PREDICTING THE LONG-TERM PERFORMANCE OF STRUCTURES MADE WITH ADVANCED CEMENT BASED MATERIALS IN EXTREMELY AGGRESSIVE ENVIRONMENTS: CURRENT STATE OF PRACTICE AND RESEARCH NEEDS – THE APPROACH OF H2020 PROJECT RESHEALIENCE.

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Abstract

Recently, in the framework of H2020, the European Commission has funded the project ReSHEALience (www.uhdc.eu), whose main goal is to develop an Ultra High Durability Concrete (UHDC) and a Durability Assessment-based Design (DAD) methodology for structures, to improve durability and predict their long-term performance under Extremely Aggressive Exposures. The project, coordinated by Politecnico di Milano, gathers 14 partners from 8 different countries (Italy, Spain, Estonia, Germany, Greece, Ireland, Israel, Malta), including 6 academic and research institutions together with 8 industrial partners, which cover the whole value chain, from producers of concrete constituents to construction companies to stake-holders and end-users. A key activity of the project will consist in the development of a theoretical model to evaluate ageing and degradation of UHDC structures, extending the modelling to predict the lifespan, and its incorporation in a Durability Assessment-based Design (DAD) methodology, which will be validated against experimental tests performed in the same project and the monitored performance of six full-scale pilots in real exposure conditions. The paper, starting from a review of the current state of art on the modelling of advanced cement based materials in extremely aggressive environments (EAE), will address the approach pursued in the project.

1. INTRODUCTION

The improvement of durability and reduction of maintenance efforts is of the utmost importance for structures exposed to Extremely Aggressive Environments (EAE). This challenge needs to be tackled through a “holistic approach”, which encompasses the concept and development of advanced materials and tailored design approaches to provide innovative structural solutions aimed to provide fit-for-the-purpose answers to the aforementioned needs.

In current design approaches, lifespan is defined by a target reference value, which, through a “structural class concept” and as a function of the exposure class, results into prescriptions deemed to guarantee the demanded level of durability. These prescriptions imply the use of high cement content, low water/cement ratios, suitable aggregates, high reinforcement covers, and the use of even new types of corrosion resistant reinforcement (e.g. epoxy-coated, stainless/galvanised steel or polymer bars), but hardly take into account new cement-based construction materials, such as Ultra High Performance (Fiber Reinforced) Concrete (UHPC/UHPFRC), neither new constituents to improve the durability (including nanoparticles or self-healing promoters), because of the lack of standards and of technical awareness by most designers and contractors. Anyway, the use of UHPC/UHFRC still has significant limitations to be overcome and the material has so far failed to stand as the market breakthrough concept/product it was expected to be. This is due to the claimed superior durability of UHPC/UHPFRC, which has been almost exclusively proven in the laboratory, and with main reference to the un-cracked state. With reference to the cracked state a "superior durability" is generally heuristically justified because of the higher crack tightness characterising the material response under tensile loads. Moreover, its use has hardly been accompanied by design considerations, due to the lack of internationally recognized regulations and a clear quantitative evaluation of the structure lifespan or service life is so far also lacking.

The EC H2020 funded ReSHEALience project (www.uhdc.eu) moves from the consideration that the long-term behaviour of structures under extremely aggressive exposure conditions can highly benefit from the use of high performance materials, in the framework of durability based design approaches. To achieve the required improvements in durability, the concept of Ultra High Performance (Fibre Reinforced) Concrete (UHPC/UHPFRC) will be upgraded to a "metamaterial" concept, through the incorporation of tailored functionalities to enhance the long-term durability performance. This will allow obtaining a new category of advanced cement based materials, named Ultra High Durability Concretes (UHDCs). Current experimental tests, numerical models and engineering design approaches are not optimized to fully exploit the whole set of potentials brought by these categories of advanced cement based materials. In order to fill this gap, the ReSHEALience project will also work on adapting and improving existing testing techniques and design criteria and/or formulating and validating new dedicated ones, so that they can be effectively and reliably applied to UHDC.

