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# NUMERICAL MODELING

## Strategies for Sustainable Concrete Structures

# Book of abstracts

Pierre Rossi  
Jean-Louis Tailhan, *Editors*

4th International RILEM Conference  
Marseille, France, July 4-6, 2022

## Preface

Cement is the main constituent of concrete, the building material most widely used today and that will continue to be in the years to come. Its production generates, among other things, CO<sub>2</sub> emissions and, so, greenhouse effects. It is, thus, of primary importance to optimize the utilization of cement in concrete constructions while checking that these constructions have a lifespan compatible with the stakes of sustainable development. It is essential to take up the challenge and use adapted quantification tools, making it possible to rigorously and reliably justify the adopted strategic and technical choices.

Numerical methods (finite elements, finite volumes, finite differences) constitute a relevant response to this challenge. They make it possible to optimize concrete constructions because they can consider complexities linked to the rheological, physicochemical, mechanical properties of concrete, the geometry of structures or even environmental boundary conditions. This optimization must also respect constraints of time, money, safety, energy, CO<sub>2</sub> emissions, and, more generally, life cycle, in a way more reliable than the codes and analytical approaches currently used.

*Numerical methods are, undoubtedly, the best calculation tools at the service of concrete eco-construction.*

After Aix-en-Provence (France, 2012), Rio de Janeiro (Brazil, 2015) and Lecco (Italy, 2019), the RILEM international Conference on ***Numerical Modeling Strategies for Sustainable Concrete Structures (SSCS 2022)*** is taking place in the city of Marseille (France).

Jean-Louis Tailhan and Pierre Rossi  
Juillet 2022

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# Artificial Neural Network-based methodology for optimization of low-cost green UHPFRC under ductility requirements

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**Keywords:** Green UHPFRC, Artificial Neural Networks, Design of Experiments, Multi-Objective Optimization, Experimental Validation, Direct Tensile Behavior.

## Abstract

Several structures and constructions in earthquake-prone areas were designed and built following old earthquake-resistant building codes, and therefore current seismic requirements are not met. Moreover, in underdeveloped nations located in earthquake-prone locations, the problem is made worse by the rampant informal construction. These circumstances require effective seismic retrofitting interventions through solutions of the acceptable cost that allow the most extensive application possible [1].

Colombia, where this research was developed, is a clear example of the latter. Owing to its location at the boundaries of several tectonic plates, Colombia is a seismically active country with a sizeable seismic risk in many areas of its territory. Furthermore, according to several studies, around 80% of the structures in Bogotá were constructed without complying with any seismic regulations. If this occurs in the country's capital, it is easy to extrapolate that it also occurs in the rest of the country [2].

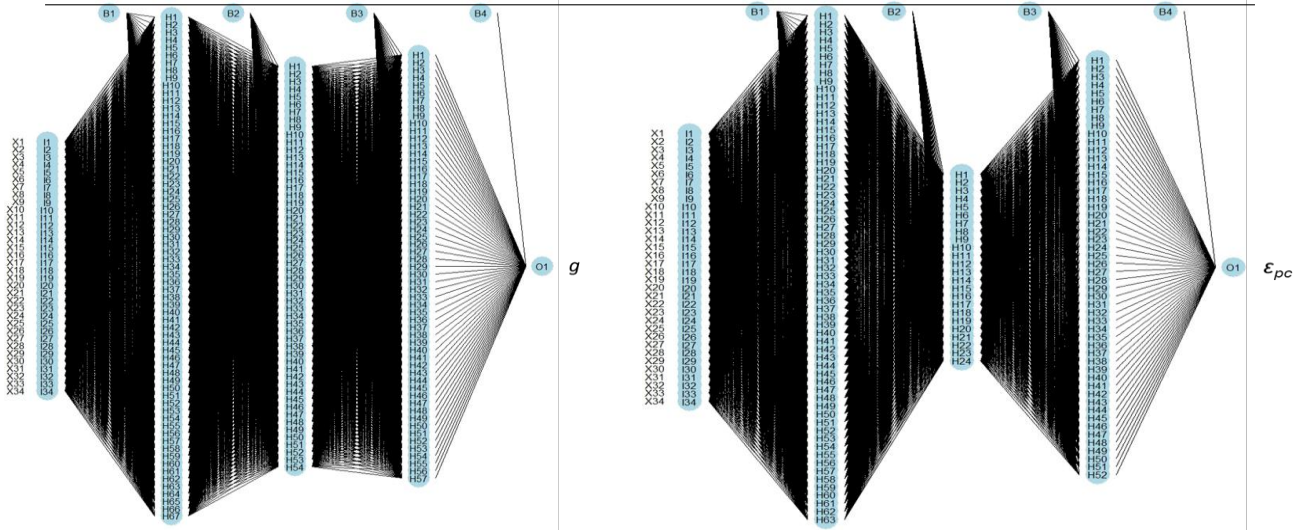
For its part, ultra-high-performance fiber reinforced concrete (UHPFRC) is an advanced construction material that provides new opportunities in the construction industry worldwide. Retrofitting and seismic strengthening of existing concrete structures are among the latest applications of UHPFRC that might be emphasized [3,4]. This research aims to develop a low-cost and green UHPFRC dosage using the highest proportion of Colombian components, to reach the ductility parameters necessary for seismic retrofitting applications. Especial emphasis was made in analyzing the utilization of green raw materials such as FC3R, slags, rice husk ash, or recycled glass.

The research herein presented is developed in different stages. First, the plain UHPC (without fibers) is optimized using various statistical and computational tools such as Artificial Neural Networks, Design of Experiments, Main Effect Plots, Response Surface Methodology, and Multi-Objective Optimization. The optimization criteria include achieving a 28-days compressive strength over 150 MPa, reaching a self-compacting behavior at the fresh state while lessening cement and superplasticizer dosages, removing quartz powder, limiting silica fume content to 100 kg/m<sup>3</sup>. The mathematically optimized dosage was experimentally evaluated.

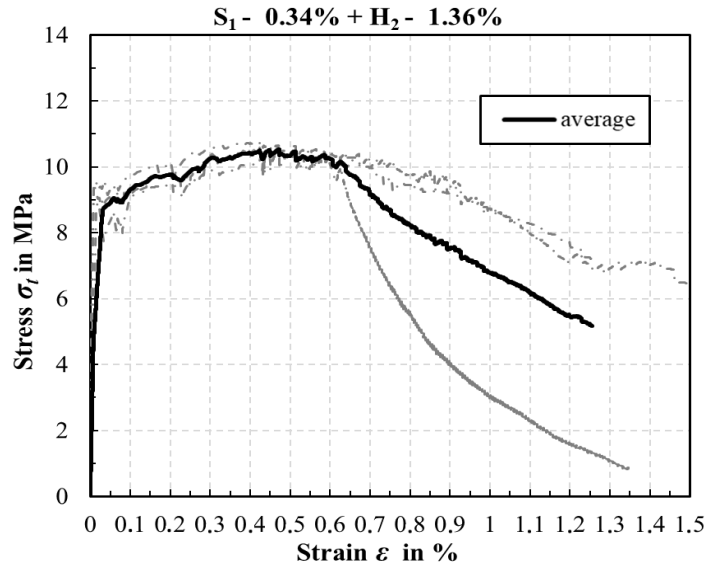
After the UHPC dosage is optimized, the objective of the second stage consists of determining the binary combination of fibers, among those available in the local market, that permit reaching the necessary ductility parameters for the desired application at a lower cost. The ductility parameters considered are, on the one hand, the energy capacity absorption ( $g$ ) and, on the other hand, the strain capacity at maximum tensile strength ( $\epsilon_{pc}$ ) measured in the direct tensile test. Two Artificial Neural Network models were created to reduce the number of tests needed during the optimization process, one for each of the ductility parameters considered (see Fig.1). Once the ANN models were adjusted, a Multi-Objective Optimization procedure was performed to determine the optimal fiber's combination. The mathematically optimized dosage was, one more time, experimentally evaluated. This case employs the JSCE-08 test set-up (see Fig.2). Lower final cost and cement content were reached when blending limestone powder with an average particle size of 2.1  $\mu\text{m}$  and recycled glass powder with 28  $\mu\text{m}$  of particle mean size as partial cement and silica fume. That optimal UHPC dosage achieved a compressive strength of 156 MPa at 28 days with a dosage of only 590 kg/m<sup>3</sup> of cement and 100 kg/m<sup>3</sup> of silica fume, providing an ultra-high-performance cementitious matrix for the next stage of the research that incorporates waste materials in its composition.

Finally, the optimal fiber volume fraction for the necessary UHPFRC ductility parameters for seismic strengthening applications ( $g \geq 50 \text{ kJ/m}^3$  and  $\epsilon_{pc} \geq 0.3\%$ ), employing the previously optimized low-cost and green UPHC, was 1.7%. This optimal fiber combination was composed of 0.34% of smooth high-strength steel ( $l_f/d_f=65$ ) fibers and 1.36% of normal strength hooked end steel fibers ( $l_f/d_f=80$ ). It is relevant to highlight that this optimized UHPFRC outperforms the ductility parameters obtained by other authors [3,5] with successful applications in the seismic strengthening of reinforced concrete structures, which supports its utility for the intended application.





**Fig. 1.** Artificial neural network models for predicting the energy capacity absorption (left) and maximum post-cracking strain (right) of UHPFRC under direct tensile test.



**Fig. 2.** Direct tensile test set-up (left) and strain-stress behavior of the optimized UHPFRC (right).

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# Long term prediction of the delayed behavior of concrete structures – The case of the Vercors mock-up of a nuclear containment

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**Keywords:** concrete, creep, shrinkage, nuclear power plant.

## 1 Introduction

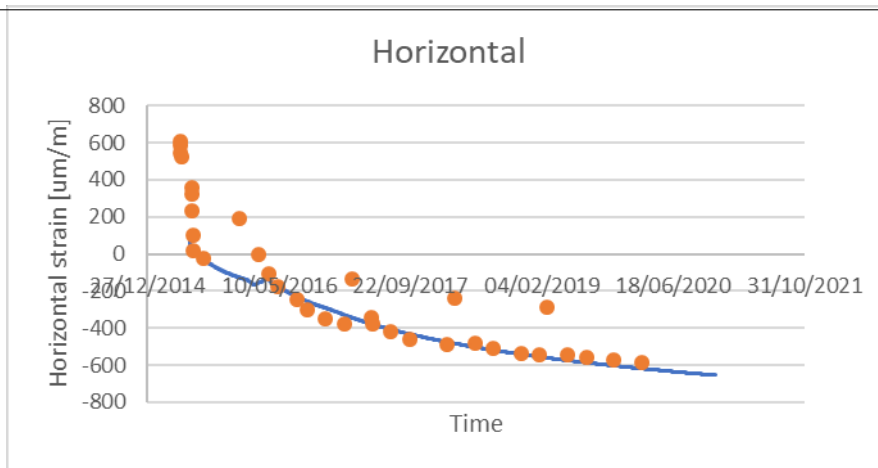
The prediction of the long-term behavior of prestressed concrete structures is important in order to assess and/or extend the service life of such structures. In the case of nuclear power plants (NPPs) where the internal vessel is a biaxially prestressed structure, the prediction of the delayed deformations is also a safety concern. Indeed, in these structures, the prestressing is there to avoid tensile stresses and cracking in case of a severe accident where internal pressure and high temperature could be generated. The prediction of the evolution of delayed strains due to creep and shrinkage of concrete and of relaxation of steel is in this case very important. Here, a modelling of the delayed strains (creep and shrinkage of concrete and relaxation of steel), based on the relations of the next Eurocode 2 (EC2), is used to predict the behavior of the internal vessel of the Vercors mock-up of a French NPP. This modelling considers the influence of the temperature and of the relative humidity (varying under service conditions). The predicted delayed strains are compared with the measurements and different hypotheses are tested to improve the prediction of the delayed strains.

## 2 Modelling of delayed strains

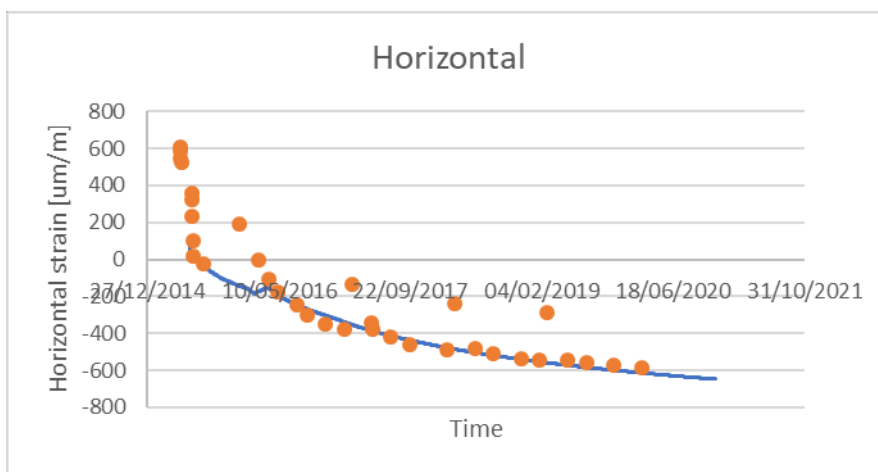
As proposed in the future version of the Eurocode 2, the delayed strains of concrete are split into four components that are adjusted to experimental results available for the Vercors containment [1]: basic shrinkage, drying shrinkage, basic creep and drying creep. The relaxation of the prestressing is also considered. An elevated temperature during service conditions (around 35°C) is observed in NPPs. This temperature affects the delayed strains. The effect of temperature is not considered in EC2. For basic creep, a thermo-activation is considered and the magnitude of drying creep is affected by the temperature as proposed in the fib MC2010 [2]. For steel relaxation, the relation proposed by the fib MC2010 is used.

