,k} \quad \text{for} \quad \text{k} = 1,2,3 \tag{4c}$$

where, $\sigma \in \text{sym}(3) \subset \mathbb{R}^3 \times \mathbb{R}^3$, $h \in \mathbb{R}^3$ and $g \in \mathbb{R}$ are the stress tensor, equilibrated force or hyper-stress and micro-body force, respectively. λ, μ, β, α, ξ and ω are the Lamé's coefficients, micro-dilatation coupling modulus, void diffusion modulus, void stiffness modulus and micro-visco-elastic modulus, respectively. According to the positive definiteness of the constitutive laws and local positivity of the total strain energy density, the forthcoming inequalities should be held in the micro-dilatation theory [29,38]:

$$\mu > 0, \quad \alpha > 0, \quad \xi > 0, \quad \lambda + \mu > 0 \quad 3\lambda + 2\mu > 0 \quad \text{and} \quad \beta^2 < K\xi \tag{5}$$

where $K = \frac{3\lambda+2\mu}{3}$ is the bulk modulus. As discussed before, the use of the micro-dilatation theory entails more material parameters and it is essential to well understand these additional material parameters for the modeling purposes. Besides the traditionally well-known material moduli, i.e. the Lamé's coefficients, there are four additional material moduli. The micro-visco-elastic features are neglected herein and consequently, ω vanishes. Other material moduli, i.e. α, β and ξ, will be focused on in the present paper.

The micro-dilatation theory has one additional equilibrium equation comparing to the classical theory. This equation deals with the equilibrium at the pore scale and it sustains the further constitutive parameters, i.e. $h \in \mathbb{R}^3$ and $g \in \mathbb{R}$. The equilibrium equations of the micro-dilatation theory can be written as follows:

$$\int_{\Omega(t)} (\sigma_{ji,j} + \rho b_i)\, dV = 0 \quad \text{for} \quad \text{i,j} = 1,2,3 \quad \text{on} \quad \Omega(t) \subset \mathbb{R}^3 \times [0, \mathcal{T}] \tag{6a}$$

$$\int_{\Omega(t)} e_{ijk}\sigma_{jk}\, dV = 0 \quad \text{for} \quad \text{i,j,k} = 1,2,3 \quad \text{on} \quad \Omega(t) \subset \mathbb{R}^3 \times [0, \mathcal{T}] \tag{6b}$$

$$\int_{\Omega(t)} (h_{i,i} + \rho_\ell \ell + g)\, dV = 0 \quad \text{for} \quad \text{i} = 1,2,3 \quad \text{on} \quad \Omega(t) \subset \mathbb{R}^3 \times [0, \mathcal{T}] \tag{6c}$$

where, $\rho b \in \mathbb{R}^3$, $e \in \mathbb{R}^{27}$, $\rho_\ell \ell \in \mathbb{R}$ are body force vector, third-rank permutation tensor or Levi-Civita tensor, and equilibrated scalar micro-body force, respectively.

3 Investigation of the micro-dilatation theory enhancement

3.1 Revision of first and second thermodynamic laws

The thermodynamic principles have been fully revised to handle the micro-dilatation materials. This issue has been achieved due to the fact that the thermodynamic principles are customarily available for the classical theory. Let us get started with the energy balance equation in the classical system:

$$\rho \frac{D\, e}{D\, t} = v_{i,i}\sigma_{ij} - q_{i,i} + \rho\, s \quad \text{for} \quad i,j = 1,2,3 \tag{7}$$

where, ρ, $\frac{De}{Dt}$, $v_{i,i}\sigma_{ij}$ and $q_{i,i}$ are the density, internal energy rate, work done by the Cauchy's body and divergence of heat flux rate vector, respectively. Based on the micro-dilatation materials, the work done would have another term in function of the porosity change rate, i.e. $\int_{\partial\Omega} (v_i\, t_i + h_i\, n_i\, \dot{\varphi} - q_i\, n_i)\, dS$. Consequently, we arrive at new expression of the energy balance as:

$$\rho \frac{D\, e}{D\, t} = v_{i,i}\sigma_{ij} + h_{i,i}\, \dot{\varphi} + h_i\, \dot{\varphi}_{,i} + \rho^\ell\, \ell\, \dot{\varphi} - q_{i,i} + \rho\, s \quad \text{for} \quad i,j = 1,2,3 \tag{8}$$

where, e, v_i, s, q_i, n_i and t are the internal energy, time-derivation of displacement vector $\frac{\partial u_i}{\partial t}$, entropy, outward heat flux rate, outward unit normal vector, and time, respectively. Based on the third balance equation of the micro-dilatation, Eq. (6c), we reach the first modified thermodynamic principle as below:

$$\rho \frac{D\,e}{D\,t} = v_{i,i}\sigma_{ij} - g\,\dot{\varphi} + h_i\,\dot{\varphi}_{,i} - q_{i,i} + \rho\,s \quad \text{for} \quad i,j = 1,2,3. \tag{9}$$