Anyway, the experimental characterization of the durability of construction materials in real structure scenarios is quite a challenging task, involving non-conventional experimental capabilities and most of all requiring the investigation to span along a time frame whose extension could hardly match with the needs of an effective and market oriented technology transfer. In this respect the availability of sound and reliable predictive modelling tools becomes of the utmost importance, since only they would allow to extrapolate the results of performed experimental characterization of the durability performance of cement-based materials to real structure service scenarios.

The modelling activity in ReSHEALience will move from the description of aging and degradation of UHDC to predict the service-life of UHDC applications under EAE conditions. Multiphysics continuum tightly coupled models will be combined into an overall numerical code and applied to macroscale phenomena. The models will take into account both the aggressiveness of the environment and self-healing of UHDC. The holistic model will link the effects of chemical reactions, transport of ions, diffusion of moisture and heat, in cracked and un-cracked concrete conditions, corrosion, damage initiation and propagation in reinforced concrete at macroscale. As a main advantage, the model can be employed not only to support the experimental results of the project but also to simulate the behaviour of real structures in service conditions. The modelling activity will incorporate all the experimentally investigated mechanisms and combine them into a unique workflow aimed at simulating the structural durability at the macroscale. It will also be validated against the performance of six pilots, which will be monitored through advanced sensors.

This paper, starting from a review of the current state of art on the modelling of advanced cement based materials in EAE, will address the approach pursued in the project.

2. MODELLING THE DURABILITY OF ADVANCED CEMENT-BASED MATERIALS: THE CURRENT FRAMEWORK

Durability models existing in the literature generally focus only on one or two of the multiple mechanisms which govern degradation and ageing of cement-based materials [1-4].

Corrosion of reinforcement is one of the most common causes of "durability failure" of R/C structures and a significant number of models has been developed with reference to it [5-10], also pursuing implementation into design codes (*e.g.* Eurocode 2). Though, generally speaking, these models do not yet consider the cracked state of the concrete [11,12].

Alkali-Silica Reaction (ASR) is another degradation phenomenon of worldwide concern. Several models can be found in the literature to simulate its mechanisms and effects [13,14], which, by the way, all consider the ASR degradation mechanism alone and never in combination with other ones.

One of the challenges posed by the project ReSHEALience is the modelling of the self-healing capacity of the advanced cement based materials which will be formulated and investigated in the framework of the project and which will be employed for the construction of the six full-scale validation pilots. A survey has been recently published by Jefferson et al. [15] highlighting that the existing models for self-healing cement-based materials have been validated using in most cases limited sets of experimental data, which are often not presented in the model papers in sufficient detail. Besides the insufficient interaction between relevant numerical and experimental research teams, the reasons for this state of affairs could be sought in the paucity of experimental data suitable for properly validating numerical models. The research group at Politecnico di Milano who is also co-authoring this paper has recently proposed a model in which the SMM (Solidification-Microprestress-Microplane) model [16-18] has been extended in order to incorporate the self-healing effects introducing an internal variable which characterizes the self-healing process, the effects of cracking on the diffusivity, and the positive recovering effect of the self-healing on the mechanical properties [19], validating it on own experimental results [20].

The concerns raised by [15] about the paucity of experimental raw data suitable as basis for durability modelling, calls into play the need of using fuzzy-probabilistic strategies to handle the same data [21]. This mathematical strategy has proven efficient for SHCC and chloride ingress but is open for application to other types of cement-based composites as well as regarding further and multiple exposures and degradation mechanisms [22,23].

3. MODELLING THE DURABILITY OF ADVANCED CEMENT-BASED MATERIALS: THE "*RESHEALIENCE*" APPROACH

The modelling activity in ReSHEALience will move from the description of aging and degradation of UHDC to predict the service-life of UHDC applications under EAE conditions. Multiphysics continuum tightly coupled models will be combined into an overall numerical code and applied to macroscale phenomena. The models will take into account both the aggressiveness of the environment and self-healing of UHDC. A model is going to be formulated, whose chain structure is shown in Figure 2, which will link the effects of chemical reactions, transport of ions, diffusion of moisture and heat, in cracked and un-cracked concrete conditions, corrosion, damage initiation and propagation in reinforced concrete. As a main advantage, the model can be employed not only to support the experimental results of the project but also to simulate the behaviour of real structures in service conditions.