## 3 Modelling of the containment

Considering the history of temperature and relative humidity, we compute the total delayed strain of concrete in horizontal (or tangential) and vertical directions using the superposition principle. The method is described in [3]. The results for the tangential strains are compared against the experimental measurement in Fig. 1 for a sensor that is in the middle of the containment, far from singularities. Two possibilities are tested to consider the effect of temperature on the basic creep. The first hypothesis considers a thermal activation of the compliance. The second possibility is the fact that, as proposed recently by Frech-Baronet [4], it is the characteristic time  $\tau$  of basic creep which is thermo-activated. Both possibilities are tested. Figure 2 shows for the two hypotheses give a correct evolution in the long term. A combination of the two effects that could exist simultaneously will be tested in the future.



**Fig. 1.** Comparison of two on-site measurements of horizontal total delayed strain with model prediction.



**Fig. 2.** Comparison of two on-site measurements of horizontal total delayed strain with model prediction, assuming thermo-activation of the characteristic time for basic creep.

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# PARALLEL FINITE ELEMENT SOLVERS FOR STRUCTURAL SCALE SIMULATIONS USING PHASE-FIELD MODELS FOR FRACTURE IN SOLIDS

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**Keywords:** Parallel computing, Finite element method, Phase-field models, Fracture mechanics, Preconditioning.

## Abstract

Phase-field models [1,2] (PFMs) are widely used to model fracture in solids. Similar to continuum damage mechanics models, material degradation is described via a scalar-valued phase/damage field ranging from zero (sound material) to unity (fully broken material) and submitted to irreversibly conditions. Damage evolution is modeled by solving a Helmholtz-like damage diffusion equation. The final boundary value problem consists in finding a vector-valued displacement field ( $\mathbf{u}$ ) and a scalar-valued damage field ( $d$ ) fulfilling the non-linearly coupled momentum balance (equilibrium) and damage diffusion equations.

Resolution strategies involve either a staggered or a monolithic approach to solve the final boundary value problem. Staggered approaches are often preferred since they ensure straightforward implementations and, depending on the chosen PFM, lead to linear sub-problems to solve. However, their main drawback is that successive solving (alternate minimization) of the equilibrium and diffusion equations are needed until convergence. Conversely, monolithic approaches allow for solving the final system of equations as a whole. Using standard Newton–Raphson methods, the linear system to solve at each iteration often loses symmetry and/or positive definiteness.

In this work, attention is focused on solvers for the "hybrid" phase-field model by Ambati et al. [3], with the primary objective of developing effective finite element implementations and to perform large-scale fracture mechanics simulations. Indeed, very refined meshes are needed for solving PFMs in the finite element framework for practical problems of interest. Large non-linear systems of coupled equations have to be solved, which makes using these models in large-scale applications a tiresome task due to the high computational workload.

Domain decomposition approaches (see, e.g. [4]) that facilitate the use of modern-day parallel computing facilities can be used to subdue these issues and considerably decrease computational workload. The computational domain is partitioned into thousands of sub-domains, and the finite element linear systems concerning the PFM equations are then concurrently assembled and eventually solved using parallel Krylov subspace methods.

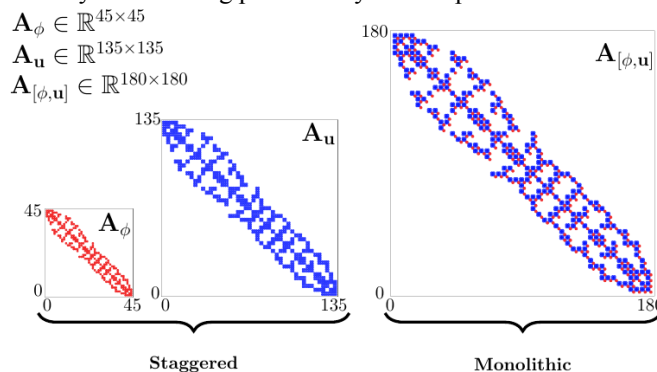


Figure 1: matrix sparsity patterns for different PFM resolution strategies.

Within this contribution, we implement and discuss two ways of setting up domain decomposition parallelism for a hybrid PFM [2] under the distributed computing framework. Particularly, a monolithic FE strategy is compared to a staggered FE strategy. The monolithic finite element scheme consists in coupling the finite element unknown fields ( $\{d, \mathbf{u}\}$ ) in a single vector-valued finite element space and solving the resulting system of equations as a whole. Conversely, the staggered scheme uses two separate scalar-/vector-valued finite element spaces for  $d$  and  $\mathbf{u}$ . Resolution is then performed in a Gauss–Seidel-like fashion. These two methods lead to different matrix sparsities (see fig. 1), as such to yield a fast and robust parallel solver, different preconditioning/parallelization strategies must be applied.

Besides presenting the two distinct ways of setting up parallelization for the considered PFM, this article presents a detailed comparison of the performance, scalability, and efficiency of the two methods at massively parallel scales. Overall, this allows for rapid solving non-trivial fracture mechanics problems with millions of unknowns [5] (fig. 2).

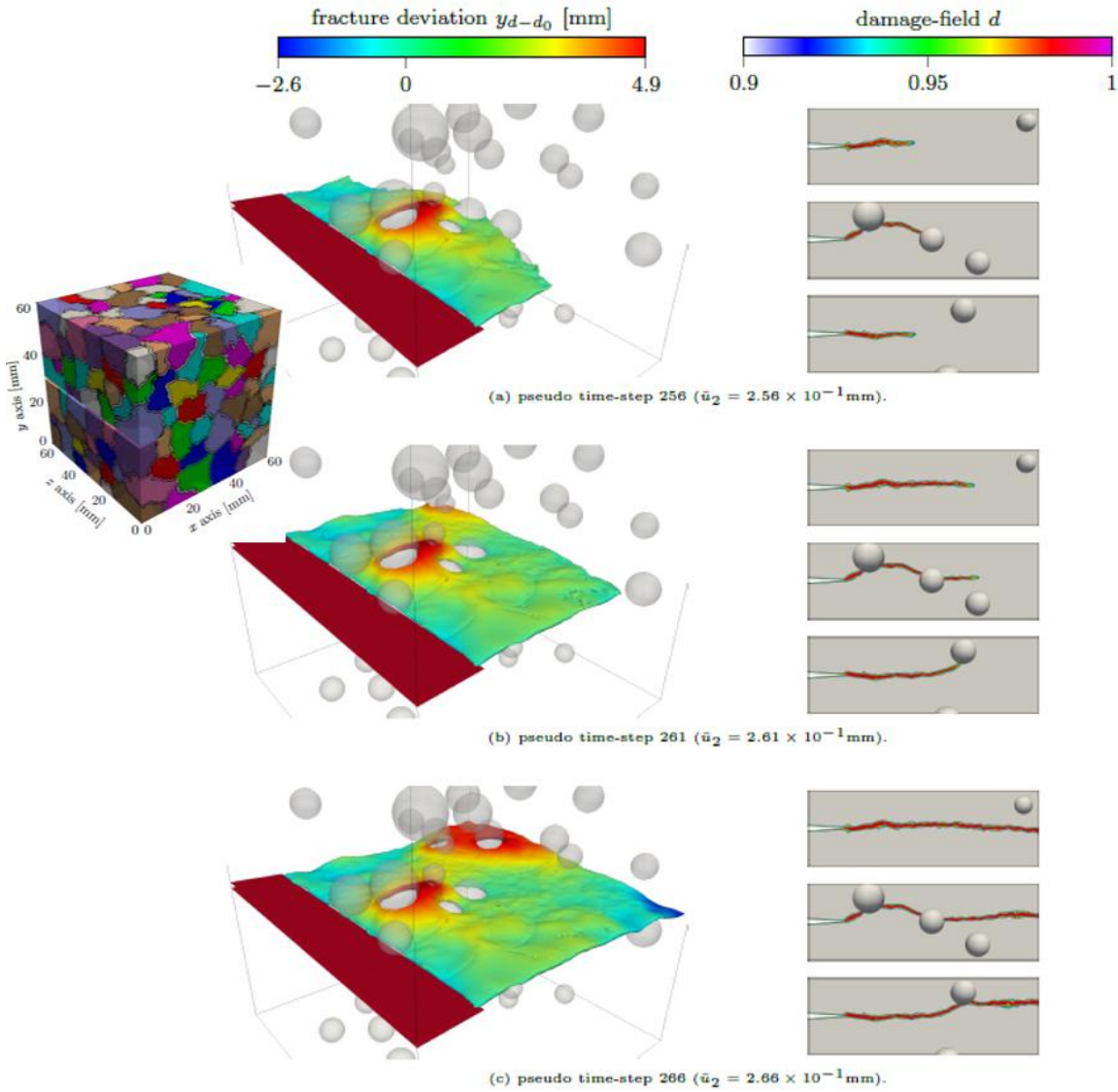


Figure 2: large-scale perforated medium. Damage propagation in a tensile test. Simulation performed using 1008 subdomains. The total number of degrees-of-freedom is about 80 millions [5].

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## INTEGRATING HYBRID REINFORCED CONCRETE TECHNOLOGY AND ADVANCED FEM-BASED NUMERICAL MODELLING FOR CRACK CONTROL IN LONG CONCRETE FOUNDATIONS WITHOUT JOINTS

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This paper describes the advanced numerical simulations and the laboratory and in situ experimental tests for the design of a relatively long concrete foundation of a packaging track executed by high precision robots. The foundation has about 22m in length, and cracking control joints cannot be adopted due to the functional requisites of the robots. For minimizing the heat generation due to cement hydration, a tubular type foundation was designed with the core formed by polystyrene blocks. Due to the relatively small thickness of wall components of this tubular system, and aiming to minimize the construction time of the foundation, a hybrid fibre reinforcement system was adopted, composed by only one layer of a steel grid mesh per wall component of the foundation, and concrete reinforced with polypropylene fibres (PFRC).

The design included the development of three-dimensional models using the FEMIX software for the numerical simulation of the behaviour of the structure, integrating models that consider the effects of temperature variation due to cement hydration, shrinkage, creep, concrete cracking and interaction of the foundation with the surrounding soil. The PFRC was designed for achieving the mechanical requisites advised by the numerical simulations and the rheological properties for an efficient casting. The evolution of the mechanical properties of the PFRC since its early age was assessed, namely the modulus of elasticity, compressive strength and post-cracking flexural behaviour.

In order to validate the assumptions adopted in the numerical models for simulating the temperature development due to the heat generation from cement hydration, the evolution of the temperatures into the PFRC of the foundation was monitored, and the obtained results were compared to the numerical ones.

The integrated design strategy followed in this case study allowed to demonstrate that fibres are a competitive solution to partially replace conventional reinforcement, with savings in material and human resources, as long as advanced design tools are used and adequate characterization of the properties of critical intervening materials are executed.

**Keywords:** Concrete reinforced with polypropylene fibres; Multiphysics simulations; Large foundations; laboratory and in situ experiments

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# Multi-physical simulation of concrete hydraulic facilities affected by alkali-aggregate reaction: from material to structure

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**Keywords:** hydraulic structures, concrete, alkali-aggregate reaction, multi-physical simulation, size effects, experimental investigations.

## Abstract

This work aims to fill the gap between experimentation on laboratory specimens and structural diagnosis of mass concrete hydraulic structures affected by alkali-aggregate reaction (AAR) by conducting numerical and experimental investigations on an existing hydroelectric facility affected by AAR.

A large experimental program was performed to characterize the mechanical properties and the kinetics of the AAR chemical reaction for the original mass concrete used in the construction of the facility (maximum aggregate size of 76 mm). The importance of considering mechanical and chemical size effects is discussed, on the basis of the asymptotic fracture energy and the free AAR expansion curve.

The developed phenomenological hygro-chemo-mechanical approach for AAR modelling in mass concrete hydraulic structures is presented. The efficient and yet simple approach is based on three analyzes: transient thermal analysis, transient hygral analysis, and final multi-physical analysis that includes mechanical loading. The modelling approach was validated with existing benchmarks from the literature and provided very promising results, despite the simplifications made and the assumptions for some uncertain input parameters.

Application of the numerical modelling approach to the existing hydraulic facility demonstrated its feasibility in an industrial context. It also provided fairly similar damage pattern if compared to the existing cracking pattern and improved the understanding of the complex structural behaviour of the facility. Comparison of displacement model predictions and available monitoring data allowed to assess an important size effect between laboratory and in-situ expansions.

# Biaxial Interaction Diagrams of a RC Section at Elevated Temperature

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**Keywords:** Biaxial interaction diagrams, reinforced concrete section, fire loading, yield design.

*Normal force-bending moment* interaction diagrams are useful tools for the design of reinforced concrete (RC) sections under the combined action of a tensile-compressive load and a bending moment. At ambient temperature, these interaction diagrams may be established within the framework of ultimate limit state design (ULSD) where the strain limitations of concrete and reinforcing steel are prescribed (see for example EN 1992-1-1 [1]). However, such a calculation procedure is rather complex for a RC section in fire conditions, essentially due to the influence of elevated temperatures on the constituent material properties (see for example Pham *et al.* [2]). The situation becomes much more complex in the case of a heated RC section under the combined action of an axial load and two bending moments about their two axes, since 3D failure surfaces (called here after biaxial interaction diagrams) are now required instead of classical 2D interaction diagrams.

This contribution is based on the lower bound static approach of the yield design (or limit analysis) theory (Salençon [3], de Buhan [4]) for deriving the biaxial interaction diagrams of a RC section. This is an extension of the work of Pham *et al.* [5] where the previous complex 3D failure surfaces are simplified here to a superposition of simple 2D interaction diagrams for different orientations of the resulting bending moment in the section (see Fig. 1). Indeed, while the classical methods are usually based on conventional limitations of strains of concrete and steel reinforcing bars (EN 1992-1-1 [1]), the yield design approach only requires that their stress (and not strain) limitations be prescribed, with no reference to other mechanical characteristics. In the present paper, material characteristics may be introduced in two steps: (i) a preliminary heat transfer analysis for evaluating the temperature distribution on the RC section and (ii) the introduction of reduced factors as functions of temperature into both the concrete and steel strength properties (see Pham *et al.* [2] for more details). As a result, a semi-analytical solution of axial load-bending moment interaction diagrams could be obtained for any prescribed temperature distribution and any prescribed orientation of bending moment. The temperature distribution of the RC cross-section may be obtained by either the use of any thermal software or available experimental results. Figure 1 (left) shows, for example, the temperature distributions predicted for instance by SAFIR program [8], while figure 1(right) displays the corresponding normal force-bending moment interaction curves for different bending moment orientation, of a RC section after 120 min of fire exposure. Due to its simplicity, the proposed method allows performing parametric studies in a rather quick way. In addition to the proposed theoretical solutions, their validation is provided by their favourable comparison with some experimental results available in the literature (see Tab. 1 for tests at ambient temperature and Tab. 2 for tests at elevated temperature).

