Elements in materials modelling

Each simulation will have its own fiche.
Metadata for these elements are to be elaborated over time

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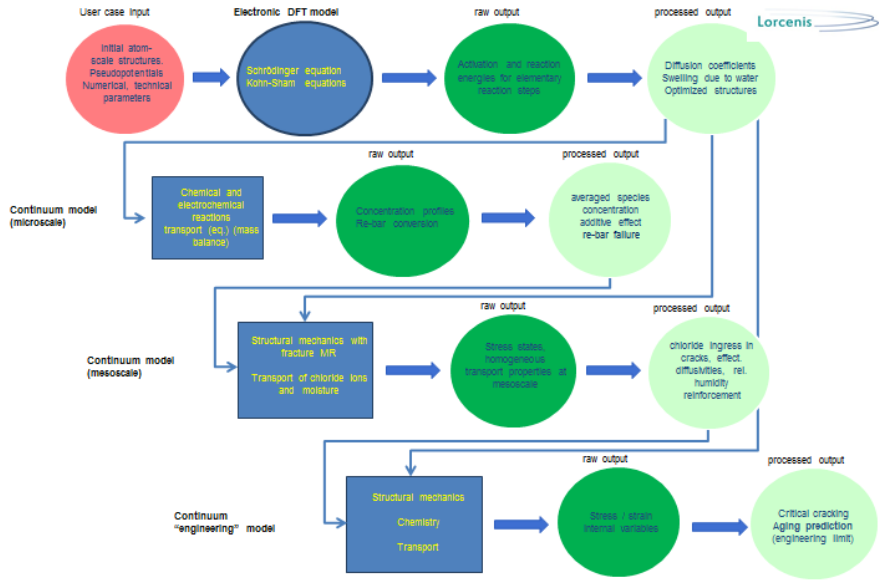
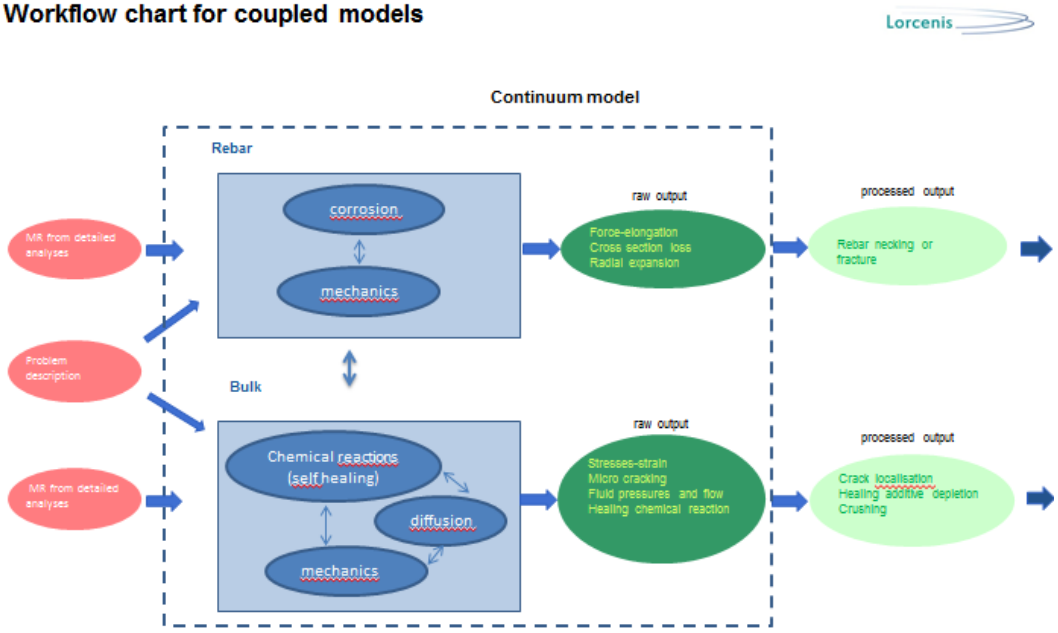
Purpose of this document:
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the modelling details.

THE SIMULATION			
1	USER CASE	The purpose is ageing control due to concrete additives and service-life prediction of energy infrastructures exposed to accelerated salt corrosive environment. The final purpose of multiscale modeling action is the extrapolation of timescale of macroscopic continuum models based on "corrosive" SVE/RVE. The newly developed elements contain information (MRs) gained from multiscale models and also include the additive effect. The MRs will be achieved by linking atomistic effects (chemical reaction engineering), continuum models of corrosion at microscale, continuum models of concrete at mesoscopic and continuum models of reinforced concrete at macroscale for damage initiation and progress. Each model does not include a full extrapolation of timescale but it delivers MRs based on respective PEs which allow to extrapolate the final continuum (SVE/RVE) simulation (initially via Abaqus) add improved forecasting accuracy. The main advantage is that the model can be applied without extensive (expensive) infrastructure which makes it attractive even for SME's.	
2	CHAIN OF MODELS	MODEL 1	*Electronic DFT model*
		MODEL 2	*Continuum model at microscale*
		MODEL 3	*Continuum model at mesoscale*
		MODEL 4	*Continuum model at macroscale*
3	PUBLICATION	-	
4	ACCESS CONDITIONS	Open access publication – yes; Open access to data – partially (restricted by project contract)	