The model consists of a continuum model for diffusion of moisture, heat and chemical species, and Law of Mass Action (LMA) models for chemical processes applied to macroscale, and electrical current equation, coupled with a continuum model applied at the macroscale for steel reinforcement bars and with a model to simulate the UHDC matrix. In the case of structural scale simulations this is likely to be a continuum model whereas for material level simulations a discrete mechanical model will be applied at the scale of material heterogeneity. The latter is based on the LDPM (Lattice Discrete Particle Model) [24] which has also been recently utilized that model with great success to simulate the degradation due to ASR [4,14].

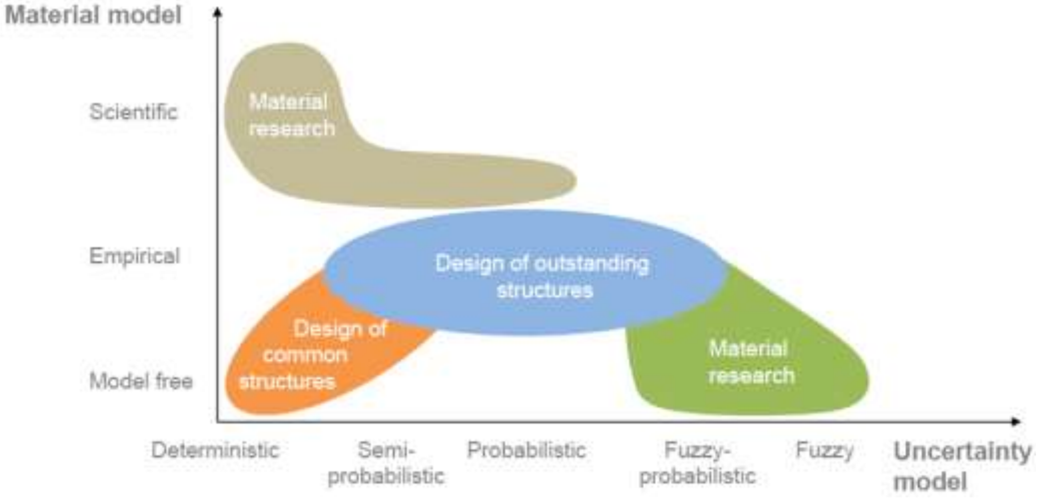

Figure 1. Coupling material model with uncertainty model in the definition of a Durability assessment-based Design approach (adapted from [21]).

