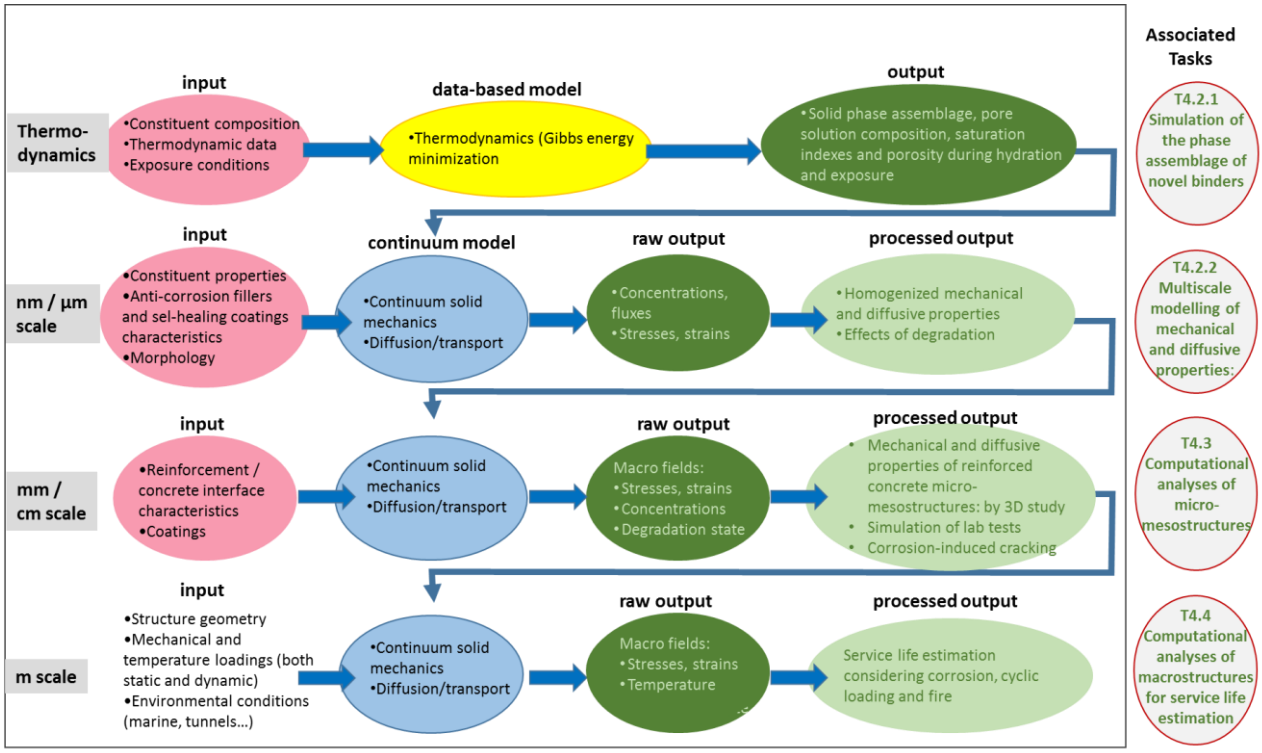
MODA for *Durability Prediction of Concrete in critical exposure conditions Simulated* in project EnDurCrete

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 since the project has not started yet.	
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 licence 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 author knowledge, 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 estimation of concrete service life and strength, in compliance with the European Standards EN 197 for cement and EN 206 for concrete1. Such	

[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.

		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. • 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 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…) in harsh environments.

Workflow picture



MODA

Application of a Data-based Model

MODEL 1

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
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.*

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:*

			$\begin{cases} G(n^{(x)}) \Rightarrow min \\ A \cdot n^{(x)} = n^b \end{cases}$ *with* $G(n^{(x)}) = \sum_j n_j^{(x)} v_j, \ \ j \in L$ *and* $v_j = {g_j^0}/{RT} + lnC_j + ln\gamma_j + \Xi, \ \ j \in L$ *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 $n^{(b)} = \left\{n_i^{(b)}, i \in N\right\}$ is the input amount of the independent components $n^{(x)} = \left\{n_j^{(x)}, j \in L\right\}$ 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 14.01 thermodynamic database (https://www.empa.ch/web/s308/thermodynamic-data)*	

3	**COMPUTATIONAL DETAIL OF DATA-BASE 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

MODA

Physics-based Model

MODEL 2

Multiscale estimation of mechanical and diffusive properties

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Simulation of the elastic, viscoelastic 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 viscoelastic properties.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION ON THIS DATA	n.a.

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 viscoelastic 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; viscoelastic properties of phases; ageing function describing the viscoelastic properties evolutions. Diffusive properties of phases.
2.4	**SIMULATED INPUT**	n.a.	

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 days for time-dependent viscoelastic 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. Explicit time discretisation for viscoelastic relations.
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	n.a.	
3.6	**ADDITIONAL SOLVER PARAMETERS**	n.a.	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	Homogenized (elastic, viscoelastic) 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.

MODA

Physics-based Model

MODEL 3
Computational analyses of micro-mesostructures

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 years.
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.

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, viscoelastic 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.	

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.	
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 and relative humidity. Homogeneous boundary conditions on the samples faces for mechanics.	
3.6	**ADDITIONAL SOLVER PARAMETERS**	n.a.	

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).

MODA

Physics-based Model

MODEL 4

Computational analyses of macrostructures for service life estimation

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.

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	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.	

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.	

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).