D4.5 Public report on EnDurCrete modelling and simulation approach – final completed MODA

Lead Partner: RINA

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Executive Summary

Work package 4 (WP4) of the EnDurCrete project focused on the theoretical understanding and modelling at different scales of the factors which affect the durability of concrete, including corrosion and ageing phenomena.

In particular, Micro-mesoscale (first two rows of the diagrams) here considered ranges from 10-100 nm (characteristic size of the smaller hydrated solid phases) to 10 cm, thereby defining representative elementary volumes of cement paste (about 1 mm), mortar (10 mm) and concrete (10 cm). Macroscale is here considered from 10 cm to several meters, representing the whole concrete infrastructures. The numerical models are calibrated using durability performance indicators experimentally determined in WP5. Long-term service life prediction of concrete macrostructures is done using computational analyses, considering corrosion phenomena and other critical conditions (e.g. cycling loading and exposure to fire). The prediction will be tuned by means of periodical reports of long-term monitoring performed in WP6.

Within this report, the implemented setup of the models is presented and described following the Modelling Data Elements (MODA) template according to the European Materials Modelling Council (EMMC).

This report provides a public summary of EnDurCrete modelling and simulation approach for dissemination and training purposes, including the final MODA.

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Abbreviations and Acronyms

[MR] – Material relation
[PE] – Physical equation
[WP] – Work package
[MODA] – Modelling Data Elements
[EMMC] – European Materials Modelling Council
[RoMM] – Review of Material Modelling

1 Introduction

The present report aims to provide a **description of the implemented models following the Modelling Data Elements (MODA) template according to the European Materials Modelling Council (EMMC).**

The description of EnDurCrete modelling and simulations approach follows the guidelines provided by the European Commission in the "Review of Material Modelling (RoMM)" in terms of modelling concepts, homogenised workflow diagrams, etc.

Micro-mesoscale (first two rows of the diagrams) is here considered from 10-100 nm (characteristic size of the smaller hydrated solid phases) to 10 cm defining representative elementary volumes of cement paste (about 1 mm), mortar (10 mm) and concrete (10 cm). Macroscale is here considered from 10 cm to several m, representing the whole concrete infrastructures. Overall, the modelling approach is based on three coupled Physics and chemistry Equations (PE) at each considered scale. Simulations results will be compared for validation with experimental characterisation of concrete samples (task 5.1) and with results of long-term monitoring on demo structures (WP6).

Table 1 MODA for durability prediction of concrete in critical exposure conditions simulated in project EnDurCrete

OVERVIEW OF THE SIMULATION			
1	USER CASE	Estimation of diffusive and mechanical (elastic, ageing viscoelastic) properties of novel materials at the scale of cement paste, mortar and concrete. Prediction of damage of concrete due to loading and corrosion product growth at steel/concrete interfaces consecutive to carbonation. Long-term service life prediction of concrete infrastructures considering corrosion phenomena and other critical conditions (e.g. cycling loading and exposure to fire).	
2	CHAIN OF MODELS	MODEL 1 - DATA BASED MODEL	Thermodynamic model (Gibbs energy minimization)
		MODEL 2	Continuum micromechanics. Continuum diffusion/transport.
		MODEL 3	Continuum micromechanics. Continuum diffusion/transport.
		MODEL 4	Continuum mechanics. Continuum diffusion/transport.
3	PUBLICATION PEER-REVIEWING THE DATA	At present, there is no publication on these data.	
4	ACCESS CONDITIONS	Open access publications and presentations.	