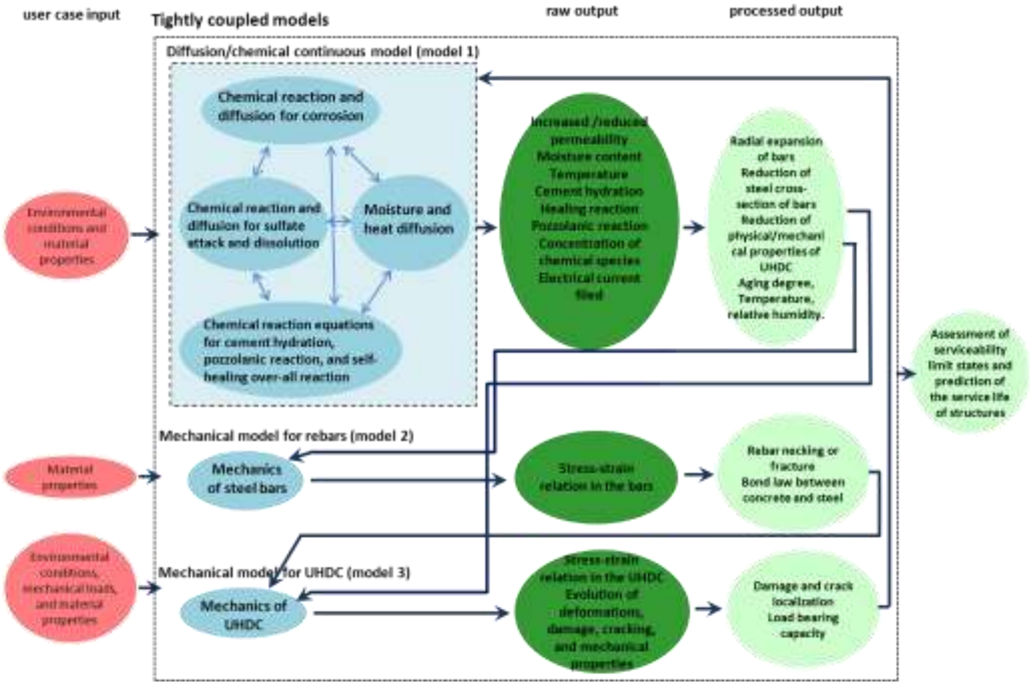

Figure 2: ReSHEALience model chain as from MODA template

3.1 Continuum model for diffusion and chemical processes at macroscale - physics of the model equations

The model combines the chemical processes of binder hydration and self-healing with heat, water, oxygen and ions transport processes and corrosion. The formers are modelled through the following Law of Mass Action equations, starting from the hydration of cement, whose evolution over time is described through a degree of cement hydration α_c

$$\frac{\partial \alpha_c}{\partial t} = A_c(\alpha_c, h) e^{-E_{ac}/_{RT}} \tag{1}$$

where A_c is a normalized chemical affinity, also depending on the relative humidity h, and E_{ac} is the hydration activation energy, with R universal gas constant and T is the temperature.

Similarly, in the case of a cementitious substitute featuring pozzolanic reaction, such as fly ash and/or silica fume, a degree of pozzolanic reaction α_s is assumed as an indicator of the process, as follows, with similar meaning of the employed notation:

$$\frac{\partial \alpha_s}{\partial t} = A_s(\alpha_s, h) e^{-E_{as}/_{RT}} \tag{2}$$

The normalized chemical affinity in the cement hydration reaction is described as [16,17]:

$$A_c(\alpha_c, h) = A_{c1}\left(\frac{A_{c2}}{\alpha_c^\infty} + \alpha_c\right)(\alpha_c^\infty - \alpha_c) e^{-\eta_c \alpha_c/\alpha_c^\infty}[1 + (a - ah)^b]^{-1} \tag{3}$$

where α_c^∞ is the asymptotic degree of hydration; η_c, A_{c1} and A_{c2} are material parameters to be calibrated through the analysis of experimental results, together with a and b for which anyway the recommended constant values $a = 5.5$ and $b = 4$ can be generally adopted. A similar relation can be proposed for the normalized chemical affinity in the pozzolanic reaction, whose parameters have to be calibrated from experimental data referring to the particular type of employed cement substitute.

With reference to the self-healing the approach proposed in [19] is going to be followed, which introduces, similarly to the degree of cement hydration and pozzolanic reaction, a self-healing recovery degree λ_{sh} which characterizes the evolution of the healing related recovery of material performance varying between 0 and 1, in case of full completion of the process.

$$\frac{\partial \lambda_{sh}}{\partial t} = A_{sh}(\lambda_{sh}) e^{-E_{ash}/_{RT}} \tag{4}$$

where the normalized self-healing reaction affinity the following expression is proposed:

$$A_{sh} = \tilde{A}_{sh}(1 - \lambda_{sh}) \tag{5}$$

The function $\tilde{A}_{sh}$ has to take into account the effect of the initial un-hydrated cement and the possible presence of additive material that accelerates the healing process together with the influence of relative humidity h and initial crack opening w, as follows :