Workflow chart for coupled models



Detailed description:

Each model used in a simulation can be documented in three chapters:

If you have a set of coupled equations, then you need a separate fiche with three chapters for each equation

1. Aspect of the User Case/ System simulated with this model
2. Model
3. Computation

Between two simulations post/pre-processing takes place. This processes the output of one simulation into input for the next simulation.

Model 1: Electronic DFT modelling

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	An atom-scale model for hydrated, hardened cement paste must be designed and evaluated. Volume changes of the cement as a function of water content may be calculated directly through a series of energy minimizations of atomistic/electronic models containing different amounts of water. kinetics of chemical changes occurring over time (oxide/hydroxide equilibria; others) may be determined by calculating activation energies of the relevant reactions, using the activation energies as input to calculation of kinetics through transition state theory; hence giving relevant insight into phenomena of importance for long-term changes (swelling, creep, changes in material properties). The energy profile for water/chloride as a function of its position in the material will be computed, resulting in activation energies for the diffusion process. From these, diffusion coefficients may be calculated using transition state theory like the kinetic parameters above.
1.2	MATERIAL	Calcium silicates; more generally oxides of calcium, aluminium, and silicon. Water.
1.3	GEOMETRY	Semi-amorphous, at the atomic scale, designed taking experimental characterization results as a starting point.
1.4	TIME LAPSE	<s; indirectly from femtoseconds to years.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Water content. Concentration gradients of water and/or chloride.
1.6	PUBLICATION ON THIS SIMULATION	-

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	DFT: Energies of atomic scale systems as a function of relative positions of atomic nuclei, computed by approximate solutions of the Schrödinger equation. In principle, any experimentally observable quantity may be computed as a function of the energies.	
2.1	MODEL ENTITY	Atoms, electrons.	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Schrödinger equation. Kohn-Sham equations.
		Physical quantities	wave function, Hamiltonian, electronic energies, bonding energies, spectroscopic parameters.
	MATERIALS RELATION MR TO PE	**Equation**	chemical kinetics, diffusion, transition state theory
		physical quantities/ descriptors	Chemical reaction rate constants, diffusion coefficients
2.3	INPUT	N/A	
2.4	PUBLICATION	Arstad, Bjørnar, Richard Blom, and Ole Swang. "CO_2 absorption in aqueous solutions of alkanolamines: mechanistic insight from quantum chemical calculations." The Journal of Physical Chemistry A 111.7 (2007): 1222-1228.	

3	COMPUTATIONAL MODELLING METADATA	
3.1	NUMERICAL SOLVER	Kohn-Sham equation solver,
3.2	SOFTWARE TOOL	The necessary software is available in the public domain (Quantum-Espresso; LAMMPS; others)
3.3	GRID SIZE	N/A
3.4	TIME STEP	<s

3.5	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION**	DFT: Plane-wave basis combined with pseudopotentials.
		MATERIAL RELATIONS	*e. g*. oxide/hydroxide equilibria ($MO + H_2O = M(OH)_2$), chloride binding
		MATERIAL	Atom-scale model comprising a number of atomic nuclei with defined relative positions. Number of electrons to ensure overall charge neutrality. Pseudopotentials.
3.6	**PUBLICATION**		

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Activation energies of diffusion from which diffusion coefficients may be computed. Swelling of cement as a function of water content.
4.2	**METHODOLOGIES**	Transition state theory.
4.3	**MARGIN OF ERROR**	DFT/diffusion: Absolute activation energies to 30 kJ/mol. Relative activation energies to 20 kJ/mol.

Model 2: Continuum model at the microscale (corrosion)

1	Aspect of the User Case/System to be Simulated		
1.1	Aspect of the User Case to be simulated	Model 2 will compute the variation of local conditions (chemical, electrochemical) within reinforced concrete and deliver information like pH change, concentration changes of active species, etc. for mesoscale models but partially also for the macroscale model	
1.2	Material	Oxides of calcium, aluminium, silicon (cement paste), chloride, steel, water	
1.3	Geometry	Idealized cavities (tubes), 3 layer domain	
1.4	Time Lapse	s-d	
1.5	Manufacturing process or in-service conditions	Corrosive exposure of scenario 1 geometry to salt environment (aging) as in-service condition	
1.6	Publication		