The second thermodynamic principle described as the Clausius-Duhem inequality can be also obtained using the first modified thermodynamic principle as following:

$$\rho\,(T\,\dot{s} - \dot{e}) + \sigma_{ji}v_{i,j} - g\,\dot{\varphi} + h_i\,\dot{\varphi}_{,i} \geqslant \frac{1}{T}\,q_i\,T_{,i} \quad \text{for} \quad i,j = 1,2,3 \tag{10}$$

where, $\dot{s}$ and T are the entropy rate and temperature, respectively.

3.2 Total strain energy density definition in the micro-dilatation theory

In the micro-dilatation materials, the total strain energy density can be denoted in terms of ε, φ and $\varphi_{,i}$. The application of Taylor series expansion of second order gives rise the following equation:

$$\begin{aligned} W(\varepsilon,\varphi,\varphi_{,i}) = {} & \frac{1}{2}\varepsilon_{ij}\,C_{ijkl}\,\varepsilon_{kl} + \frac{1}{2}\varepsilon_{ij}\,B_{ij}\,\varphi + \frac{1}{2}\varepsilon_{ij}\,D_{ijk}\,\varphi_{,i} + \frac{1}{2}\varphi\,\xi\,\varphi + \frac{1}{2}\varphi\,B_{ij}\,\varepsilon_{ij} \\ & + \frac{1}{2}\varphi\,F_i\,\varphi_{,i} + \frac{1}{2}\varphi_{,i}\,A_{ij}\,\varphi_{,j} + \frac{1}{2}\varphi_{,i}\,D_{ijk}\,\varepsilon_{jk} + \frac{1}{2}\varphi_{,i}\,F_i\,\varphi \quad \text{for} \quad i,j,k,l = 1,2,3 \end{aligned} \tag{11}$$

C_{ijkl}, B_{ij}, D_{ijk}, F_i and A_{ij} are the fourth-rank stiffness tensor, micro-dilatation coupling modulus matrix, third-rank zero-centrosymmteric stiffness tensor, zero centrosymmteric coupling vector and void diffusion modulus matrix, respectively. Based on the linear elastic materials, we can get the stress-strain relation:

$$\sigma_{ij} = \frac{\partial\,W}{\partial\,\varepsilon_{ij}} = C_{ijkl}\,\varepsilon_{kl} + B_{ij}\varphi + D_{ijk}\varphi_{,i} \quad \text{for} \quad i,j,k,l = 1,2,3. \tag{12}$$

The above linear stress-strain relation can be re-written for the centro-symmetrical materials involving the isotropy assumption as:

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} + \beta\varphi\delta_{ij} \quad \text{for} \quad i,j,k = 1,2,3. \tag{13}$$

By taking advantage of the linear relation into the porous media, the porosity change and so-called micro-force parameter can be denoted as below:

$$h_i = \frac{\partial\,W}{\partial\,\varphi_{,i}} = A_{ij}\,\varphi_{,j} + D_{ijk}\varepsilon_{ij} + F_i\,\varphi \quad \text{for} \quad i,j,k = 1,2,3. \tag{14}$$

The above relation can be re-written for centro-symmetrical materials involving the isotropy assumption as:

$$h_i = \alpha\varphi_{,i} \quad \text{for} \quad i = 1,2,3. \tag{15}$$

The micro-pressure inside the pores can be found out in the same manner.

$$-g = \frac{\partial\,W}{\partial\,\varphi} = \xi\,\varphi + B_{ij}\varepsilon_{ij} + F_i\varphi_{,i} \quad \text{for} \quad i,j = 1,2,3. \tag{16}$$

This can be denoted for the centro-symmetrical materials excluding the micro-void-elastic counterpart ($\omega = 0$) as following:

$$-g = \xi\varphi + \beta\varepsilon_{kk} \quad \text{for} \quad k = 1,2,3. \tag{17}$$