$$\tilde{A}_{sh} = \tilde{A}_{sho}\, f_h(h)\, f_w(w) \tag{6a}$$

$$\tilde{A}_{sho} = \tilde{A}_{sh1}\,(1 - \alpha_c^{sh0})c + \tilde{A}_{sh2}\, sh_{st-adm} \tag{6b}$$

$$f_h(h) = \frac{1}{1 + (a_h - a_h h)^{b_h}} \tag{6c}$$

$$f_w(w) = \{1 - [a_w - a_w(1 - w)]^{b_w}\}^{-1} \tag{6d}$$

In Equation (6b), the coefficient $\tilde{A}_{sho}$ takes into account the effect of the initial un-hydrated cement and the possible presence of additive material that accelerates the healing process, with c cement content and α_c^{sh0} is the value of the hydration degree when the healing process starts (that isn't generally uniform in the volume). The term $(1-\alpha_c^{sh0})c$ thus represents the amount of unhydrated cement available at the beginning of the healing phenomenon.

Similarly, the term $\tilde{A}_{sh2}\ sh_{st-adm}$ has been introduced to take into account for the presence of a self-healing stimulating admixture (at a dosage equal to $sh_{st\text{-}adm}$), including cementitious substitutes in case, on the healing process as a whole [20].

Material parameters $\tilde{A}_{sh1}$ and $\tilde{A}_{sh2}$ in Equation (6b), which have the dimension of volume/mass/time together with constant a_h and b_h in Equation (6c) and a_w and b_w in Equation (6d) have to be calibrated on the basis of experimental results.

It is worth here remarking that the proposed preliminary formulation for self-healing does not take into account other influencing factors, such as:

(1) the water pressure: a liquid flowing faster through the crack would wash out the deposited healing products, preventing the self-healing from occurring [25, 26];
(2) the leaching or dissolution, since an aggressive fluid that leads to a leaching or dissolution reaction can affect the healed crack;
(3) the stability of the crack over time, as affected by sustained through-crack stresses [27].

Heat transport is modelled through the well-known energy conservation equation

$$\rho c_t \frac{\partial T}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{q} + \dot{Q}_c + \dot{Q}_s \qquad (7)$$

where $\mathbf{q}$ is the heat flux, linked to the temperature gradient $\boldsymbol{\nabla}T$ through the Fourier equation and the material conductivity, c_t is the heat capacity and ρ is the concrete density. The two heat source terms, $\dot{Q}_c + \dot{Q}_s$ describe the heat of hydration of cement and the enthalpy of the generic cementitious substitute and have to be calibrated through experimental results.

As for the transport processes of water, oxygen and other phenomena, mass conservation equations are used, also implementing formulations proposed in [3,18,19]. In detail:

- <u>diffusion of water:</u>

$$-\frac{\partial w(h,\alpha_c,\alpha_s)}{\partial t} = \boldsymbol{\nabla}\cdot\boldsymbol{J_w} \qquad (8)$$

where w is the water content and $\boldsymbol{J_w}$ is the water flux, linked through the Fick's law for water transport $\boldsymbol{J_w} = -D_h(h,T,d)\boldsymbol{\nabla}h$ to the gradient of relative humidity $\boldsymbol{\nabla}h$, with $D_h\ (h,T,d)$ water permeability coefficient;

- <u>diffusion of oxygen:</u>

$$-\frac{\partial C_o}{\partial t} = \boldsymbol{\nabla}\cdot\boldsymbol{J_o} - \boldsymbol{J_w}\boldsymbol{\nabla}C_o + \dot{O} \qquad (9)$$

where C_o is the oxygen concentration, $\boldsymbol{J_o}$ is the oxygen flux, and $\dot{O}$ is the source or sink term of oxygen due to chemical reactions (before depassivation of steel is $\dot{O} = 0$);

- <u>chloride ions</u>

$$-\frac{\partial C_c}{\partial t} = \boldsymbol{\nabla}\cdot\boldsymbol{J_c} - \boldsymbol{J_w}\boldsymbol{\nabla}C_c + \frac{\partial C_{cb}}{\partial t} \qquad (9)$$

with C_C and C_{Cb}, concentration of free and bound chlorides and $\boldsymbol{J_C}$ chloride ions flux;