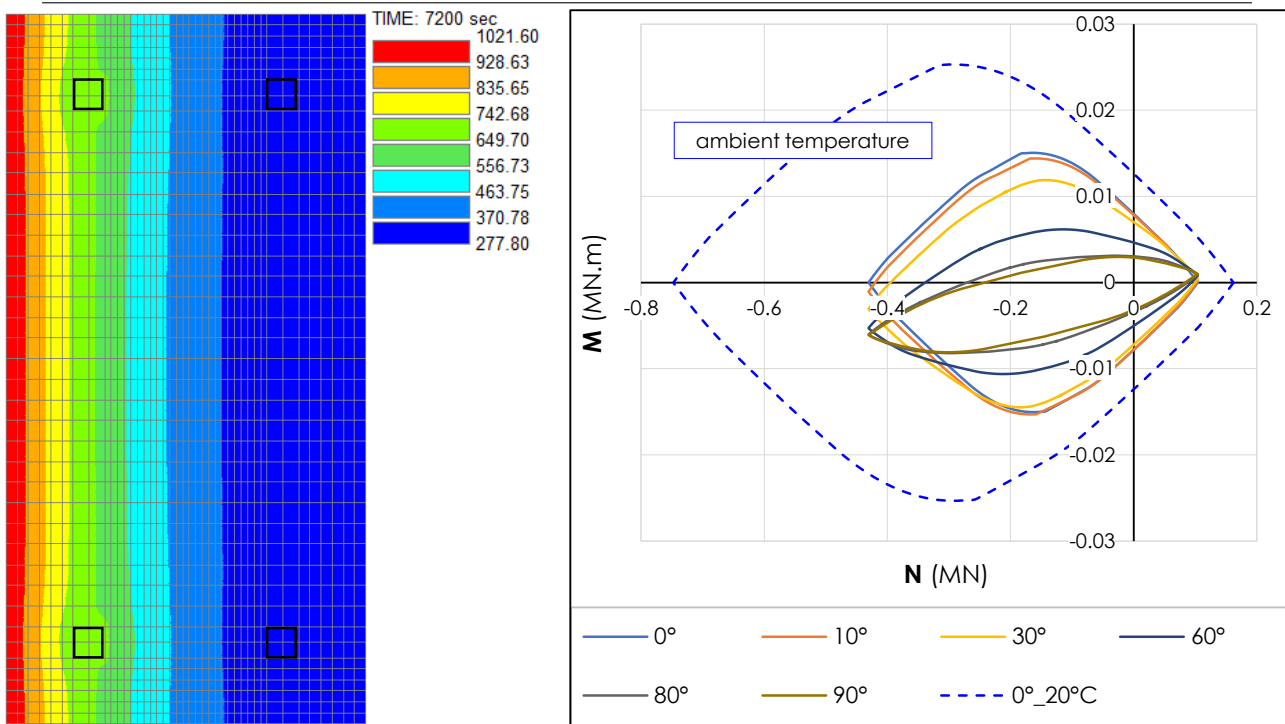
**Table 1.** Comparison between theoretical predictions with the results of tests at ambient temperature of Kim et Lee [6].

Test	Orientation (°)	Ntest (kN)	Mtest (kN.m)	Mpred.	Mpred/Mtest
SS-0-1	0°	119	6.664	6.165	1.08
SS-0-2	0°	126	7.3206	6.152	1.19
SS-30-1	30°	112	5.822	5.140	1.13
SS-30-2	30°	104	5.436	3.780	1.44
SS-45-1	45°	103	5.500	4.983	1.10
SS-45-2	45°	106	5.514	4.975	1.11

**Table 2.** Comparison between theoretical predictions with the results of tests at elevated temperature of Tan et Nguyen [7].

Test	Orientation (°)	Ntest (kN)	Mtest (kN.m)	Mpred.	Mpred/Mtest
C3-1-25	45°	860	74.27	79.82	0.93
C3-2-40	45°	680	73.83	85.28	0.87
C3-3-60	45°	530	68.29	88.64	0.93





**Fig. 1. 1.** Example of interaction diagrams for a rectangular RC section subjected to fire on one side.

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# Probabilistic modelling of containment building leakage at the structural scale: application to the PACE mock-up

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**Keywords:** Reinforced concrete, leakage, correlated random fields.

## Abstract

Despite the recent progress over the last decade and especially during the French research program MaCEnA (PIA), accurate prediction of air leakage through a reinforced (and prestressed) concrete structure remains a difficult issue. Indeed, as mentioned by the international Benchmark Vercors (phase 2) restitution report, only very few teams are able to predict the leakage and discrepancy of at least one order of magnitude between participants are observed. Even when global leakage is quite well predicted, the repartition between localized leakage (through cracks for instance) and diffuse one (through the porous network of cementitious material) is poorly estimated. However, reinforced concrete tightness estimation is of the utmost importance for confinement vessels but also to assess concrete structures durability.

One of the reasons for these difficulties lies in the fact that air leakage prediction is the last step of nonlinear multiphysic simulations. On the one hand, to predict concrete permeability (i.e. flow through the connected porous media), saturation evolution (in time and space) of the porous network needs to be correctly addressed as well as the description of the porous network. On the other hand, crack predictions (numbers, openings, and appearance time) is essential but not sufficient since their roughness, tortuosity and connectivity also strongly influence the leakage rate. Moreover, localized phenomena (cracking) and diffuse one (stresses, strains, saturation) are strongly coupled. Indeed, saturation evolution (inducing shrinkage), creep strains, early age behavior, stresses may lead to localized cracks due to reinforced concrete heterogeneity (material or structural ones). To represent the heterogeneous nature of concrete structures, the most employed technics is to deal with random fields applied to one (or more) concrete behavior parameter.

The aim of this contribution is to quantify the effect of the use of correlated random fields on the concrete structural leakage prediction. On contrary to structural tests that are very expensive and cannot be reproduced, numerical simulations can be performed for many realizations of a random field with identical parameters. In this contribution, the results of about 30 realizations for 3 different set of random fields) of a VSR (structural representative volume) involving rebars and prestressed tendons and based on a real structural experiment [2] will be analyzed. For this calculation, regularized damage model is used and the leakage rate is computed from the mechanical fields (damage and strains) through the recently developed coupling law between damage and leakage that could take into account leakage rate evolution during cracks closure [3]. The results highlight that for the same random field parameters, the air leakage prediction can easily vary from one decade. Moreover, during mechanical loading, observation of the crack evolutions (numbers, openings and positions) allows to quantify the prevalence between material and structural heterogeneity and to explain sudden evolution of leakage rate.

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# Toward a Material Agnostic Model of Microstructure Hydration and Deterioration in Concrete

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**Keywords:** Thermodynamics, Microstructure, Hydration, Kinetics

Concrete mixtures are becoming increasingly complex amid market pressures to reduce both its cost and environmental impact. At the same time, performance criteria are becoming more demanding due to the rise of rapid construction methods like 3D printing. Improved numerical models are needed to guide material design, and these models must be formulated to directly link the materials chemistry and physics to the evolving material properties. That direct link is a realistic representation of the material's microstructure. Such microstructure models have existed for a while, most of them being designed to handle a particular material or to require extensive parameter fitting via experimental observations. This presentation will describe progress toward a combined model of geochemical speciation and 3D microstructure evolution to simulate changes to the material properties over time under a range of compositional and environmental conditions. Examples will be shown of how the same modeling framework accommodates ranges of mineral admixtures, curing temperatures, and moisture conditions. A variety of engineering properties are tracked by direct finite element or finite difference models of the microstructure as it changes. Finally, some limitations of this model, and some potential approaches to overcoming them, are offered as subjects of future research.

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# Digital twin for modelling structural durability

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**Keywords:** reinforcement corrosion, chloride ingress, carbonation, fracture mechanics, nonlinear simulation.

## 1 Introduction

The reinforcement corrosion due to carbonation and chloride ingress are important damaging mechanisms. They can significantly reduce the service life of reinforced concrete structures.

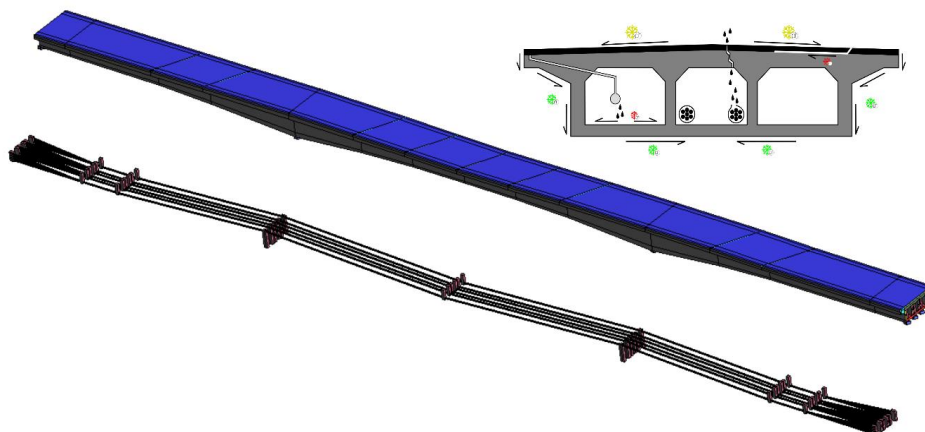
The paper presents a chemo-mechanical model covering initiation and propagation of chlorides or carbonation as well as resulting reinforcement corrosion. The paper will discuss the efficient application of a coupled model for large scale analysis and its application for the assessment of Wonka bridge in Czech Republic (see Fig. 1).

The integrated bridge assessment method utilizes an online bridge monitoring system with finite element method (FEM) modelling [1] for structural durability prediction. The material models used for the numerical simulations can realistically describe non-linear behaviour such as concrete tensile cracking and compression crushing [2] as well as yielding and rupture for the steel reinforcement. Furthermore, an advanced, coupled chemo-mechanical model is applied to evaluate deterioration mechanisms, namely chloride and carbonation-induced reinforcement corrosions [3]. For the deterioration phenomena, the diffusion-driven induction phase is assumed first and, after the depassivation of the reinforcement, the reduction of the reinforcement cross-section is calculated. The coupled model accounts for the impact of mechanical cracks on the acceleration of the ingress of the external environment substances while the compromised structural performance contributes to further growth of the cracks.

## 2 Digital twin model

Digital twin represents a combination of a computational model, which is calibrated and continuously validated by a monitoring system. In this case, the monitoring system iBWIM (Bridge-Weigh-In-Motion) from Petschacher Consulting, ZT-GmbH was used [4].

The FE model of the bridge is shown in Fig. 1. The model was created using layered shell elements with smeared reinforcement. Two types of pre-stressing cables are in the model, unbonded cables inside of the girder box and the bonded cables in the webs. The deterioration of the structure due to chloride attack was considered under the loading by dead loads. Then the loading by the design load combination was increased to determine the ultimate load-bearing capacity of the bridge for different ages as shown in Fig. 2-left. This main result of this approach is the development of the structural design resistance in time (see Fig. 2-right)



**Fig. 1.** Model of the Wonka with shell elements for the bridge girder the unbonded pre-stressing cables. The top cross-section shows the application of the chloride ingress boundary condition.

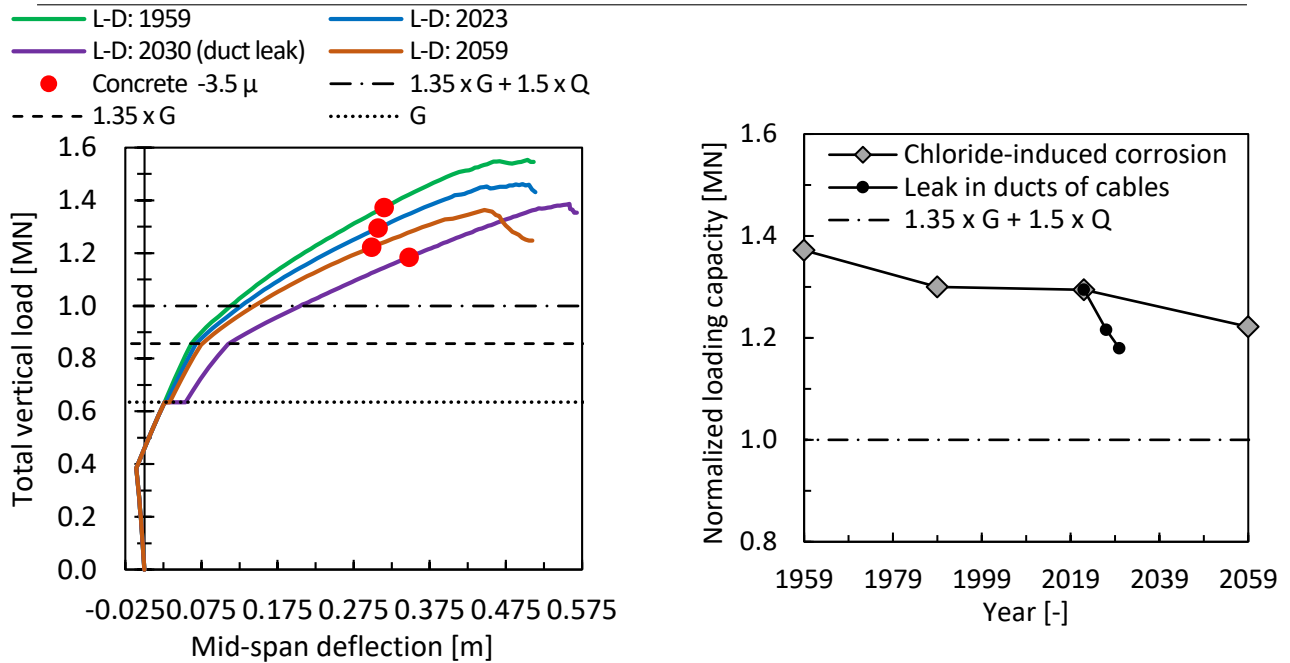


Fig. 2. (left) L-D diagrams for different bridge ages and deterioration levels, (right) time development of bridge load carrying capacity

### 3 Conclusions

The paper presents a chemo-mechanical model for durability analysis of reinforced concrete structures. The model application is presented using the “Digital twin” concept on Wonka Bridge located in Pardubice, Czech Republic. The long-term assessment is based on the integrated system, which is composed of an online system for bridge monitoring and a numerical model. Using the measured data, the numerical model is calibrated and then used for evaluation of the structural deterioration due to de-icing agents. The effect of the chloride attack was evaluated using the chloride transport and reinforcement corrosion models implemented in the framework of non-linear FE analysis. This allowed for the prediction of the development of the design load-bearing capacity of the bridge.