3.3 Micro-damage model proposal

We assume that the internal energy expression of the micro-dilatation includes one additional variable, damage scalar variable, d as $W(\varepsilon, \varphi, \varphi_{,i}, d)$. Based on the Taylor series expansion of second order,

$$\begin{aligned} W(\varepsilon, \varphi, \varphi_{,i}, d) = & \frac{1}{2}\varepsilon_{ij}\, C_{ijkl}\, \varepsilon_{kl} + \frac{1}{2}\varepsilon_{ij}\, B_{ij}\, \varphi + \frac{1}{2}\varepsilon_{ij}\, D_{ijk}\, \varphi_{,i} + \frac{1}{2}\varepsilon_{ij} d_{ij} d \\ & + \frac{1}{2}\varphi\, \xi(d)\, \varphi + \frac{1}{2}\varphi\, B_{ij}\, \varepsilon_{ij} + \frac{1}{2}\varphi\, F_i\, \varphi_{,i} + \frac{1}{2}\varphi \Lambda\, d \\ & + \frac{1}{2}\varphi_{,i}\, A_{ij}\, \varphi_{,j} + \frac{1}{2}\varphi_{,i}\, D_{ijk}\, \varepsilon_{jk} + \frac{1}{2}\varphi_{,i}\, F_i\, \varphi + \frac{1}{2}\varphi_{,i} \Lambda_{,i}\, d \\ & + \frac{1}{2} d\, d_{ij} \varepsilon_{ij} + \frac{1}{2} d\, \Lambda \varphi + \frac{1}{2} d\, \Lambda_{,i} \varphi_{,i} + \frac{1}{2}\, d\, c\, d \quad \text{for} \quad i, j, k, l = 1, 2, 3. \end{aligned} \tag{18}$$

Therefore, the internal energy rate can be derived as following:

$$\dot{W} = \frac{\partial W}{\partial \varepsilon}\dot{\varepsilon} + \frac{\partial W}{\partial \varphi}\dot{\varphi} + \frac{\partial W}{\partial \varphi_{,i}}\dot{\varphi_{,i}} + \frac{\partial W}{\partial d}\dot{d}. \tag{19}$$

Now, we set that, $\dot{s} = 0$ and $T_{,i} = 0$ for the micro-dilatation materials, Eq. (19) is applied into the modified Clausius-Duhem inequality in Eq. (10) and it can be inferred:

$$\rho\dot{e} - \sigma_{ji} v_{i,j} + g\, \dot{\varphi} - h_i\, \dot{\varphi}_{,i} \leqslant 0 \quad \text{for} \quad i, j = 1, 2, 3. \tag{20}$$

Now, introducing the internal energy rate again into Eq. (20), we can derive again the Clausius-Duhamel inequality as following

$$\rho\left(\frac{\partial W}{\partial \varepsilon} - \sigma_{ji}\right)\dot{\varepsilon} + \rho\left(\frac{\partial W}{\partial \varphi} + g\right)\dot{\varphi} + \rho\left(\frac{\partial W}{\partial \varphi_{,i}} - h_i\right)\dot{\varphi_{,i}} + \rho\frac{\partial W}{\partial d}\dot{d} \leqslant 0. \tag{21}$$

By taking advantage of the above-mentioned equation, the left hand-side terms are assumed to be equal to zero. Therefore, we can derive three relations as defined earlier in Eq. (12), Eq. (14) and Eq. (16). And finally, we can obtain a thermodynamic elastic force which starts damage phenomenon, F_{d} at micro-pore scale.

$$\frac{\partial W}{\partial d} := F_{\mathrm{d}}. \tag{22}$$

Based on the centro-symmetry assumption, the thermodynamic macro-poro-damage force can be denoted as below:

$$F_{\mathrm{d}} = c\, d + \Lambda\, \varphi + \frac{1}{2}\frac{d\,(\xi(d))}{d\,(d)}\, \varphi^2. \tag{23}$$

4 Pore scale material parameters identification

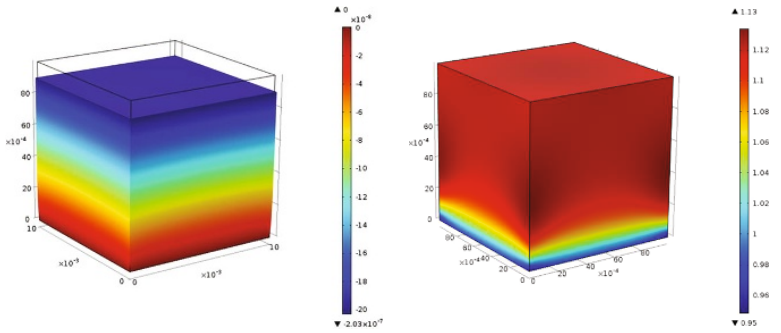
4.1 Some numerical experiments via 3D-FEM

In order to scrutinize the materials parameters related to the porous body, some numerical experiments have been achieved via the unit cube (1×1×1 [cm]) with macro-scale and micro-scale parameters in Table 1.