		Calculation of homogenized properties will be carried out with the commercial software Mathematica (http://www.wolfram.com/mathematica/). FE simulations at the concrete material scale will be performed in the FE code developed at CEA (http://www-cast3m.cea.fr/); this code is open-source for research use, but a license is required for commercial applications. Continuum models at the macroscale will be based instead on the commercial package Sap2000 (https://www.csiamerica.com/products/sap2000). The software which will be used for the thermodynamic modelling is GEM – Gibbs Energy Minimization software. The GEM software is distributed "as is" by the Laboratory for Waste Management (LES) of the Paul Scherrer Institute (PSI). Permission to download (http://gems.web.psi.ch/) and use GEM Software is hereby granted free of charge for educational and academic research purposes.
5	**WORKFLOW AND ITS RATIONALE**	To the authors' knowledge, the durability of complex concrete structures, including innovative materials, is far from being either fully understood or predicted in real application scenarios. Analytical mathematical models have been used for the estimation of concrete service life and strength, in compliance with the European Standards EN 197 for cement and EN 206 for concrete[1]. Such predictive models focus on service life with respect to carbonation and to chloride penetration, based on a system of non-linear differential equations built on reaction engineering principles. Such systems are easy-to-use, but fail to predict the behaviour of structures where new materials are applied. In EnDurCrete a multi-scale and multi-physic modelling approach is followed, validated by experimental data acquired during the project by the EnDurCrete advanced monitoring and testing tools. In this context: • Multiscale homogenization techniques are widely used and well adapted to estimate physical properties of cement-based materials, including ageing linear viscoelastic ones. • The analysis of concrete samples including explicitly coarser aggregates and steel reinforcement provides an accurate description of initiation and propagation of damage induced by corrosion products formation consecutive to carbonation. • The material parameters and Material Relation (MR) resulting from the micro and meso scale models, validated through experimental tests, will be used for macro-scale simulations aiming at service-life prediction of concrete structures (e.g. ports, tunnels, bridges, offshore structures, etc.) in harsh environments.

[1] Demis S and Papadakis VG 2016; Estimation and Validation of Concrete Strength and Service Life Using Software Packages based on Predictive Models; Granja 2016.