*Acknowledgement:* digital twin model was supported by TAČR project: CK03000023 „Digital twin for reliability and durability of concrete bridges“.

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# Assessing 3D concrete structures at ULS with robust numerical methods

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**Keywords:** Concrete structures, ULS, numerical methods, optimization

## 1 Introduction

Assessing the full state of a concrete structure at ULS is often challenging. By definition, the ULS imposes to consider nonlinear law of material and concrete is known to have a complex heterogenous behavior. Not only the reinforced bars must obviously be taken into account, but the concrete itself can show scattered values of limit strength, especially in tension. Eurocodes ease the analysis for engineers by defining a compressive strength limit for concrete, assuming a tensile limit generally null for conservative purpose, and by applying general safety factors to the analysis. This point of view is only one-dimensional, and some adaptations must be made when dealing with multi-axis stressing like confined concrete (see for instance [4]).

On one hand, from a design office point of view, the engineers find themselves with two possibilities for analyzing concrete structures at ultimate states:

- Applying the codes, generally by boiling down complex problems to easier ones. For instance, transversal sections of slender structures are classically calculated thanks to 2D tools, providing the ULS normal reinforced bars ratio. For more complex geometries, engineers can apply the strut-and-tie method (an illustration of limit analysis, see [1], [2], [3]) to find compressive and tensile parts of concrete, and then find the design of the needed reinforcement. Although this method is still used nowadays, it requires a certain level of expertise.
- When the above methods cannot be easily applied, like on complex massive 3D structure, as a last resort, engineers turn to full 3D finite elements nonlinear elastoplastic analysis. This solution, which can be very time-consuming, is not so easy to put in practice, and often leads with more questions than answers: which software to use? What kinds of finite elements? What kind of 3D nonlinear law to use for concrete? How to take into account the reinforced bars (which are one-dimensional) into a 3D model? And even so, once the analysis has been made, how to efficiently post-process the 3D results?

On the other hand, for several years, academics have proposed different solutions for modeling reinforced concrete, but often with complex 3D law, using many different parameters difficult to tune for classic engineer. Hence a gap between the research and the practical world has emerged. This state of art being made, we think this gap can be narrowed down by developing innovative easy-friendly software to the profession. To this end we present hereafter a new numerical method to assess the ULS of reinforced concrete.

## 2 A general optimization formalism to asses ULS in reinforced concrete

### 2.1 The static approach or how to find the best equilibrium state

The presented method proposes to take advantage of the strut-and-ties however needed 3D model in order find the best equilibrium state numerically. On this model, the algorithm tries to maximize the complementary energy, which only depends on the stress field, among stress values complying with the materials limit values. Different kind of behavior can be prescribed: elastic, elastoplastic or rigid-plastic (each with frictional contact if needed). The major advance of the presented method is the mathematical formulation of the problem. It inherits from the work of [5] and [6] which brought out the interest of conic constraints in limit analysis. This formulation gives access to robust solver and allows to deal with all the kind of analysis (elastic, elastoplastic, limit analysis) in the same extended framework.

This numerical robustness is enhanced by the ability to lead limit analysis. Indeed, limit-analysis is on its own a very direct and robust approach to assess an ULS state. While it is commonly used in geotechnical studies, structural studies hardly take advantage of this method, mainly for traditional reasons. For a civil engineer confronted to a complex RC structure, limit analysis can be seen as a very efficient tool giving access to the largest load scaling value accepted by

the loaded structure. This scaling value is all the more interesting as the associated stress state is provided, illustrating the equilibrium scheme. Thus, static limit analysis can be seen as the optimal strut-and-ties scheme according to an automatically found safety factor.

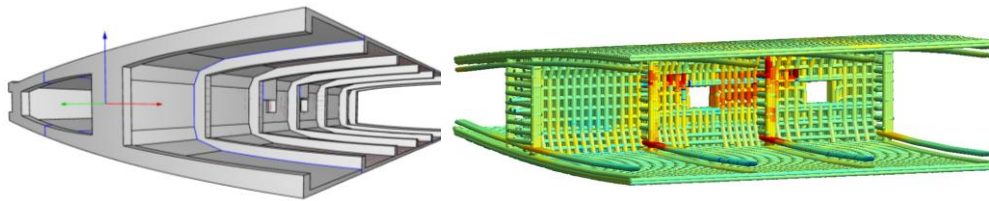
## 2.2 The kinematic approach or how to find the worst mechanism

Regarding the presented method, what is called kinematic approach is the search of a displacement field minimizing the potential energy plus the dissipation. Constrains on this minimization are about boundary conditions and slack variables. The kinematic information completes the information already given by the equilibrium stress field, knowing that its computation cost is much less important than the static approach's. The retrieved displacement field gives access to a failure mechanism in adequation with the static approach stress field.

Dual approach comparisons show that the choice to lead a static or a kinematic approach is far from having no impact. Indeed, with the access to a kinematic result and a static result at the same time it becomes possible to compute the distance between the two solutions. As the dual approach complies with all the mechanical equations except the constitutive law, this distance can be seen as an error in constitutive law ([7]).

## 3 Results on a real project

Application on a real project illustrates the method achievements and its limitations.



**Figure 1: 3D Application example - CAD model and reinforcements stress**

## 4 Conclusion

RC complex structures raise many questions that current standards and evaluation methods can't answer. The presented below numerical method is a powerful engineering tool, based on strong physical basis, that gives access to new responses on the structure behavior. It opens the door to a deep understanding of phenomenon, essential to a safe and sound evaluation of structures.

As for friction and steel [8], a formulation in convex optimization framework for reinforced concrete can be established. Once again, convex optimization appears to be an efficient way to tackle tricky mechanical problems. Its numerical implementation gives very readable results enhanced by the access to an error assessment, as shown on the illustrative example.

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# Numerical modeling of water transport in Ultra-High-Performance Fiber-Reinforced Concrete under dry-wet cycles

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**Keywords:** UHPFRC, transport model, finite element method, DVS, dry-wet cycles

## Abstract

Chloride induced corrosion has been an important issue for many reinforced concrete structures. Over the past decades, numerous transport models have been developed to simulate the process. Most existing transport models focused and are validated only on well-known traditional materials such as regular concrete and cement paste. New materials such as Ultra-High-Performance Concrete (UHPC) and High-Performance Fiber-Reinforced Concrete (UHPFRC), however, are less studied from the numerical perspective. The objective of this study is to propose a new transport model for UHPC and UHPFRC to simulate the water transport process in these less permeable materials. The model has been implemented in an in-house finite element method (FEM) software TransChlor2D and validated with experimental results from Dynamic Vapor Sorption (DVS) test on crushed UHPFRC samples subjected to dry-wet cycles. Experimental measurements on DVS also gave the sorption isotherm curves for the studied UHPFRC material, where the desorption curve was bilinear and the adsorption curve had a non-linear trend as an exponential growth. An analytical sorption hysteresis model of UHPFRC was therefore established and integrated in the transport equations. It is also realistic to state that the transport process is essentially diffusive without capillary suction effect for the tested specimens. Overall, the research provides a 2D numerical model allowing to estimate durability of UHPC and UHPFRC structures under realistic dry-wet boundary conditions.



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# Predicting early age temperature evolution in massive structures from non-standard characterization test

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**Keywords:** heat of hydration, massive structures, early age behavior, temperature evolution

## Introduction

In concrete massive structures, heat generated during the exothermic hydration reaction of the binder can lead to important temperature at core. The risk associated to an excessive temperature is nowadays well known and has been largely communicated in the concrete industry (see for example [1]). The consequence is that today, for all big construction projects, thresholds are imposed on the maximal temperature and on the maximal gradient temperature. It is therefore necessary to have an accurate prediction of early age temperature at any point and any time in the structure. Different methods and recommendations have been published in the last two decades for predicting temperature evolution [2, 3]. These methods are usually based on the characterization of the binder hydration by using a quasi-adiabatic test, at one or better at two temperatures [4, 5]. Unfortunately, depending on the country and on the local standards, such a test can not be accessible, and just a temperature monitoring of a mockup is available. The objective of this study is to propose a general framework allowing to predict temperature evolution in massive structures, whatever the type of hydration characterization test.

## 1 Temperature prediction study

The first part of this study is dedicated to the characterization of the thermal fingerprint of a binder. The procedure of the identification from a quasi-adiabatic test is recalled, with a particular highlight on the predominant parameters. Then, a proposal to extend the procedure to uncalibrated insulated tests is given: a numerical model of the characterization test is built, in which an Arrhenius function is chosen to take into account the coupling between the hydration reaction rate and the temperature [6]. A finite element solver is used to solve the heat equation. The thermal fingerprint identification is done through a minimization algorithm. Two assumptions are evaluated: for the first assumption, a predefined form of the chemical affinity is imposed; for the second assumption, a predefined form of the heat loss is imposed. We show that both assumptions allow to identify the thermal fingerprint of the binder. The choice of the assumption depends on the binder type.

The second part of the study gives an objective analysis of the temperature prediction, using the thermal fingerprints identified in the first part. Comparison of the results obtained with or without calibrated tests are given, with an estimation of the accuracy that can be expected depending on the characterization test. Results obtained with different binders are given, with a particular focus on blended binders.

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# Life time extension of wind tower foundations via numerical predictions

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**Keywords:** wind tower, soil-structure interaction, shear behaviour, size effect, fibre reinforced concrete.

## Abstract

The current effort towards the progressive switch from carbon-based to renewable energy production is leading to a relevant spreading of both on- and off-shore wind turbine towers. Regarding reinforced concrete shallow foundations of onshore wind turbine steel towers, possible reductions of reinforcement obtainable by employing SFRC may increase their sustainability, speed of erection, and competitiveness. At the same time, there is a strong need to extend the life of foundations erected more than 15 years ago, originally designed for only 20 years [1,2].

The paper presents a Finite Element investigation on full scale structures based on a previous numerical simulation of experimental results collected in a research programme in progress at Politecnico di Milanowith ENEL on prototypes at different reduced scales (1:4 and 1:15; [3], Fig.1), concerning the reinforcement with steel fibres of concrete shallow foundations embedded in a sandy soil subjected to both monotonic and cyclic loadings.

The paper will introduce also some ideas to develop a rational approach, based on simplified numerical predictions and mechanical parameters identified on site [4], to evaluate the residual life of existing wind tower foundations and eventually to extend it [5], if required.

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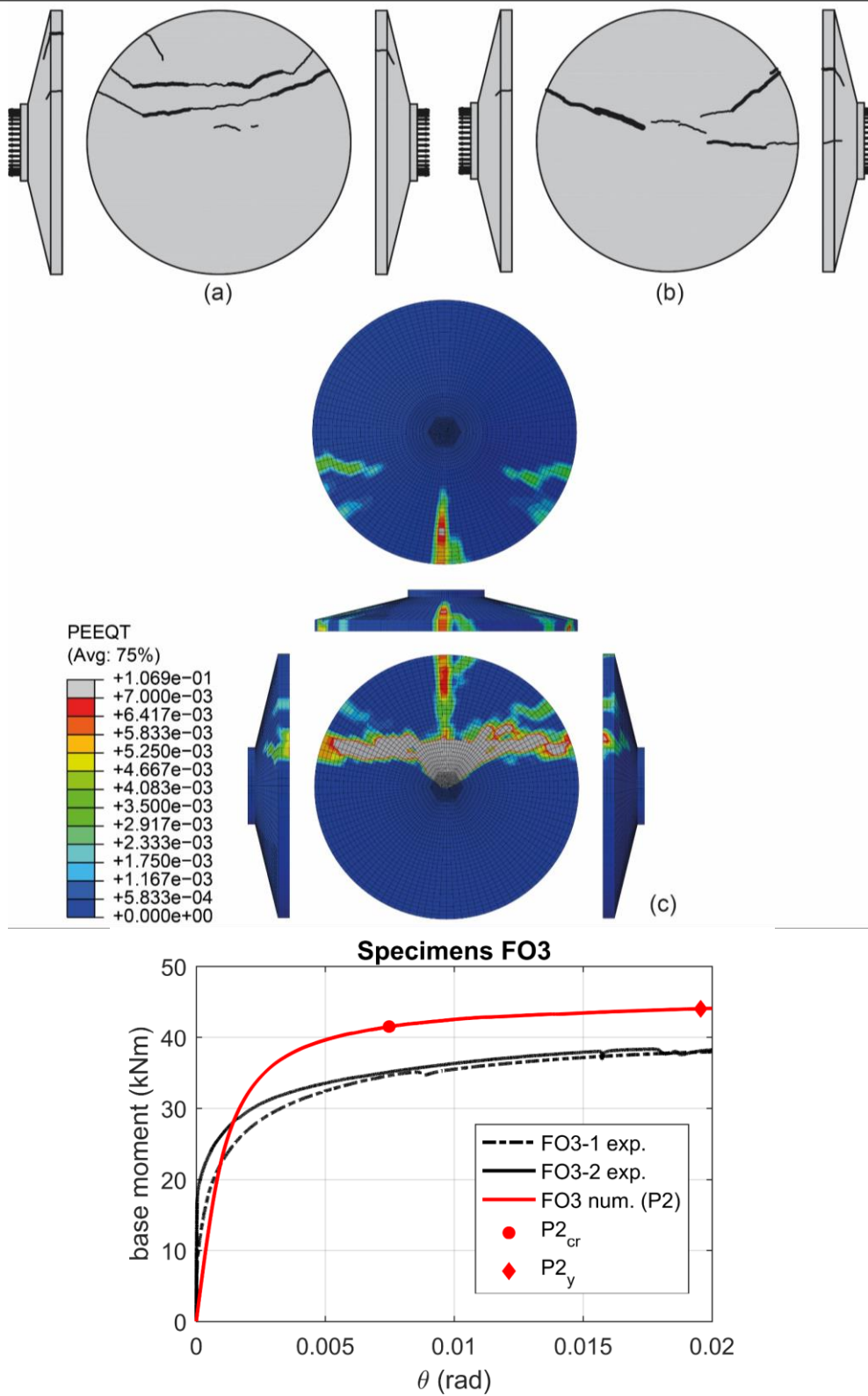


Figure 1 – Numerical simulation of a 1:15 prototype experimental test on a R/FRC foundation of a wind tower: (a, b) experimental crack patterns; © numerical simulation; (d) bending moment vs. rotation prediction.