The cube is subjected to the compressive loading on the top while the bottom is clamped. The obtained displacement value is presented in Fig. 3a and the current

Table 1. Presentation of the macro-scale and micro-scale material parameters.

Macro-scale parameters	Values	Micro-scale parameters	Values
Modulus of elasticity, E	50 [GPa]	Initial porosity	1.5 in [%]
Poisson's ratio, ν	0.2 [–]	Void diffusion modulus, α	0.1 in $[N]$
–	–	Void stiffness modulus, ξ	30 in [kPa]
–	–	Coupling number, N	0.3 in [–]



(a) (b)

Fig. 3. Numerical results of the unit cube specimen under uni-axial compressive loading a) extracted displacement field and b) current porosity distribution.

porosity is in Fig. 3b. It is observed that the current porosity is between 0.96% at the bottom and 1.13% at the top in Fig. 3.

Based on the α value from very small $\alpha = 0.001$ $[N]$ until very large $\alpha = 100$ $[N]$ value, the role of α is highlighted. According to the numerical experiments, α deals with the stiffness of the pore and then the high porosity gradient should be expected with the smallest α value while the porosity gradient should be nearly zero with higher α values[2].

4.2 Modeling of shrinkage due to CO_2 carbonation and highlighting the coupling number, N)

The micro-dilatation theory has been applied to modeling of CO_2 shrinkage of the cement-based materials like cement mortar. In fact, the CO_2 gas is introduced through the mortar and then dissolved in pore-water to product $CaCO_3$ which is crystallized around the pore [39–43]. The mentioned chemical process leads to the shrinkage of the materials. The experimental tests in which cement mortars are subjected to CO_2 diffusion have been performed in laboratory and the porosity change and shrinkage deformation have been determined according to different CO_2 concentrations in Fig. 4a. Assuming that the material has $\alpha = 0.01$ $[N]$ referred to the previous numerical experiment results and no visco-elastic behavior $\omega = 0$ $[Pa.s]$, some numerical experiments have been done with different coupling numbers N which can be written as:

$$N^2 := \frac{\beta^2}{K\xi} \quad \text{where} \quad N^2 \in [0, 1[. \tag{24}$$

[2] It should be mentioned that the ξ value is more complicated parameter depending on either stiffness of the pore or degree of macro-micro coupling. Therefore some numerical experiments are required to find out the most appropriate values.

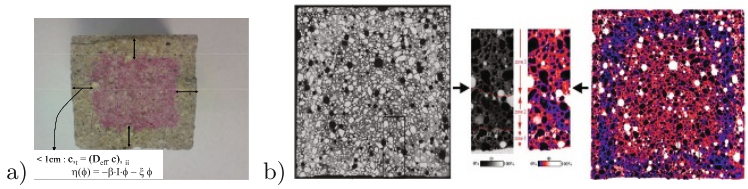


Fig. 4. Left: autoradiograph of a section perpendicular to the surface of mortar sample. Low porosity zones (grains) are white, bubbles are dark and cement is medium gray regions. Center left: detailed view of the porosity map computed from the autoradiograph. Center right: detailed view of the porosity map displayed using an adapted color look up table; nonporous grains are black, bubbles are white, blue color is centered in porosity = 12% (carbonated cement), red color is centered in porosity = 26% (undisturbed cement). Right: porosity zonation of the whole section of the sample is clearly revealed by a porosity map displayed in this false color mode.

The porosity variation on the mortar subjected to CO_2 carbonation is computed by various N values[3]. The most appropriate N value has been determined via the ^{14}C-PMMA method (polymethylmethacrylate) impregnation method [37,43–45] which is a radiographic image techniques developed by POSINAM European project. This method permit us to obtain the porosity on the mortar.