- carbon dioxide (CO_2):

$$-\frac{\partial C_{CO_2}}{\partial t} = \nabla \cdot \boldsymbol{J}_{CO_2} + \dot{C}_{CO_2} \tag{10}$$

- sulfate ions:

$$-\frac{\partial C_s}{\partial t} = \nabla \cdot \boldsymbol{J_s} - \boldsymbol{J_w} \nabla C_s + \dot{C}_S \tag{11}$$

- calcium ions:

$$-\frac{\partial C_{Ca}}{\partial t} = \nabla \cdot \boldsymbol{J_{Ca}} - \boldsymbol{J_w} \nabla C_{Ca} + \dot{C}_{Ca} \tag{12}$$

All three equations (10-12) have a common structure where the ion concentration *C*, the ion flux $\boldsymbol{J}$ and a sink term due to chemical reactions $\dot{C}$ appear.

With reference to numerical implementation, the previous system of partial differential equations in the strong form is rewritten into the weak form and discretized in space using Galerkin finite element method. Time discretization of the partial differential equation system is obtained by the well-known Crank–Nicolson method (a central difference method) that has been proven to be unconditionally stable in the case of constant matrix coefficients. When solving the aforementioned equations for diffusion and chemical processes at macroscale it is assumed that damage is constant, i.e. physical and chemical properties are controlled by mechanical properties (damage) from the previous time step as obtained in input from the mechanical model for UHDC (discrete model at the scale of material heterogeneity).

The output of the model is interpolated for the discrete material description of the UHDC mechanical model, calculating the values on each facet of the cells, to provide it in input

- all the chemical quantities that characterized the hydration and self-healing;
- moisture and temperature field
- volume expansion and reduction of physical/mechanical properties.

Moreover, the cross-section reduction and the radial expansion of the re-bars are obtained and reinforcement deterioration are provided in input to the continuum mechanical macroscale model of steel bars, for which a classical elastic-plastic model is employed.

3.2 Discrete model at the scale of material heterogeneity

UHDC is here idealized as an assembly of rigid particles whose equilibrium generates a system of equations like the finite element method in general. The particle generation is carried out by assuming that each aggregate piece can be approximated as a sphere. From the grain size distribution of the investigated UHDC, the spheres are randomly placed in the volume. The topology of the particles is obtained by means of a Delaunay “tetrahedron tessellation”, from which the (rigid) polyhedral cells containing one particle are generated and the facets associated with each cells is where the constitutive law is formulated [24] (Figure 3).

Discrete compatibility equations (strains vs. displacements) are formulated through the relative displacements (and rotations) of adjacent nodes (particles). Equations of force and moment dynamic equilibrium for each discrete cell that, after the assembling, give

$$\boldsymbol{M}\frac{d^2\boldsymbol{Q}}{dt^2} + \boldsymbol{P}(\boldsymbol{Q}) = \boldsymbol{F}(t) \tag{13}$$

where $\boldsymbol{M}$ is mass matrix, $\boldsymbol{P}$ is the vector of internal static quantities, which are obtained by assembling the contributions from all the discrete cell, $\boldsymbol{Q}$ the vector of kinematic variables, i.e. displacements and rotations of all cells, $\boldsymbol{F(t)}$ given external action history.