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# Numerical modeling of new conceptions of 3D printed concrete structures for Pumped Storage Hydropower

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**Keywords:** Pumped Storage Hydropower, 3D printing, , Forth Keyword, Sixth Keyword.

## Abstract

Pumped-storage hydropower (PSH), also called “the world’s water battery”, represents one of the most sustainable, economical, and efficient solutions for energy storage, being an excellent alternative to store energy from intermittent sources such as wind and solar. PSHs have two reservoirs at two different levels and water is pumped from the lower reservoir to the upper one when energy generation is greater than demand, and its drop is released for the generation of energy when there is an increase in demand.

In Brazil, the hydroelectric potential of rivers is greatly explored, which has generated positive results in terms of self-sufficiency in energy production. However, in recent times, the solar and wind energy sources have been increasingly explored and for these types of energies to expand, it is necessary to install "water batteries" to ensure the constancy of energy supply. PSHs are relatively new energy storage systems and in the case of Brazil they are still little implemented. In addition to allowing the expansion of the wind and solar generation network, it can provide projects with the use of reservoirs with smaller surfaces.

This paper explores the possibilities of this new type of hydroelectric development, checking the possibilities of using new engineering tools such as 3D printing. The use of such technology for concrete has gained rapid development in recent years due to the advantages in structural optimization and economy with formwork in conventional construction. Practical engineering applications have proven the applicability of 3D printing in the large-scale construction of building components and compared to conventional manufacturing methods, this advanced technique has several advantages and offers almost unlimited potential for arbitrary geometric complexities.

We explore the potentials of using 3D printing for the construction of PSH structures with the help of numerical modeling in two ways: (i) during the early ages considering the phenomena of hydration; (ii) after hardening of concrete verifying the possibility of introducing new design concepts. The results indicated that numerical modeling can point to new solutions that will help address the challenges posed by greater sustainability in energy generation and storage in the 21st century.

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# The role of modelling in structures operation or rehabilitation

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**Keywords:** Modelling, Durability, Dam, Swelling, Rehabilitation.

Almost thirty percent of hydraulic structures in the world suffer from internal concrete swelling pathologies. For dams, this pathology creates damages that can compromise the global stability of the structure at long term. For power plants, this can lead to various disorders: misalignment of turbines, ovalization of units, blocking of valves ?, etc.

However, it is not always essential to reinforce the structures affected. Numerical models are able to precisely describe the internal state of concrete as well as its probable evolution, which can be an effective tool in order to continue the safe operation of structures.

But, in some cases, reinforcements are necessary. The models then make it possible to design the most relevant restoration projects and optimize the cost of the works. In this context, a methodology to manage the overall of structures, based on monitoring, laboratory tests and numerical modeling has been developed by EDF.

This methodology was applied in the context of the renovation of Chambon dam. A presentation through the case of this dam will be offered.

The dam is located on the Romanche river, upstream of Bourg d'Oisans. It was built in the 1930s on the site of a former glacial threshold, which formed a constriction in the valley with a much larger space upstream. The water reservoir forms an artificial lake called Lac du Chambon.

After twenty years of operation, a network of cracks gradually appeared in the lower part of the blocks on the left bank. Then the development of cracking spread to the entire dam, accompanied by irreversible movements, in particular by raising of the crest, and deformation of blocks towards upstream in the left bank side of the dam and towards downstream in the right bank side. The evolution of cracking and irreversible displacements therefore required special monitoring and investigations.

Between 1960 and 1980, numerous laboratory tests were carried out on concrete samples, which concluded, with the state of the art at the time, in an alkali aggregate reaction phenomenon.

The development of swelling had led to a first renovation campaign in the 1990s. And in the 2000s, a new study and modeling campaign was launched in order to better understand:

- the behavior of the structure,
- remove any remaining doubts,
- propose an efficient renovation of the dam,

These studies were followed by a new campaign of reparation works.

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# The multi-scale multi-technique multi-physics framework required to model the thermal properties of cement-based materials

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**Keywords:** Heat capacity, Thermal conductivity, Thermal Expansion, Molecular simulations, Micromechanics.

Thermal deformations are a major cause of cracking in cement-based materials. The physical origins of the properties controlling the thermal response of micro- and mesoporous materials are fundamentally related to atomic-scale processes. Therefore, techniques well-suited to assess the atomistic scale are required to properly understand the thermal behavior of cement-based materials or, in a more ambitious perspective, bottom-up engineer materials with a target thermal performance.

Fundamental component data regarding the properties of the main phases present in cement systems are critical input in multiscale modeling. However, such data is missing for some key phases (e.g., AF-phases). Also, the effects of water content in the thermal properties of hydrated phases (especially C-S-H and AF-phases which exhibits variable water content) are not fully understood.

In this paper, we review the techniques of classical molecular simulations that can be used to link the structure of materials to their thermal properties, namely, the heat capacity, thermal expansion, and thermal conductivity. We show that the molecular simulations of the heat capacity of materials with crystalline domains, as it is the case of crystalline phases (e.g., tricalcium silicate) or microporous hydrated phases (e.g., C-S-H, ettringite, monosulfoaluminate, alkali-silica crystalline products), requires the incorporation of quantum corrections. As a result, the thermal properties of tricalcium silicate, ettringite, and C-S-H computed from classical molecular dynamics are presented and confronted with experimental data available from the literature. The fundamental property data provided in this work for the thermal properties of these phases are valuable input for multiscale modeling and prediction of the thermal behavior of cement-based materials.

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# Elastic and failure behavior of main hydrated cement phases interfaces using Molecular Dynamics simulations

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**Keywords:** Calcium-Silicate-Hydrate, Portlandite, Ettringite, Molecular Dynamics, Multiscale, Tensile Test

## 1 Introduction

Concrete are by far the most used materials in the construction field and it is estimated that cement and concrete industry produce the global CO<sub>2</sub> emission for about 7-8% nowadays [1]. Concrete consists of a particulate phase (aggregates) and a binding phase (cement matrix) as a complex composite. As a result, the cement matrix affects the mechanical properties of concrete. Cement paste is a porous multiscale substance with varying physical properties at different length scales [2]. Calcium-Silicate-Hydrate (C-S-H) is a major component of hardened hydrated cement paste, which occupies more than 50% volume in the paste [3]. Another major phase in hydrated cement is Portlandite (Ca(OH)<sub>2</sub>) which occupies 20-25% of the volume fraction of the total mass [4].

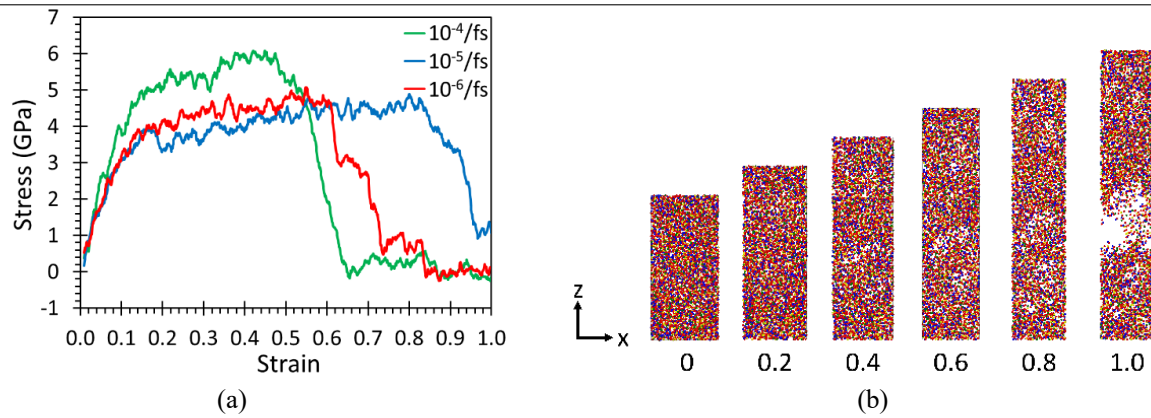
Macro-scale fracture is originated from the breakage of interatomic bonds at the nano-scale. It is now necessary to grasp the adhesion properties between different hydrated cement paste phases and to take them into account at the micro-structure scale of the cement paste. It is indeed the break in adhesion between these phases themselves (inter-phases and non-intra-phases breaks). There are many problems related to micro-cracking simulations at nano-scale. For example, the durability of the concrete is reduced by the micro-cracking. The storage of nuclear or gas could leak and causes the problem because of the micro-cracking. Thus it is interesting to study the micro-cracking using the Molecular Dynamics simulations at nano-scale which is related to interatomic potential between atoms.

## 2 Numerical Approach

Molecular Dynamics (MD) is a computer simulation technique for analyzing the physical movement of atoms and molecules. Atoms and molecules can interact for a period of time, giving insight into the dynamic "evolution" of the system. In this research, reactive force field (ReaxFF) [6] is used. Firstly, each individual supercell was created from the replication in x, y and z directions, respectively and then they were changed from triclinic cell to orthogonal cell. It was simulated in three dimensions and in real units with periodic boundary condition along three dimensions. Secondly, the random velocity was set to the supercell with the temperature of 300 K. After that, an energy minimization of the system was performed. Thirdly, they were relaxed in the NPT ensemble with the pressure of 0 atm along x, y and z directions and with temperature of 300 K for 50 ps. Finally, the relaxed supercells were deformed along z direction while the NPT ensemble with the pressure of 0 atm and with temperature of 300 K were set to perpendicular directions.

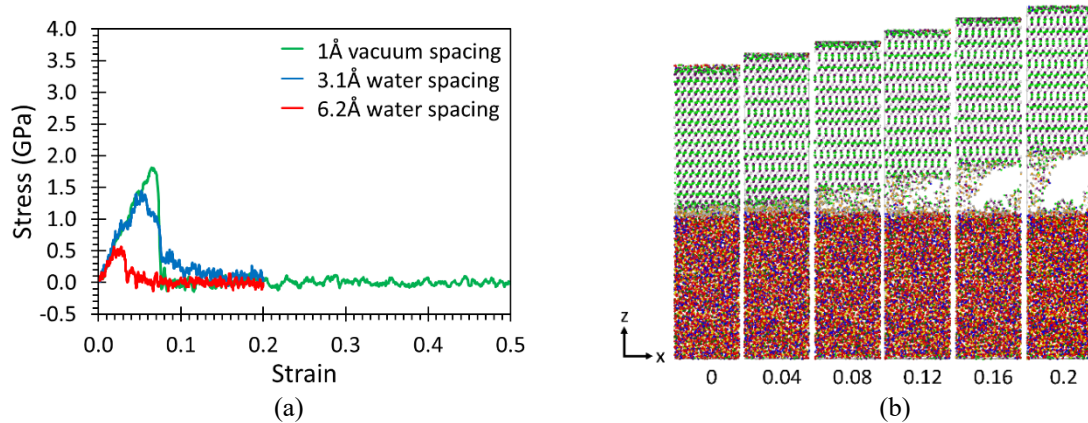
## 3 Results

In the first case, we have used the annealed amorphous supercells of C-S-H (I) which are replicated 5×5×3 in x, y and z directions. In order to see the effect of strain rate, the strain rates are set to 10<sup>-4</sup>/fs, 10<sup>-5</sup>/fs and 10<sup>-6</sup>/fs. **Fig. 1a** shows the stress-strain curves with three different strain rates and **Fig. 1b** shows the tensile failure of C-S-H (I) supercell. It could be seen clearly that the supercell and strain rate have effect on the stress-strain curves of supercell C-S-H (I). It can also be observed that the rupture is starting at the middle of the supercell 5×5×3.



**Fig. 1.** (a) Stress-strain curves supercells of C-S-H (I) (b) Tensile failure of C-S-H supercells at strain rate of  $10^{-5}/\text{fs}$  (Green balls are calcium atoms (Ca); yellow balls are silicon atoms (Si); red balls are oxygen atoms (O); blue balls are hydrogen atoms (H))

CH supercell was also placed on top of C-S-H (I) supercell with three different cases which are  $1 \text{ \AA}$  vacuum spacing,  $3.1 \text{ \AA}$  water spacing and  $6.2 \text{ \AA}$  water spacing between them. **Fig. 2a** showed that the values of peak stress and peak strain decrease with the increasing of spacing. The rupture along  $z$  direction happens into the phase of CH with the spacing of vacuum while the ruptures occur at the interface between the C-S-H (I) and CH with water in between them as shown in **Fig. 2b**. The Young's modulus of C-S-H (I)/CH are ranging from 22.193 GPa to 47.639 GPa.