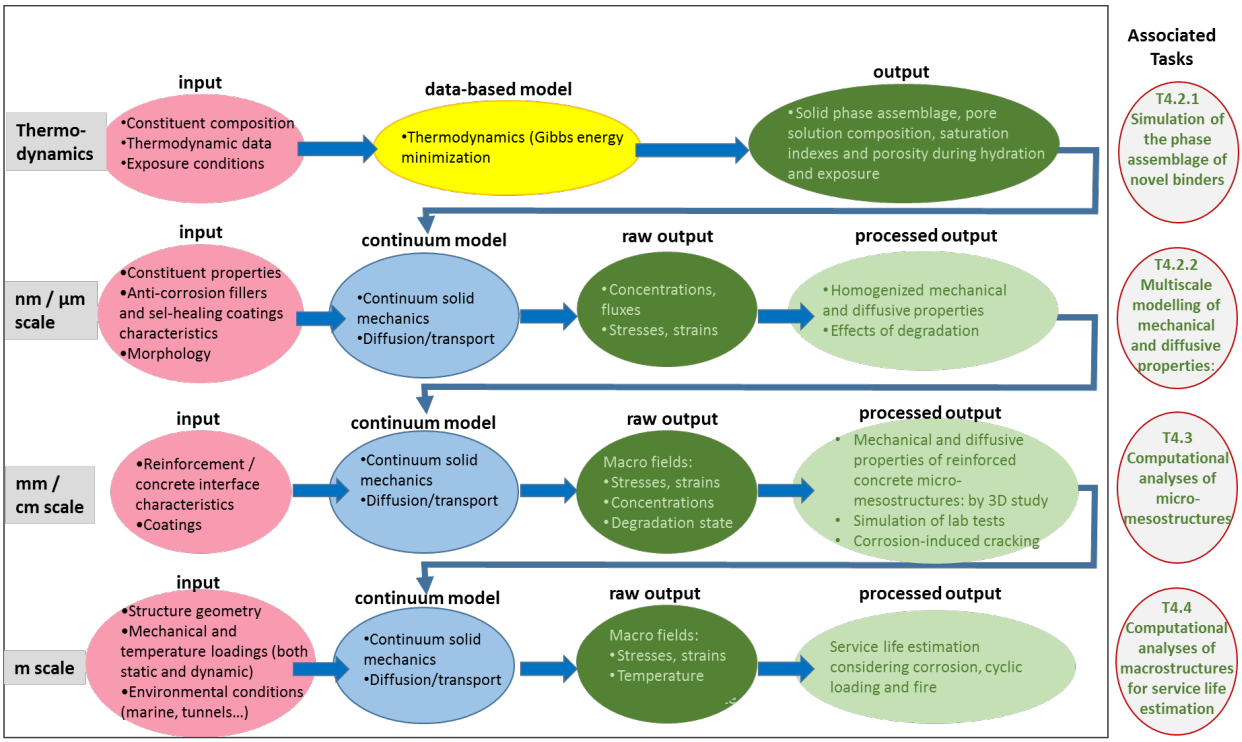

Figure 1 Workflow picture

The first step is dedicated to multiscale modelling of mechanical and diffusive properties of cement paste, mortar and concrete (Task 4.2). The model addresses in a first stage (T4.2.1) the calculation of the phase assembly in the hydrated cement paste through appropriate chemical reactions describing hydration, based on concrete constituent properties and the novel additives characteristics studied in WP2 and WP3. The changes in the phase assembly (including porosity) upon exposure to aggressive environments will also be predicted.
The second stage consists in calculating the homogenized mechanical and diffusive properties of cement paste, mortar and concrete components (T4.2.2) by applying mean-field upscaling techniques, considering the phase volume fractions obtained in stage 1 for the various studied exposure conditions. These physical properties serve as input for the second step. The second step focuses on computational analyses of micro-mesostructures (T4.2), with the aim to provide mechanical and diffusive properties of reinforced concrete through 3D simulations explicitly including the coarser aggregates and the steel rebars, and to study corrosion-induced cracking consecutive to carbonation.
At this mesoscale, cracking in the matrix will be described through a variable damage introduced in the mechanical behaviour of the material (this behaviour MR is involved in the conservation of momentum PE), and whose evolutions are controlled by the positive (extension) strains via a dedicated MR. Carbonation will be described by specific mass conservation PE for CO_2 and water species, completed by a MR modelling the calcite formation. Corrosion will be reproduced via a particular phenomenological MR characterizing the progressive formation of an expansive layer of corrosion products at the steel/concrete interfaces subjected to carbonation. The models will be validated on the lab tests carried out in WP5 and will provide inputs for the third step.
The third step will use such information to perform computational analysis of macrostructures for long-term service life prediction of concrete infrastructures considering corrosion phenomena and other critical conditions (e.g. cycling loading and exposure to fire). The prediction will be tuned by means of periodical reports of long-term monitoring performed in WP6 and will result in service life plans including graphical representations. The analysis will contribute to perform effective life-cycle cost analysis of the EnDurCrete products.

Task activity coordinated by RINA-C (who will also provide technical contributions related to Task 4.4. activity) receives technical contributions from NTNU (models developed in Tasks 4.2) and CEA models (developed in Tasks 4.2 and Task 4.3).

In particular:

- Chapter 2 provides the description for Micro-mesoscale (first two rows of the diagrams) considered from 10-100 nm (characteristic size of the smaller hydrated solid phases) to 10 cm defining representative elementary volumes of cement paste (about 1 mm), mortar (10 mm) and concrete (10 cm).
- Chapter 3 provides the description for Macroscale here considered from 10 cm to several meters, representing the whole concrete infrastructures.

2 MODA – Micro & Mesoscale

2.1 Application of a Data-based Model - MODEL 1

Table 2 User Case

1	USER CASE:	
1.1	ASPECT OF THE USER CASE TO BE CALCULATED	We will model the hydration phase assemblage of the novel binders upon hydration and under different exposure conditions
1.2	MATERIAL	The input is the bulk chemical composition of the cement and the reactive phases of the supplementary cementitious materials which have reacted
1.3	GEOMETRY	The modelling will be performed for specific amounts of water e.g. 50 g and cement e.g. 100 g replaced with different amounts of supplementary cementitious materials
1.4	TIME LAPSE (DURATION OF THE PROCESS TO BE DESCRIBED)	days, years
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	We will simulate: - Different compositions and degrees of reaction of the cement and the supplementary cementitious materials - Different exposure solutions e.g. chloride-rich solutions and CO_2
1.6	PUBLICATION ON THIS USE OF THE DATA-BASED MODEL	*Lothenbach, B. and F. Winnefeld (2006), Thermodynamic modelling of the hydration of Portland cement. Cement and Concrete Research 36, 209-226.* *De Weerdt, K., Ben Haha, M., Le Saoût, G., Kjellsen, K. O., Justnes, H., Lothenbach, B. (2011) Hydration mechanisms of ternary Portland cements containing limestone powder and fly ash. Cement and Concrete Research 41, 279-291.* *Machner, A., Zajac, M., Ben Haha, M., Kjellsen, K. O., Geiker, M. R., De Weerdt, K. (2018) Stability of the hydrate phase assemblage in Portland composite cements containing dolomite and metakaolin after leaching, carbonation, and chloride ingress. Cement and Concrete Composites 89, 89-106.*