4.3 Modeling of Delayed Ettringite Formation and highlighting micro-volume force inside pore

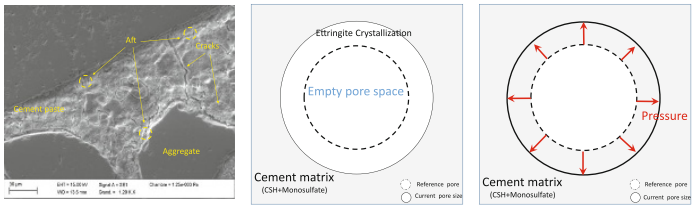
Another important pathology of the cement concrete materials is the Delayed Ettringite formation (DEF) [46–53]. For DEF phenomenon, the third equilibrium equation in Eq. (6c) has been focused on again. It is required to mention that the third equilibrium equation, particularly, the role of $\rho_\ell \ell$ has never been studied yet. The DEF phenomenon takes place when the cement-based materials have experienced a high temperature during the cure period and then this high temperature can decompose the ettringite and it can be replaced by the mono-sulfate which crystallizes in any empty space like pore or cracks (Fig. 5a). As a consequence, the cement-based materials sustain the bulk expansion under DEF crystallization and then, the crystallization pressure is applied inside pore spaces (Fig. 5b and Fig. 5c). Hence, it is assumed that crystallization pressure corresponds to the micro-volume force of the micro-dilatation in Eq. (25). This is our main assumption for modeling of the DEF inside the cement-based materials.

$$\rho_\ell \ell := -\Delta P. \tag{25}$$

Based on the open litterature, the pressure crystallization value is available and it is applied in the current study. The pressure value depends on the pore size and this value should not be the same for the whole specimen but rather it is randomly distributed[4]. Consequently, the Monte Carlo method is used to apply randomly the crystallization pressure in the whole specimen. To extract the stress distribution in

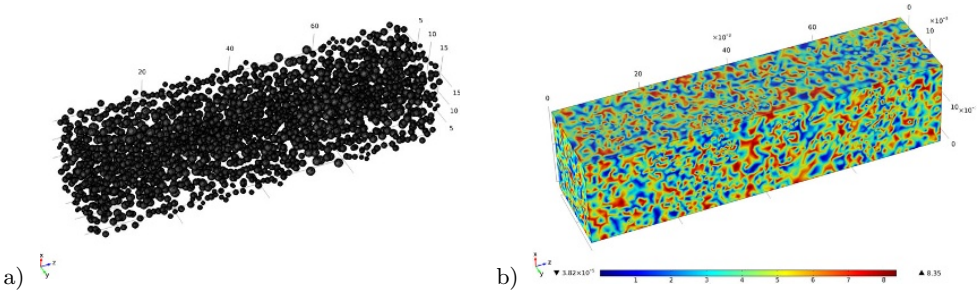
[3] The very weak couplings lead to the zero coupling number ($N^2 = 0$) and very strong couplings take place while $N^2 = 1$. The determination of the coupling number is an important task in the micro-dilatation theory.

[4] It is important to mention that the cement-based materials have an extremely complex micro-structure due to the their components and porosity. The porosity can be seen from some nano meters to some micro meters.



(a) (b) (c)

Fig. 5. Delayed Ettringite Formation (DEF) pathology phenomenon in the cement-based materials [54], a) crack formation on the cement paste due to the DEF, b) schema of the ettringite crystallization inside empty pore and c) crystallization pressure application towards cement paste matrix.



a) b)

Fig. 6. Numerical mortar bar specimen using one-quarter symmetry assumption ($80 \times 20 \times 20$ [mm]) under random DEF application [54], a) mesh presentation of perfect spherical aggregates of the mortar bar specimen and b) induced stress distribution.

the cement matrix, the spatial stochastic crystallization pressure has been generated several times and the relevant actions have been achieved by means of the obtained numerical samplings via the Monte Carlo method. In Fig. 6, the numerical mortar specimen with spherical aggregates is shown as well as the induced stress distribution. The maximum tensile stress is greater than 8 [MPa]. The extracted tensile stress is high enough to create micro-crack through the specimen and this matter is observed by Scanning Electronic Microscopy (Fig. 5a).

5 Conclusion and perspective

In the current paper, the micro-dilatation theory is investigated for the chemically motivated mechanical phenomenon modeling on the porous materials. The thermodynamic laws are revised for the porous-system and the internal energy expression including three variables, i.e. strain, porosity change and gradient of porosity change. All additional micro-scale material parameters are studied via two concrete pathologies. The analytical damage model which induces the micro-crack at the pore scale without mechanical behavior modification at macro-scale is also proposed and it would be put into practice in the next studies.

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