**Fig. 2.** (a) Tensile stress-strain curve of C-S-H (I)/CH composite (b) Tensile failure of C-S-H (I)/CH composite (In C-S-H (I) phase at lower part; green balls are calcium atoms (Ca); yellow balls are silicon atoms (Si); red balls are oxygen atoms (O); blue balls are hydrogen atoms (H). In CH phase at the upper part, white balls are calcium atoms (Ca); lime balls are hydrogen atoms (H); purple balls are oxygen atoms (O). In water between them, silver balls are hydrogen atoms (H); orange balls are oxygen atoms (O))

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# Numerical Model for Explosive Spalling of High-Strength Concrete and Carbonation during and after Fire Exposure

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**Keywords:** Multi-scale Modeling, Explosive Spalling, High-Strength Concrete, Tension Softening, Carbonation, Fire

## Abstract

This paper investigates the explosive spalling of high-strength concrete and the shear capacity of high-strength reinforced concrete (RC) beams in considering an impact of carbonation during and after a fire. Explosive spalling at a fire accident causes severe damage to structural concrete. Thus, numerical and experimental investigations have been conducted [e.g. 1]. Carbonation after high-temperature heating is also an important thermodynamic event in terms of the durability of RC [e.g. 2]. Recently, carbonation during a fire is paid an attention [3]. In this study, numerical model is built for behavioral simulation of high-strength RC during and after a fire when spalling and carbonation are simultaneously combined. The authors have tried to extend the applicability of current multi-scale modeling [4,5] up to 1,000°C [6,7] and carried out verification of the updated model [6,7]. It has been verified on carbonation in ambient environments [4] and during a fire including the conditions of high concentration of carbon dioxide (CO<sub>2</sub>). Here, an explosive spalling and moisture transport were focused on as a critical point of development [8].

This study is a part of strengthening the multi-scale platform. First, the spalling model of the multi-scale platform [6] was upgraded. In the case of ultra-high-strength concrete (the compressive strength is more than 120MPa), significantly early spalling of cover concrete occurred after fire exposure compared to the case of normal high strength one. But the computed spalling by the previous modeling took place later than the reality [6]. In this study, the limit state of spalling was upgraded in consideration of the strain threshold of concrete under strain softening range. This upgraded spalling model was validated by experiments of ultra-high-strength concrete during high-temperature heating.

Second, carbonation which may change the micro-pore structures during a fire was investigated by using the upgraded spalling model. According to the simulation results, it was computationally predicted that the explosive spalling in the case of high concentration of CO<sub>2</sub> begins earlier than the case where no carbonation is considered. This event attributes to the densification of the microstructure which may suppress the vapor in motion owing to the reduced diffusivity and results in the higher pore gases pressure.

Third, shear failure of high-strength RC subjected to high-temperature fire heating was analytically investigated. The coupled analysis of the upgraded thermodynamic model with the multi-directional crack model of structural concrete was examined to be able to roughly reproduce the shear capacity and ductility after high-temperature heating. Although the effects of high concentration of CO<sub>2</sub> during a fire was not large to the shear behaviors, the carbonation during post-fire-curing has a great impact to the behavior of RC subjected to fire exposure. These post fire behaviors can be explained with the multi-scale modeling as well as the one during the fire.

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# Modelling of rock-shotcrete interfaces using a novel bolted cohesive element

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**Keywords:** Interface, rock-shotcrete, finite element method, user-defined element, cohesive element.

Rock-shotcrete interfaces are common in mining and civil engineering infrastructures including underground tunnels and excavations. These interfaces are important to investigate since they represent irregularities that usually cause stress concentration. Factors such as rock roughness, shotcreting irregularities, properties of reinforcing elements (e.g. rock bolts and/or fibres), and the conditions of their installation influence the behaviour of these interfaces. These irregularities can be attributed to the heterogenous nature of rocks and also to the excavation process that is often based on drilling and blasting or mechanical digging, which makes it difficult to obtain smooth surfaces free of local defects. Shotcrete is usually sprayed on these surfaces to prevent detachment of loose rocks, especially in the presence of workers and/or heavy equipment. Naturally, shotcrete spraying results in non-uniform layers that slightly smoothen the original rock surface and strengthen it. The interface between the rock mass and the shotcrete layer relies essentially on the bonding that occur due to cement hydration reactions. Additional strength is gained by reinforcing the structure with rock bolts.

To the author's knowledge there are no cohesive element approaches in the literature to predict the behaviour of rock-shotcrete interfaces, especially when support systems such as rock bolts are used. Existing approaches to predict describe the behaviour of rock-shotcrete interfaces are essentially analytical as shown by the authors in previous contributions [1,2] and they ignore the effect of reinforcing systems. The present formulation builds on a similar element that the authors suggested for fiber-reinforced concrete [3]. However, the different scales between fibers and bolts as well as the absence of interface in plain concrete make this approach fairly different. It is worthwhile noting that the proposed formulation does not apply only to mining and civil engineering infrastructures embedding such interfaces but also to other applications where detachment between different materials can occur in a localized manner.

In this study, we introduce a new technique to model rock-shotcrete interfaces embedding rock bolts using the finite element method. We developed a so called 'bolted cohesive element' through the user-defined element (UEL) subroutine of Abaqus to describe this complex interface. The proposed model takes into account the uneven interface roughness and the complex interaction between its components. The cohesive stiffness of the model degrades proportionally to the damage that occurs due to this interaction. The stiffness of the bolt connection and its location are also considered in the proposed mathematical formulation. The present bolted cohesive element has been validated experimentally; good agreement has been obtained between the measurement and numerical simulation under the conditions of direct shear test and bolt pull-out tests. Mesh independence has also been verified by examining the effect of mesh size on the overall force-displacement response of typical structures. With the model at hand, the effects of key installation parameters such as number of bolts, their inclinations and material properties have been investigated.

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# Numerical Simulations of CNT/CNF Reinforced Concrete Using ANSYS

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**Keywords:** concrete mix design, nano-reinforced concrete, numerical simulations, mechanical properties.

Concrete mix design is an important stage in the design of concrete structures, especially in the case of specific structures such as high-rise buildings, long bridges, and other massive structures, or when a specific type of concrete is used, such as green, recycled, high-strength, lightweight, etc. The proper design of the mix proportions assures that the concrete is as economical as possible, and that the successful construction and exploitation stages are provided. Concrete mix design methods include analytical, experimental, and statistical methods. Determination of the optimal mix proportions of concrete, according to the relevant concrete property is commonly obtained by using a hybrid of these methods, called the semi-experimental methods which usually include some statistical method combined with experimental testing. This paper determines the feasibility of application of ANSYS for the mix design of concrete reinforced with carbon nanotubes or carbon nanofibers. The work here explores the possibilities given by the program, examines the feasibility of numerical modeling in concrete mix design, and compares the results of the numerical simulations with the results of previous experimental testing of CNT/CNF reinforced concrete.

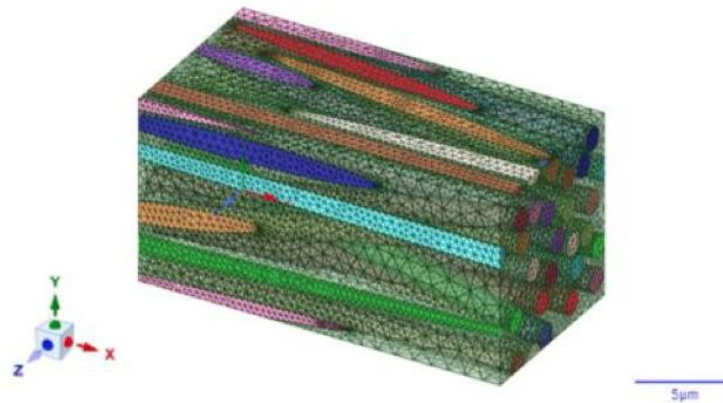


Fig. 1. Random UD Composite RVE of concrete matrix with CNTs.

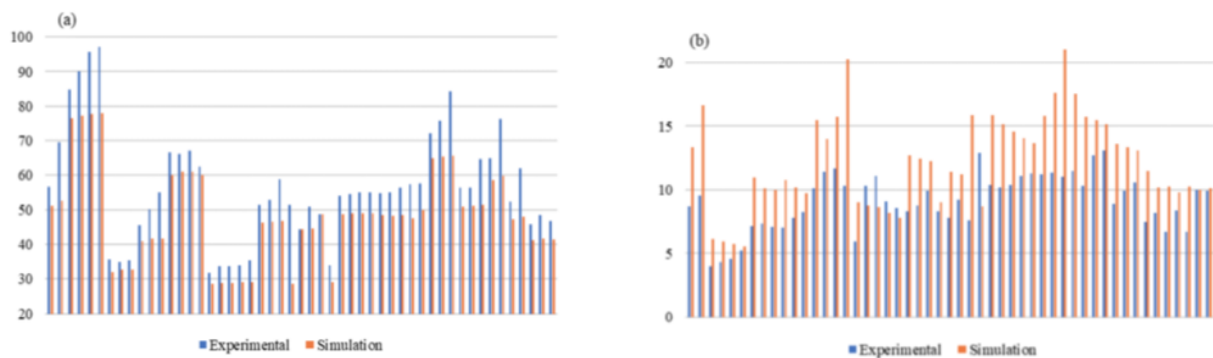


Fig.2 Validation samples compared between experimental and simulated testing: (a) compressive strength; (b) flexural strength.

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# Computational performance assessment and failure analysis of reinforced concrete wall buildings under seismic loads

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**Keywords:** Reinforced concrete buildings, Core wall, Performance-based seismic design, Nonlinear analysis, Seismic damage, Shear-flexure interaction, System effects.

## 1 Introduction

Reinforced concrete structural walls (RCSW) constitute a common seismic force-resisting system for multistory buildings in seismically active regions. Understanding the inelastic behavior and failure modes of RC walls is of uttermost importance for detecting and eliminating potential vulnerabilities of the building inventory and ensuring the safety and resilience of earthquake-prone communities. Currently employed seismic analysis and design procedures for multistory buildings employ simplified models which may neglect crucial aspects of the behavior, such as the interaction between flexural and shear damage in nonplanar walls and the impact of the inelastic behavior of coupling beams and/or slabs.

This study employs computational simulation to investigate the seismic performance of a prototype 14-story building with core-walls, located in Downtown Los Angeles and designed [1] in accordance with the pertinent minimum code requirements. The plan configuration of the building is presented in Fig. 1a. The core-wall, located in the center of the plan, consists of two coupled C-shaped walls whose planar segments are aligned with axes X and Y shown in Fig. 1a.

## 2 Overview of Computational Study and Main Findings

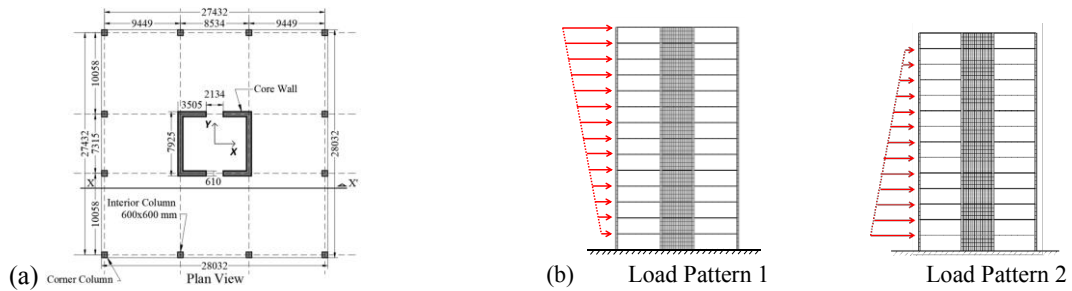
The computational representation of the building, which accounts for the material and geometric nonlinearity of all structural components, employs the beam-truss model (BTM) for the walls and floor slabs. The BTM [2] allows capturing the cyclic inelastic behavior of RC walls and slabs, while being conceptually simpler than, e.g., continuum finite element models. The capability of the method to capture the cyclic hysteretic response, damage patterns, and failure of RCSW components has been extensively validated [2-4] over the last decade. Nonlinear static and dynamic analyses are conducted for a combination of gravity and seismic loads. The static analyses are conducted for two different load patterns, i.e. distributions of lateral forces with height, termed Load Patterns 1 and 2, as schematically shown in Fig. 1b. The lateral loads are cyclic, and each cycle corresponds to an increasing value of roof lateral displacement. The dynamic analyses consider a set of triaxial ground motions scaled at two intensity levels, namely, those of the design earthquake and the risk-targeted maximum considered earthquake (MCE<sub>r</sub>).

The analyses provide insights into the evolution of structural system damage and lateral strength degradation, while also elucidating the complex interaction between the webs and flanges of the core-wall and the system effects associated with coupling between the walls, beams, slabs, and columns. Figure 2a compares the level of shear stresses for application of Load Pattern 2 along the X-direction of the building. The figure also shows the upper and lower limit values for the shear stresses in the webs per the Los Angeles Tall Building Seismic Design Council (LATBSDC) performance-based seismic design guidelines [5]. The significant amount of shear stresses leads to damage patterns which include extensive shear damage in wall webs, as deduced from the maximum principal strain contour plots shown in Fig. 2b.