Table 3 The Data-Based Model

2	**THE DATA-BASED MODEL**		
2.0	**TOOL OR EQUATION TYPE AND NAME**	Thermodynamics Gibbs Energy Minimization Selector (GEMS3.3)	
	PHYSICS QUANTITIES IN THE DATA-BASED MODEL	**HYPOTHESIS**	*For a given T, P, n^b, and standard state thermodynamic data of the dependent components, the amount of dependents components $n^{(x)}$ and the chemical potentials u of the independent components can be calculated from the following set of convex equations:* $\begin{cases} G(n^{(x)}) \Longrightarrow min \\ A \cdot n^{(x)} = n^b \end{cases}$ *with* $G(n^{(x)}) = \sum_j n_j^{(x)} v_j, \;\; j \epsilon L$ *and* $v_j = {g_j^0}/{RT} + lnC_j + ln\gamma_j + \Xi, \;\; j \epsilon L$ *Using the Karush-Kuhn-Tucker necessary and sufficient conditions* $\begin{cases} v - A^T u \geq 0; \\ A\hat{n}^{(x)} = n^b;\ \hat{n}^{(x)} \geq 0; \\ \hat{n}^{(x)}(v - A^T u) = 0 \end{cases}$
		PHYSICAL QUANTITIES	*Where:* *T* is temperature *P* is pressure $n^{(b)} = \left\{ n_i^{(b)}, i \epsilon N \right\}$ is the input amount of the independent components $n^{(x)} = \left\{ n_j^{(x)}, j \epsilon L \right\}$ is the calculated amount of the dependent component u is the chemical potential of the independent components $G\left(n^{(x)}\right)$ the total Gibbs free energy of the system A is the matrix constructed from the stoichiometric coefficients of independent components in formulae of dependent components v_j is the normalized chemical potential of the j^{th} dependent component g_j^0 is the standard state molar Gibbs energy function of the j[th] dependent component *R* is the universal gas constant C_j the concentration relative to the chosen standard concentration scale for the respective phase γ_j the activity coefficient of the j[th] dependent component

			Ξ the nonlogarithmic asymmetry term
2.1	**DATASET AND ORIGIN OF DATA**	*PSI-Nagra TDB and CEMDATA 18.01 thermodynamic database (https://www.empa.ch/web/s308/thermodynamic-data)*	

Table 4 Computational Detail Of Data-Based Application

3	**COMPUTATIONAL DETAIL OF DATA-BASED APPLICATION**	
3.1	**NUMERICAL OPERATIONS**	Convex minimization problem solved by a IPM (Interior Point Method) algorithm using Karush-Kuhn-Tucker conditions
3.2	**SOFTWARE TOOL**	The software which will be used is GEM – Gibbs Energy Minimization software. The GEM software is distributed "as is" by the Laboratory for Waste Management (LES) of the Paul Scherrer Institute (PSI). Permission to download (http://gems.web.psi.ch/) and use GEM Software is hereby granted free of charge for educational and academic research purposes. Further information can be found in the following publication: Kulik D.A., Wagner T., Dmytrieva S.V., Kosakowski G., Hingerl F.F., Chudnenko K.V., Berner U. (2013): GEM-Selektor geochemical modeling package: revised algorithm and GEMS3K numerical kernel for coupled simulation codes. Computational Geosciences 17, 1-24. Wagner T., Kulik D.A., Hingerl F.F., Dmytrieva S.V. (2012): GEM-Selektor geochemical modeling package: TSolMod library and data interface for multicomponent phase models. Canadian Mineralogist 50, 1173-1195.
3.3	**MARGIN OF ERROR**	The accuracy is strongly dependent on: - Accuracy of the determination of the degree of reaction of the cement and supplementary cementitious materials - Deviation of equilibrium due to e.g. topochemical differences, or kinetics - Thermodynamic data available