2	Generic Physics Of The Model Equation			
2.0	Model type and name	Continuum modelling of chemical and electrochemical reactions and related species transport		
2.1	Model entity	FE		
2.2	Model Physics/ Chemistry equation PE	**Equation**	PE1: Chemical and electrochemical reactions according to diluted solutions / electrolyte (aqueous) exposure PE2: Dissolved species transport equation (mass balance) incl. , Gauss law, Nernst equation, and at the rebar boundary modified Butler-Volmer, Tafel	
		Physical quantities	Concentrations, local potential, pH, current density, porosity, deposit rates, surface conversion, rebar surface chemistry	
	Materials relation MR to PE	**Equation**	Expressions for chemical kinetics, diffusion, electrochemical kinetics partially derived from model 1 e.g. spatially resolved stability constants under severe exposure conditions	
		Physical quantities/ descriptors	forward/ -backward reaction coefficients, anodic/ -cathodic coefficients at re-bars, surface coverage via corrosion products	
2.3	"Redundant" Physics quantities	-		
2.4	Publication	Höche, D., Simulation of Corrosion Product Deposit Layer Growth on Bare Magnesium Galvanically Coupled to Aluminium. Journal of The Electrochemical Society, 2015. 162(1): p. C1-C11.		

3	Computational Modelling Metadata		
3.1	Numerical Solver	FEM	
3.2	Software tool	COMSOL	
3.3	grid size	adapted	
3.4	Time step	adapted	
3.5	Computational Representation	Physics Equation	Written up for finite volumes
		Material Relations	Functionals (as matrix) of time dependent e.g. concentration profiles, and constants (as numbers) like chemical and electrochemical coefficients
		Material	calcium, aluminium, silicon (cement paste), chloride, steel, water
3.6	Publication	-	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Raw output for fine volumes is averaged for finite volumes of (100 nm – 10 µm)
4.2	METHODOLOGIES	Computed via an coupled equation set via direct solver → Data - matrix as input for model 3 and 4 (as averaged finite micro volume)
4.3	MARGIN OF ERROR	Based on experience the accuracy remains high until the driving mechanism changes (e.g. from diffusion driven process to convection driven process)

Model 3: Continuum model at mesoscale

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Material properties pertaining to the physical phenomena of mass transport in concrete are ultimately derived from material heterogeneities found at different subscales. At the mesoscale level, these heterogeneities are mainly characterized by the presence of embedded aggregates in the cement paste, together with cracks. Model 3 will compute moisture and chloride transport in concrete and deliver information regarding deformational characteristics, where the mesoscale heterogeneities are explicitly accounted for by means of geometrical and constitutive descriptions along with computational homogenization.
1.2	MATERIAL	Mesoscale constituents cement paste, aggregates and the highly porous interface material
1.3	GEOMETRY	**Aggregate representation and FE discretization** In 2D, the aggregate representation will be based on octagons and the randomness in shape of the aggregate will be rendered by adding a random variation to each corner point in the octagon. The finite element discretization will be carried out using a Delaunay triangulation algorithm. In 3D, the aggregates will be modelled as spheres. In contrast to the 2D representation, no random variation in shape will be applied. The spatial discretization technique will be based on voxelization to create a structured grid of identically sized voxels (cubes). The concept is to subdivide the continuous SVE into a discrete set of voxels which are considered solid finite elements.
1.4	TIME LAPSE	h-d
1.5	MANUFACTURING P CONDITIONS	Homogeneous transport properties at macroscale
1.6	PUBLICATION ON THIS SIMULATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum modelling of moisture and chloride transport	
2.1	MODEL ENTITY	Finite elements – two- and three-dimensional Statistical Volume Elements (SVEs) of mesoscale concrete	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	Equation	**Moisture transport** • For saturated conditions, pressure gradients are the main driving forces for moisture transport. • For unsaturated conditions, moisture exists simultaneously in two phases as liquid and as vapour. The driving forces for the liquid phase are pressure gradients in addition to capillary forces. For the vapour phase, diffusion and convection are the two main transport mechanisms. **Chloride transport** Chlorides are solved only in the liquid phase of moisture, not in the vapour phase. This phenomenon makes the transport of chloride ions intrinsically coupled to the transport of moisture. The three main transport processes are diffusion, convection and migration. **Coupled chloride ions and moisture transport** The constitutive model will be a modified expression of Fick's law by Ababneh and Xi *et al.* for the cement paste, which cross-couples the fluxes of chloride ions and moisture in the following way: $J_{\emptyset} = -D_{\emptyset}\nabla_{\emptyset} - \varepsilon_c D_c \nabla_c$ $J_c = -\varepsilon_{\emptyset} D_{\emptyset}\nabla_{\emptyset} - D_c \nabla_c$