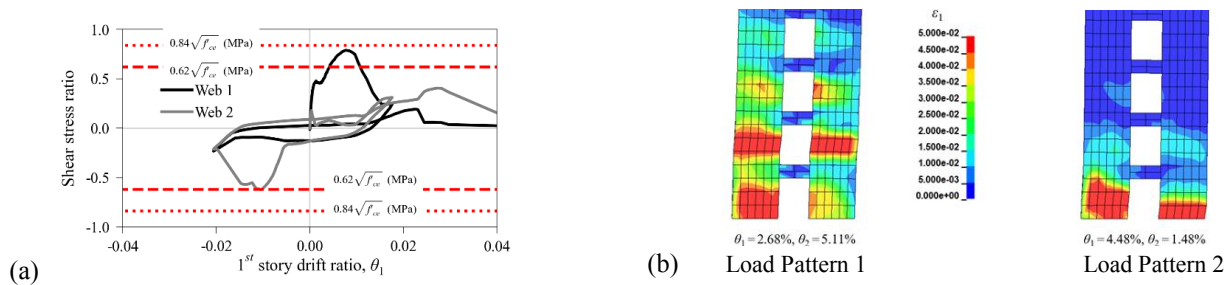
Figure 3a shows the deformed shape of the building model corresponding to a roof story drift ratio of 3%, for cyclic static loading in the Y-direction with Load Pattern 1. The deformed shapes in the figure also include vertical displacement contours. The axial elongation and rotation of the core-wall imposes significant flexural deformations in the slab. The vertical displacement contours of Fig. 3a indicate the formation of yield lines in the slabs associated with downwards vertical displacement. It is worth mentioning that the slab coupling also affects the demands in the columns.

The potentially detrimental effect of the multidirectional nature of the seismic motion on the inelastic deformability of the wall components is also demonstrated. For instance, several of the MCE<sub>r</sub> ground motions led to vertical concrete crushing of the confined corners of the core wall. This is illustrated in Fig. 3b which depicts vertical strain contours at

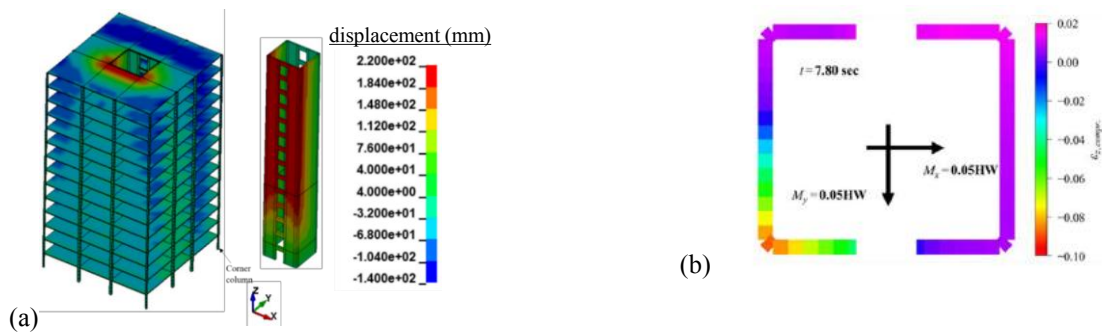
the base of the wall, for a given instant in the analysis. The core wall moment in the X- and Y-directions is similar for that particular instant, indicating lateral loading at nearly  $45^\circ$  while the compression strain of the bottom left corner of the wall section 8%. This type of damage is critical not only for the collapse prevention and seismic safety of the building but also for the accurate calculation of residual deformations (lateral and vertical) that determine the functional recovery performance of earthquake-prone communities.



**Fig. 1.** Building model considered in analytical study: a) Plan configuration, b) Load patterns considered in nonlinear static analyses.



**Fig. 2.** Results obtained from nonlinear static analysis: a) Comparison of shear stresses on web piers to upper-bound values allowed in performance-based guidelines by the LATBSDC [5], b) Deformation and principal strains at end of analysis.



**Fig. 3.** Analysis results: a) Deformed shape and vertical displacement contours for building and core wall obtained in static analysis, b) Vertical strain contours of the core wall for dynamic analysis involving an  $MCE_r$  ground motion.

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# Fuzzy logic-based approach for the uncertainty treatment in cementitious materials modelling

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**Keywords:** Fuzzy Logic, Uncertainty Treatment, Material Modelling, Cementitious Materials, Fibre Reinforced Concrete, Lattice Discrete Particle Model, Hygro-Thermo-Chemical model, ONIX.

## Abstract

In the context of the Horizon 2020 project ReSHEALience, the concept of Ultra High Durability Concrete (UHDC) is introduced to refer to those materials belonging to the wide family of cementitious materials, whose mixture recipe is tailored to enhance the performance in terms of durability compared to ordinary concretes [1]. The target is achieved through the full exploitation of the inherent capacity of autonomously repairing the cracks which characterises the cement-based composites. For this reason, supplementary cementitious materials, such as slag and crystalline admixtures, are included into the mixture [2]. The UHDC concept is validated by means of either extensive and complex experimental programmes in the laboratory, and monitoring campaigns on structures in real service scenarios. However, the disruptive impact of such advanced materials on the construction market can be materialised only by modelling their behaviour accurately, in order to reliably predict the performance in different scenarios.

The behaviour of UHDC is well-captured by physics-based models, of which the Lattice Discrete Particle Model (LDPM) [3], for the mechanical problems, and the Hygro-Thermo-Chemical (HTC) model [4], for the simulation of moisture, heat and chemical phenomena, are two worthy examples. Recently, these models were extended for the autogenous and stimulated healing in ordinary and fibre-reinforced concretes at the Politecnico di Milano [5, 6]. However, the afore-mentioned models present a significant number of parameters that need to be calibrated against experimental measurements, which are almost always unavailable. This represents the most relevant issue to tackle for their use. In addition, accurate small-scale models, such as LDPM and HTC, are particularly suitable for the modelling at the material level. The upscaling to structural members, or even entire structures, requires the identification of *bridging* parameters, in charge of bringing the small-scale models' accuracy into the engineering models adopted for the long-term prediction at the structural level.

Among other methods for mathematically describing and quantifying uncertainty, the probability theory and fuzzy set theory could be used [7]. The probability theory is a mathematical theory of chance, stating the likelihood that an event will occur, by quantifying it with a number between zero and one. On the other hand, the logic of fuzzy set theory allows the quantification of degrees of truth or membership to a set [8]. Therefore, the latter is used to describe epistemic uncertainty, in particular the uncertainty resulting from insufficient information or lack of (experimental) data to deal with in complex systems, such as the cross-influence between the material composition, the chemistry, and environmental conditions on the material response. The fuzzy-set theory enables a flexible assessment of the possibility, which is necessary to deal with complex governing parameter systems and limited experimental databases.

The content of this paper focuses on the uncertainty featuring the models' calibration in case of limited experimental data on modelling material properties at microscopic and mesoscopic scales. To the purpose, a fuzzy logic-based approach is presented and tested for one of the UHDC mixtures identified within the activity of the project ReSHEALience. The accuracy of the fuzzy logic-based predictions is compared to the values of the models' parameters, gained through the calibration against experimental data. In particular, the proposed approach consists of five steps (see Fig 1).

1. Collection of the expert knowledge on the material itself and on the relationships between peculiar aspects, such as material composition, environmental conditions, loading regimes, and the models governing parameters.
2. Definition of a fuzzy cognitive map, namely a fuzzy graph for representing causal reasoning [9], which allows the extraction, analysis, and visualisation of the knowledge based on hard evidence as well as subjective expert judgement.
3. Implementation of a fuzzy rule base with if-then conditions. This fuzzy rule base is serving as the main combination between the membership functions, the causal relations, as it is stated in the cognitive map, and the expert knowledge provided by surveys or literature of similar materials.

4. Fuzzification of the parameters, which govern the models adopted, by associating a membership function to each of them. This operation is carried-out for those parameters whose value is affected by a scenario-related uncertainty.
5. De-fuzzification process: the membership functions, interval limitations and expert knowledge are combined into an inference system to identify a crisp value for each models governing parameter.

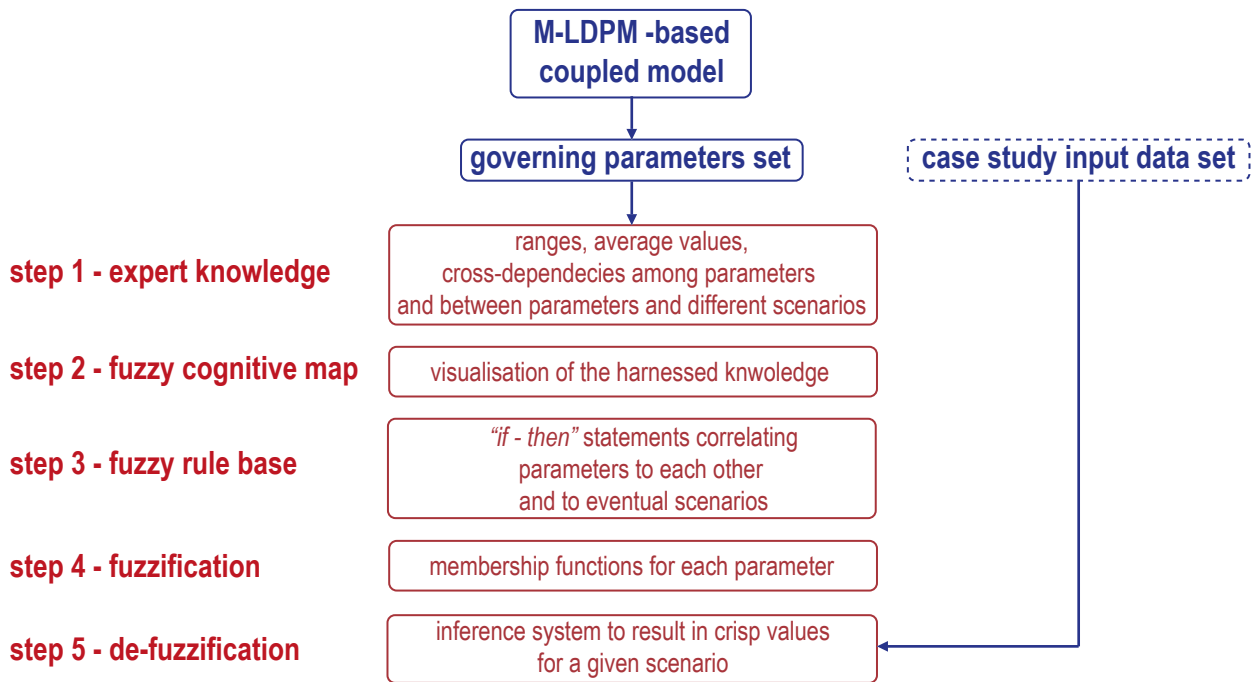


Fig. 1. Fuzzy logic and set theory-based approach for the calibration of the governing parameters in five steps.

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**Keywords:** permeability, cracks, mesoscale

The coupling between cracking and permeability of geomaterial members such as concrete and rock is of great interest for numerous problems. In most case the structure is wanted to be tight in order to prevent fluid or gas to migrate, this is as an example the case of nuclear waste disposals, nuclear plant confinement vessels, or other simple civil engineering infrastructures. In other cases, like hydraulic fracture for gas or geothermal wellbores, the geomaterial is wanted to be permeable. If the material is uncracked, the overall permeability is driven by the migration into the porosity, in a case of macrocracking the flow into the cracks governs the overall permeability. The coupling between cracking and permeability can be introduced by the way of the damage variable (Picandet et al., 2001, 2009; Chen et al., 2014), but the application of this method must be restricted to the initiation of damage in particular conditions. Another way is to use directly the value of the crack width and to compute the permeability through the so called "cubic law". The crack width could be a direct result of the computation for discrete methods, embedded crack element or X-FEM methods, or the result of a post processing for continuous damage approaches (Matallah et al., 2010; Rahal et al., 2017; Rastiello et al., 2016; Wang et al., 2022). In most cases the direct use of the cubic law overestimates the flow and authors use a tortuosity or flow coefficient which value ranges from 0.01 to 1.

This flow coefficient is generally attributed to tortuosity, roughness, recirculation into a single crack (Boussa et al., 2001; Rastiello et al., 2016) among others. Some experiments show that the flow coefficient may vary with the crack width to reach the value of 1 or not far from 1 when the crack is width reaches a given value (Rastiello et al., 2014).

Simulations made at the mesoscopic scale (Gangnant et al., 2016; Grassl, 2009; Nguyen et al., 2010) can reproduce the transition between diffuse cracking to localize cracking and it is interesting to perform the simulation of the coupling between cracking and permeability at this scale.

The experiments done by Rastiello et al. are simulated at the mesoscopic scale and authors show that the cubic law applies directly at this scale without use of any flow coefficient. The flow coefficient evolution measured during the experiments is correctly reproduced by the numerical simulation. This shows that, for this example, the existence of a flow coefficient that must be applied at the macroscopic scale is more due to the multicracking than to tortuosity.

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# Bayesian Inverse Modelling of Early-Age Stress Evolution in GGBFS Concrete Due to Autogenous Deformation and Aging Creep

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## ABSTRACT

Stress evolution of restrained concrete is directly related to early-age cracking (EAC) potential of concrete, which is a tricky problem that often happens in engineering practice. Due to the global objective of carbon reduction, Ground granulated blast furnace slag (GGBFS) concrete has become a more promising binder comparing with Ordinary Portland Cement (OPC). Although GGBFS concrete produces less hydration heat which further prevents thermal shrinkage, the addition of GGBFS highly increases the autogenous shrinkage and thus increases EAC risk. This study presents experiments and numerical modelling of the early-age stress evolution of GGBFS concrete, considering the development of autogenous deformation and creep. Temperature Stress Testing Machine (TSTM) tests were conducted to obtain the autogenous deformation and stress evolution of restrained GGBFS concrete. By a self-defined material subroutine based on the Rate-type creep law, the FEM model for simulating the stress evolution in TSTM tests was established. By characterizing the creep compliance function with a 13-units continuous Kelvin chain, forward modelling was firstly conducted to predict the stress development. Then inverse modelling was conducted by Bayesian Optimization to efficiently modify the arbitrary assumption of the codes on the aging creep. The major findings of this study are as follows: 1) the high autogenous expansion of GGBFS induces compressive stress at first hours, but its value is low because of high relaxation and low elastic modulus; 2) The codes highly underestimated the early-age creep of GGBFS concrete. They performed well in prediction of stress after 200 hours, but showed significant gaps in predictions of early-age stress evolution; 3) The proposed inverse modelling method with Bayesian Optimization can efficiently adjust the aging terms which produced best modelling results. The adjusted creep compliance function of GGBFS showed a much faster aging speed at early ages than the one proposed by original codes.