2.2 MODA - Physics-Based Model – MODEL 2 Multiscale estimation of mechanical and diffusive properties

Table 5 Aspect Of The User Case/System To Be Simulated

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Simulation of the elastic and diffusive properties based on a simplified representation of the material microstructure and its evolution (ageing, degradation).
1.2	MATERIAL	Mineral phases of the cement paste, sand and aggregates (volume fraction, morphology and spatial arrangement) Chemical composition of the cement paste (volume fraction of hydrated products), as calculated with the databased model (model 1).
1.3	GEOMETRY	Simplified infinite Representative Volume Element of Hydrated Cement Paste (HCP) = pores + hydrated phases + unhydrated cement; mortar = homogenized HCP + sand + Interfacial Transition Zones; concrete = homogenized mortar + aggregates.
1.4	TIME LAPSE	Years for time-dependent elastic et diffusive properties.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION ON THIS DATA	n.a.

Table 6 Generic Physics Of The Model Equation

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum Micromechanics. Diffusion/transport.	
2.1	MODEL ENTITY	Finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Mechanical equilibrium equation (conservation of momentum): $\mathrm{div}\boldsymbol{\sigma} = 0$ where $\boldsymbol{\sigma}$ is the stress tensor. Diffusion equation (conservation of mass): $\frac{\partial \phi C_k}{\partial t} = \mathrm{div}(\boldsymbol{J}_k)$ with ϕ the porosity, C_k the concentration of species k, $\boldsymbol{J}_k$ the diffusive flux of species k.

		Physical quantities	Stresses and strains; displacements and forces. Ionic concentrations and fluxes.
2.3	**MATERIALS RELATIONS**	**Relation**	Mechanical equations defining the behaviour of each solid phase *i*: - Hook's law: $\boldsymbol{\sigma} = \mathbf{K_i}: \boldsymbol{\varepsilon}$ with $\mathbf{K_i}$ the stiffness matrix for elastic properties, - linear ageing elastic behaviour: $\boldsymbol{\sigma}(\mathbf{x}, t) = \int_{\tau=-\infty}^{t} \mathbf{R_i}(\mathbf{x}, t, \tau): \frac{\partial \boldsymbol{\varepsilon}(\mathbf{x},\tau)}{\partial \tau}\, d\tau$ with $\mathbf{R_i}$ the relaxation tensor for viscoelastic properties. Fick's law for diffusive transport: $\boldsymbol{J}_k = -D_i.\nabla C_k$, with D_j the diffusion coefficient of phase *i*.
		Physical quantities/ descriptors for each MR	Volume fractions of phases. Elastic properties of phases. Diffusive properties of phases.
2.4	**SIMULATED INPUT**	n.a.	

Table 7 Solver And Computational Translation Of The Specifications

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	Linear solver for physical properties calculations from analytical homogenization approaches.	
3.2	**SOFTWARE TOOL**	Mathematica.	
3.3	**TIME STEP**	Seconds to years for time-dependent elastic and diffusive behaviours.	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Idealized representation of the microstructure defining one material point subjected to homogeneous stresses or strains (for mechanics) and homogeneous concentration or fluxes (for diffusion) boundary conditions at infinity. Hardcoded functions for material relations.
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	n.a.	

3.6	**ADDITIONAL SOLVER PARAMETERS**	n.a.

Table 8 Post Processing

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	Homogenized elastic mechanical and diffusive properties of representative finite volumes of cement paste, mortar and concrete.
4.2	**METHODOLOGIES**	Volume averaging procedures. Application of analytical mean-field homogenization methods (Mori-Tanaka, self-consistent and generalized self-consistent schemes) to calculate both mechanical and diffusive homogenized properties.
4.3	**MARGIN OF ERROR**	Errors related to particle idealization (spherical or ellipsoidal shapes) and simplified microstructure representation. Approximations due to application of mean-field homogenization methods.

2.3 MODA Physics-based Model – MODEL 3 Computational analyses of micro-mesostructures

Table 9 Aspect Of The User Case/System To Be Simulated

1	**ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED**	
1.1	**ASPECT OF THE USER CASE TO BE SIMULATED**	Mechanical response (strain and stress levels, damage) of an Elementary Volume of concrete, including steel reinforcement. Carbonation due to CO_2 diffusion. Progressive corrosion product formation at steel/concrete interface.
1.2	**MATERIAL**	Concrete samples including mortar matrix, aggregates, steel rebar.
1.3	**GEOMETRY**	3D cubic (or parallelepipedic) numerical samples with typical size of 10-15 cm.
1.4	**TIME LAPSE**	Seconds to decades.