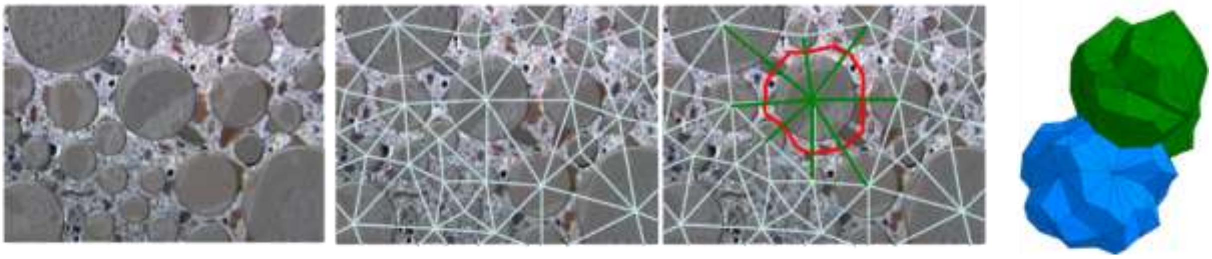

Figure 3: from material heterogeneity scale to polyhedral discretization

The system of equations is solved using the classical solution procedures for nonlinear finite element discretization, such as explicit and implicit methods for transient problems. The numerical time is scaled for the integration of rate-type creep formulation since coincides with the real time lapse of the simulated cases.

Stresses and strains, i.e. static and kinematic quantities at each facet between particles, are related by means of constitutive relationships that consists of [4,18,24]:

- age dependent constitutive law, depending on the aging degree, self-healing, volumetric expansion and reduction of mechanical/physical properties from model 1;
- viscoelastic behaviour based on Solidification and Micro-Pre-Stress theory dependent on aging degree, relative humidity, temperature from model 1;
- hygrometric and thermal strains.

When solving the model equations, it is assumed that all the physical and chemical properties from model 1 are constant in the time step. The computed deformation and damage (crack opening) state is interpolated on the finite element discretization mesh utilized in the model 1 and exported as a “previous step” input for the same model.

This proposed formulation will be first calibrated on relevant experimental tests performed in the experimental validation task, including, *e.g.*, calorimetry, water diffusion, chloride diffusion and healing tests. After, the whole numerical framework will be adopted to simulate the performance of the six pilots built and monitored in real exposure conditions.

4. CONCLUSIONS

In order to fully exploit the potential of advanced cement based materials a breakthrough durability-based material concept and design is necessary in which durability is not a bonus (as currently is for UHPC/UHPFRCs) but becomes the governing objective. This requires a robust durability experimental evaluation in real service conditions, to identify and quantify the parameters to be used in a durability-based design and their threshold values, and for monitoring the evolution of these parameters in the real structure. This is quite a challenging task, involving non-conventional experimental capabilities and most of all requiring the investigation to span along a time frame whose extension could hardly match with the needs of an effective and market oriented technology transfer. For this reason, a likewise robust modelling of the durability, encompassing different physical/chemical degradation mechanisms, aging and interaction with mechanical loads is required.

In this paper the modelling activity which is going to be performed by the consortium involved in the H2020 project ReSHEALience has been presented. The project will upscale the concept of UHPFRCC to the “metamaterial concept” of a Ultra High Durability Concrete, through the incorporation of tailored functionalities to enhance the long-term durability performance. The proposed modelling approach incorporates the investigated physical/chemical degradation mechanisms and combines them into a unique workflow aimed at the simulation of the structural durability at the macroscale. Moreover, the experimentally garnered raw data suitable as basis for durability modelling, will be handled through fuzzy-probabilistic strategies, to be consistently extended to a design-format which professional engineers may confidently employ. Material durability model parameters will be calibrated through a dedicated and thorough experimental campaign and the model predictions will be also validated against the real-life monitoring, through advanced fit-for-the-purpose sensors able to measure the “in-structure durability performance” of the materials in six full-scale pilots. These have been selected as representative of cutting edge economy sectors, such as green energy, blue growth and conservation of R/C heritage and include a cooling tower water basin and a geothermal mud-collection basin based in Italy, a floater for off-shore wind turbine and a mussel-raft to be installed in the Mediterranean sea offshore from the Valencia coast, a precast breakwater elements to be installed along the British Isles coast and a severely damaged water tower in the Valletta Grand Harbour region in Malta to be retrofitted. This stands as a one-of-a-kind feature of the project aimed at providing a breakthrough change from a prescription- to a performance-based material and structural durability concept targeting to the overall resilience of engineering applications built of/retrofitted with advanced cement based materials.

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