		Physical quantities	Relative pore humidity (ϕ), free chloride ion concentration (c), Flux (J.) and diffusion coefficient (D.)
to be repeated if necessary	**MATERIALS RELATION MR TO PE**	**Equation**	relation between pore chemistry and composition and crack initiation parameters
		Physical quantities/ descriptors	micro convection, humidity
2.3	**"REDUNDANT" PHYSICS QUANTITIES**	N/A	
2.4	**PUBLICATION**		

3	**COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	Finite Element Method (FEM) The SVEs will be employed numerically using the finite element method (FEM) to simulate mass transport—for both stationary and transient conditions—in order to compute macroscale diffusivities.	
3.2	**SOFTWARE TOOL**	MATLAB; access to source codes are restricted by project contract	
3.3	**GRID SIZE**	Adapted	
3.4	**TIME STEP**	Adapted	
3.5	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION**	The computation is done according to standard FEM. Dirichlet boundary conditions will be used in the numerical implementations and all numerical results will be — as a consequence — upper bound solutions.
		MATERIAL RELATIONS	Constitutive models for cement paste and aggregate in compression and tension. Constitutive model for ITZ governing normal and tangential traction and displacement.
		MATERIAL	Cement paste, aggregates and the highly porous interface material
3.6	**PUBLICATION**		

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	(Finite volumes) Homogeneous transport properties on the macroscale, chloride ingress in cracks
4.2	**METHODOLOGIES**	Matrix-based computation of: Normalized effective diffusivities as a function of aggregate contents for varying diffusivities in the ITZ, time evolution of macroscale relative humidity, and Effective diffusivities as functions of SVE size and ITZ diffusivities and volume aggregate contents.
4.3	**MARGIN OF ERROR**	The accuracy remains reasonably high until at least one of the following assumptions is violated: (1) The mass transfer of chloride ions and moisture are concentration gradient-driven processes, allowing for Fick's law to be used, (2) the macroscale fields of moisture and chloride ions vary linearly within the SVE, and (3) the mesoscale constituents are assumed to be homogeneous, and the laws of continuum physics are assumed to apply at the mesoscale level.

Model 4: Continuum model at the macroscale

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Structural integrity and aging behaviour of concrete structure (Scenario 1)
1.2	MATERIAL	Oxides of calcium, aluminium, silicon (cement paste), chloride, steel
1.3	GEOMETRY	Structure/structural component. (test beam Scenario 1)
1.4	TIME LAPSE	Years
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Corrosive exposure to salt environment (aging) under steady mechanical loads
1.6	PUBLICATION	-

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Coupled multiphysics, macroscale, continuum model: "Engineering model"	
2.1	MODEL ENTITY	FE (finite elements)	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	**Continuum mechanics** Strain definition Stress as dual of strain Equilibrium/virtual work principle Re-bar expansion **Mass transport (from model 3)** Conservation of mass Chemical equilibrium or kinetics **Corrosion (from model 2)** Conservation of mass (oxygen) in the corrosion process
		Physical quantities	**Continuum mechanics** Displacement, stress, strains, surface forces **Mass transport** Solute concentrations/partial pressures **Corrosion** Loss of cross section Increase in effective diameter
to be repeated if necessary	MATERIALS RELATION MR TO PE	**Equation**	**Bulk** Strain is related to the smeared cracking, itself related to stress, mass transport (from model 3) **Re-bar** Oxygen absorption is related to loss of cross section and increase in volume (from model 2)
		Physical quantities/ descriptors	**Bulk** Strain, stresses, mass-diffusivity, smeared-crack tensor. **Re-Bar** Remaining cross section, mass-absorption, diameter
2.3	"REDUNDANT" PHYSICS QUANTITIES	-	
2.4	PUBLICATION		

3	COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	FEM	
3.2	SOFTWARE TOOL	Abaqus, user defined elements for a) re-bars and b) bulk	
3.3	GRID SIZE	The model is to be "light" enough for engineering purposes. To this effect, specialised elements must be developed: – a beam element (re-bars) with additional mass diffusion and expansion degree of freedom - A volume element (bulk) with additional degrees of freedom for radial expansion around a re-bar, and degrees of freedom for mass diffusion	
3.4	TIME STEP	Of the order of weeks or months	
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	Coupled differential equations to be discretized using Galerkin finite element method.
		MATERIAL RELATIONS	To be determined from models 2 and 3. Phenomenological models will probably be introduced.
		MATERIAL	**Bulk** Internal variables for smeared cracking **Re-bar** No internal variables foreseen
3.6	PUBLICATION		

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Finite volumes **Bulk** Coalescence of micro-cracks into macro-cracks (cracking, spalling), which can be defined as an engineering limit state. **Re-bars** Stresses in the re-bars in excess of yield or ultimate stresses, again an engineering limit state
4.2	METHODOLOGIES	-
4.3	MARGIN OF ERROR	-