1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	External CO_2 pressure and relative humidity conditions, mechanical loading.
1.6	PUBLICATION ON THIS DATA	n.a.

Table 10 Generic Physics Of The Model Equation

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum Mechanics. Diffusion/transport.	
2.1	MODEL ENTITY	Finite volumes.	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Mechanical equilibrium equation (conservation of momentum). Diffusion-reaction equation (conservation of mass).
		Physical quantities	Stresses and strains; displacements and forces. Damage variable. Aqueous concentrations, gas pressures and fluxes.
2.3	MATERIALS RELATIONS	**Relation**	1. Hook's law and linear ageing viscoelastic behaviour for mechanical equation. 2. Mazars damage model controlled by positive (extension) strains. 3. Fick's law for diffusive transport of CO_2 and water; semi-empirical relations describing the influence of partial saturation. 4. Semi-empirical relation for CO_2 reactions with calcium in mineral phases. 5. Empirical relation for the progressive formation of corrosion products at steel/concrete interface.
		Physical quantities/ descriptors for each MR	1. Elastic and diffusive properties of phases. 2. Material dependent parameters controlling the damage evolutions. 3. Initial pressures, material properties dependent on the saturation degree. 4. Kinetics constant of reaction. 5. Kinetics constant, corrosion rate.
2.4	SIMULATED INPUT	Homogenized mechanical and diffusive properties at the microscale.	

Table 11 Solver And Computational Translation Of The Specifications

3	Solver And Computational Translation Of The Specifications		
3.1	Numerical Solver	Finite elements. The equations are solved successively and iteratively (fixed point method).	
3.2	Software tool	Cast3M (www-cast3m.cea.fr)	
3.3	Time step	Seconds to days.	
3.4	Computational Representation	Physics Equation, Material Relations, Material	Finite element discretization of all equations. Hardcoded material relations as function of variables (e.g. damage evolution law, mechanical and diffusive properties, kinetics constant, corrosion rate). Explicit representation of coarse aggregates and steel reinforcement.
3.5	Computational boundary conditions	External pressure of CO_2 and relative humidity. Homogeneous boundary conditions on the samples faces for mechanics. Prescribed values of ionic species.	
3.6	additional Solver Parameters	n.a.	

Table 12 Solver And Computational Translation Of The Specifications

4	POST PROCESSING	
4.1	The processed output	Statistical analysis of degradation rate (carbonation depth) and of global corrosion rate at steel/concrete interfaces in the heterogeneous samples. Damage index. Macroscopic stress and strain response.
4.2	Methodologies	Volume or surface averaging.
4.3	Margin Of Error	Errors related to idealized aggregate shapes (polyhedrons) and limited number and size of aggregates. Errors due to simplification in the approaches (constant temperatures, constant external pressures, absence of drying/imbibition cycles).

3 MODA – Macroscale

3.1 MODA Physics-based Model – MODEL 4 - Computational analyses of macrostructures for service life estimation

Table 13 Aspect Of The User Case/System To Be Simulated

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Mechanical response (strain and stress levels, damage) of an aged concrete structure, including steel reinforcement. Aging of the structure in terms of material properties and rebar size after corrosion is informed by results from previous models.
1.2	MATERIAL	Concrete, aggregates, steel rebar. Reinforcing fibers (homogenized properties as derived from previous models).
1.3	GEOMETRY	Geometry will depend on the identified structures to be analysed, as selected in WP1.
1.4	TIME LAPSE	Seconds to years.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Mechanical loadings (both static and dynamic), fire conditions.
1.6	PUBLICATION ON THIS DATA	n.a.

Table 14 Generic Physics Of The Model Equation

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum Mechanics. Diffusion/transport.	
2.1	MODEL ENTITY	Finite volumes.	
2.2		**Equation**	

	MODEL PHYSICS/ CHEMISTRY EQUATION PE		Mechanical equilibrium equation (conservation of momentum). Diffusion-reaction equation (conservation of mass).
		Physical quantities	Strains, displacements and forces. Temperature.
2.3	**MATERIALS RELATIONS**	**Relation**	1. Hook's law and elasto-plastic behaviour for mechanical equation. 2. Palmgren-Miner's cumulative damage model controlled by stress variations and depending on material S-N curve. 3. Fourier's law for the rate of flow of heat energy per unit area through a surface.
		Physical quantities/ descriptors for each MR	1. Elasto-plastic properties of material. 2. Material dependent parameters controlling the damage evolutions. 3. Thermal conductivity.
2.4	**SIMULATED INPUT**	Homogenized mechanical and diffusive properties at the macroscale.	

Table 15 Solver And Computational Translation Of The Specifications

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	Finite elements.	
3.2	**SOFTWARE TOOL**	Sap2000 (https://www.csiamerica.com/products/sap2000).	
3.3	**TIME STEP**	Fraction of seconds to hours.	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Finite element discretization of all equations. Hardcoded material relations as function of variables (i.e. mechanical and diffusive properties). Implicit representation of steel reinforcement in 1D (beam) or 2D (shell) elements.
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	Structural restraints depending on kind of foundations. Distributed or concentrated loads on structure. Environmental temperature.	

3.6	**ADDITIONAL SOLVER PARAMETERS**	n.a.

Table 16 Solver And Computational Translation Of The Specifications

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	Assessment of residual service life according to safety prescriptions in reference standards (i.e. EN 1990, EN 1992).
4.2	**METHODOLOGIES**	Residual service life is proportionally derived from the minimum value of capacity/demand ratio among the mandatory safety checks for the structure at hand.
4.3	**MARGIN OF ERROR**	Errors related to homogenization of material properties. Errors due to simplification of geometry (details, restraints) and approaches (limited number of load cases).

4 Conclusions

The main purpose of the EnDurCrete research project, funded through the Horizon 2020 scheme, is to develop new economically and environmentally sustainable concretes for long-lasting application.

The thermodynamic model was used to predict the development of the phase assemblage and pore solution composition during the hydration of the novel PCCs developed within the EnDurCrete project. From the results obtained in this study the following conclusions can be drawn:

- The experimentally obtained results from WP2 were used as planned as input for the models in this study.
- The experimentally obtained portlandite content, as determined within WP2, and the predicted portlandite content over time in this study agree very well. The correction of the Ca/Si ratio of the predicted C-S-H phase was not possible due to a lack of data.
- A separation between capillary water and gel water was performed based on literature data on the H_2O/Si ratio of C-S-H and commonly observed gel water quantities per mol C-S-H.
- The results of the hydration modelling agree well with the hydration phase assemblage determined within WP2.

In addition, changes in the hydration phase assemblage and pore solution composition upon exposure of hydrated PCCs to chloride solutions or carbonation were modelled. The results obtained were used as input for the durability models of carbonation and chloride ingress.

Analytical upscaling techniques were applied to estimate the mechanical and diffusive properties of cement paste, mortar and concrete in different configurations, i.e. upon hydration, carbonation and migration of chlorides. The results from thermodynamic model were used as input for characterising the phase changes in these estimations. Simulations of 3D concrete samples numerically generated were performed and the results showed good agreement with the analytical predictions in the case of hydration.

Simulations of carbonation kinetics with a simplified coupled drying-carbonation model were also carried out and compared to laboratory tests performed in WP5. With this model, the cracking of concrete cover due to corrosion induced by carbonation was subsequently investigated through the simulation of numerical 3D concrete samples at mesoscale. The role and performance of the new materials were analysed.

Last, simulations of the chloride ingress tests carried out in WP5, based on a simplified model describing the chloride migration and binding in cementitious materials, were performed for mortar and concrete made with the new CEM II/C-M (S-LL) and CEM VI (S-V) binders. Both chloride profiles and peaking behaviour for materials exposed to either NaCl or NaCl + KOH were correctly reproduced.

The macroscale model investigated the influence of the developed New Concrete mix design on the service life estimation.

The quantification of the service life improvement is made through the comparison of different kinds of structures in their operational scenarios (i.e. piers in marine environments, tunnel in continental environment, etc.) considering the case with or without the adoption of the developed technologies.

The service life estimation is considered through the time needed to reach the collapse of the structure, due to the degradation phenomena. Two main degradation phenomena were analyzed, chloride migration in marine environment and carbonation penetration in continental environment.