**Keywords:** Concrete; Bayesian Optimization; Early age cracking; Creep; Relaxation; Autogenous shrinkage.

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# Contribution of rib-scale modelling to study the bond mechanisms of reinforcement in UHPFRC

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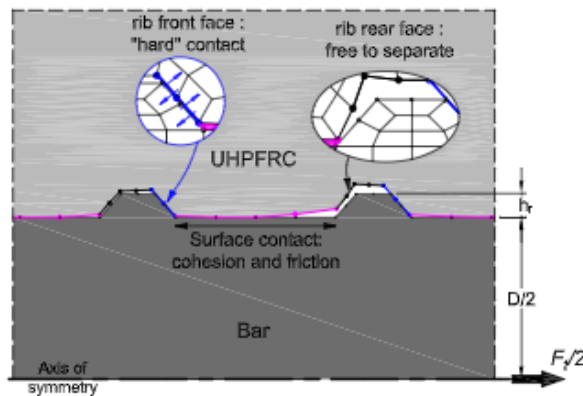
**Keywords:** Bond, Nonlinear analysis, Finite element, UHPFRC

## 1 Introduction

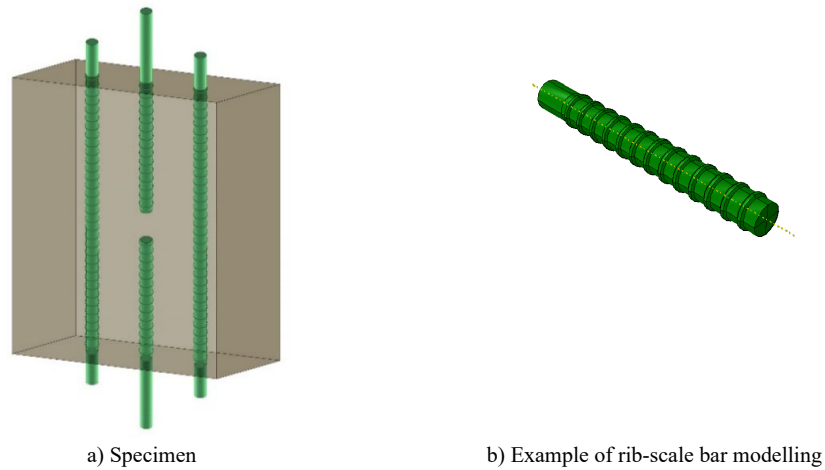
Using ultrahigh-performance fibre-reinforced concrete (UHPFRC) for reinforcement lap splice field connections simplifies construction details, reduces on site labour work and overall enhances connection performance and durability. Existing design equations for determining the required development length for normal concrete cannot be used for fibres reinforced concrete. With the rapid increase of popularity of UHPFRC field connections in North America in precast construction, a new set of equations that describe the failure mechanisms must be derived from new test data.

## 2 Rib-scale modelling strategy

This paper presents the development of a refined nonlinear finite element model at rib-scale using the 3D concrete constitutive model EPM3D implemented in ABAQUS which enables explicitly expressing the bond performance of lap splices in UHPFRC according to the tensile properties of the concrete, the cover thickness and the bonded length (see Fig. 1). Such model can be used to develop the required equations but also to contribute to developing relevant testing procedures (see Fig. 12).



**Fig. 1.** Schematic view of different surface interaction properties at the steel-concrete interface.



**Fig. 2.** Direct tensile bond test specimen.

### 3 Results

The numerical results show accurate simulation of the maximum strength, splitting failure mode, crack pattern, and steel stress distribution over the bonded length from different configurations of experimental bond tests. The analyses also highlighted one of the most important challenges in UHPFRC design: the selection of an accurate estimation of the actual tensile properties in the structures in terms of strength, strain hardening and softening stage that account for the fibre orientation and dispersion. This methodology illustrates the value of nonlinear finite element analysis towards the harmonisation of a bond test configurations and its contribution into the development of design guidelines for UHPFRC lap splice connections.

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# Modelling the nonlinear seismic performance of bridge piers

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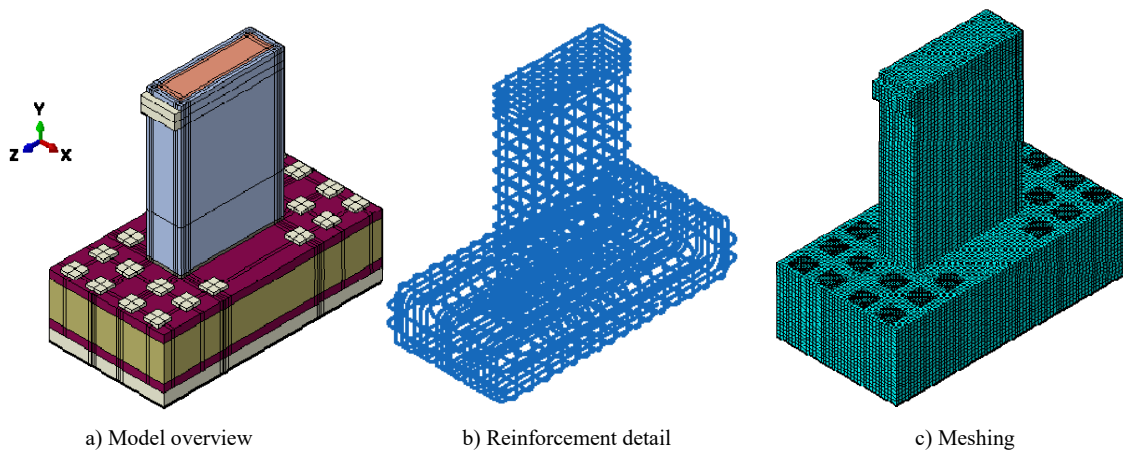
**Keywords:** Seismic performance, Ductility, Nonlinear analysis, Finite element, UHPFRC, Strengthening, Precast elements

## 1 Introduction

Bridges in regions of moderate to high seismicity must be designed to dissipate earthquake-induced energy through the nonlinear behaviour of some portions of their supporting elements, called plastic hinged regions, while the other region of these members and the other elements of the structure must stay intact. Bridge design codes are moving toward performance-based design approaches for the plastic-hinge zones with prescriptions applying essentially to cast-in-place construction. Although some systems have been proposed, recommendations for precast pier elements are not yet available in design codes. Moreover, achieving the prescribed performance standards for existing structures designed with requirements prior to the introduction of modern reinforcement detailing practice is hardly feasible. An extensive research program has been carried out at Polytechnique Montreal in the past 15 years for developing criteria aimed at designing cast-in-place and precast bridge columns meeting the most stringent seismic performance requirements. Furthermore, the research program also included developing a strengthening technique using UHPFRC covers aimed at correcting existing detailing deficiencies. These developments relied on large scale testing as well as on extensive nonlinear finite element analysis. Large scale testing provides essential information and allow observing the actual structural element behaviour. However, their applicability is limited to the tested geometries and scale whereas their cost is prohibitive. The use of refined nonlinear finite element analysis has provided essential insight for understanding the actual behaviour of bridge piers using UHPFRC connections for the lap-splice of reinforcement.

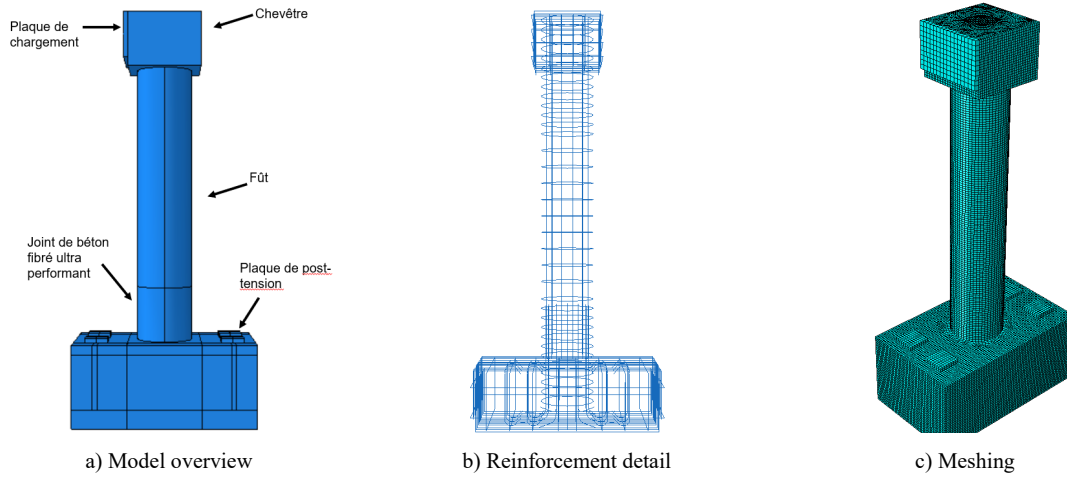
## 2 Nonlinear finite element modelling

A methodology for modeling bridge piers using Abaqus software and the EPM3D concrete constitutive model was developed for studying the ductility of these elements in seismic applications. Modelling of existing bridge pier strengthening using UHPFRC cover in the lap-splice region is shown in Fig. 1 whereas the model of a precast column element connected to the footing using lap-splice connections in UHPFRC at column base is shown in Fig. 2.



**Fig. 1.** Finite element model for the seismic strengthening of existing rectangular bridge piers

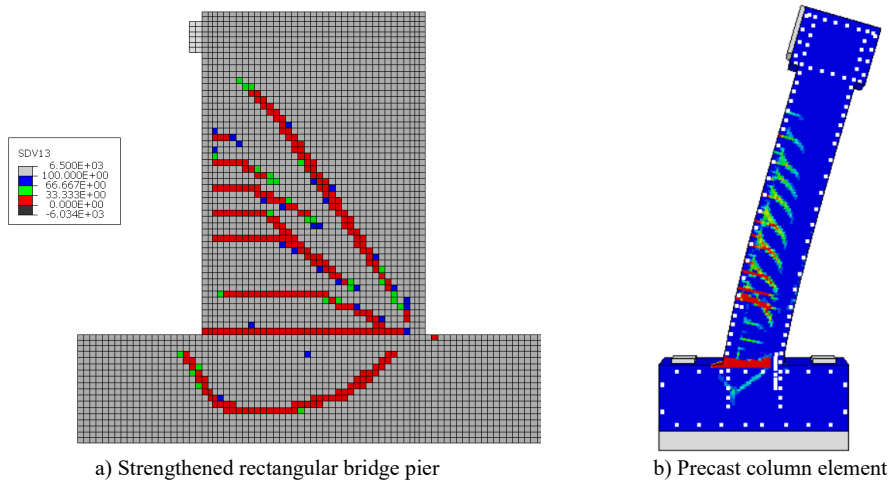
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**Fig. 2.** Finite element model for studying the seismic behaviour of precast bridge pier connection at the column base

### 3 Results

For both types of applications, the nonlinear static pushover analyses carried out with the finite element model made it possible to reproduce with a high level of precision the behaviour of the specimens observed experimentally, for the envelope of the hysteretic force-displacement curves, the crushing of the concrete, the yielding pattern of the longitudinal bars, the length of the plastic hinge and the crack pattern (see Fig. 3).



**Fig. 3.** Modelled crack patterns.

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# Numerical modeling of 3D concrete printing wall structure to reliably estimate the failure mechanisms

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**Abstract.** 3D concrete printing technology (3DCP) have gained wide attention. They indicated their potential to become a serious supplement to conventional concrete casting in molds. The main reason for this is it directly addresses the challenges related to the sustainability and productivity of the construction industry.

However, the current practice is based on the trial-and-error procedure, which makes the research of the 3DCP process expensive and time-consuming. One of the reasons is that there exist significant knowledge gaps regarding the relations between the design, material, and process parameters. Therefore, it is of vital importance to establish a relation between the process parameters and the printed product to avoid unreliability and failure. By implementing a numerical simulation of the 3DCP process, a more fundamental understanding of the relations between the printing process, the process parameters, and the properties of the printed product could be achieved.

In this study, Layer-wise Finite Element Method (FEM) combined with a pseudo-density approach, following the soft-killing approaches in topology optimization is applied. Along with the progressing printing process, all material parameters vary spatially and temporarily due to the time dependency of the curing process. The numerical simulations allow to reliably estimate the failure mechanisms that might occur during the 3D concrete printing of a wall structure.

**Keywords:** 3D concrete printing, Numerical modeling, SFEM simulation, Pseudo-density approach, Random Process, Reliability, Time dependency.

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# Numerical simulation of concrete fracture by means of a 3D probabilistic explicit cracking model

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**Keywords:** concrete fracture, probabilistic cracking model, scale effect, tensile failure, FEM.

The fracture process of concrete involves phenomena of considerable complexity, such as scale effect and softening behavior, which are directly linked to the heterogeneity of this material. These phenomena pose great challenges to the fracture modeling. Probabilistic models that deal directly with heterogeneity are a powerful tool to overcome these challenges, since they consider the natural variability of the mechanical responses. The present work refers to the simulation of concrete fracture by means of a 3D probabilistic finite element model in which interface elements are employed to explicitly represent the cracks. Friction between crack surfaces is also taken into account in the model. The three-dimensional modeling of cracks allows the fracture process to be analyzed in a more realistic way. The statistical parameters that define material heterogeneity were determined through inverse analysis procedures for which empirical reference data were used. Different sample sizes were considered to enable the assessment of the scale effect prediction. The possibility of occurrence of different softening levels was also investigated.



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# Incremental formulation of early age concrete in the finite strain range for the modelling of 3D concrete printing

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**Keywords:** Additive manufacturing, Incremental formulation, Early age, Large deformations, Instabilities.

Concrete cracking at early age is a major issue, especially for massive structures. By essence, a thermo-chemo-mechanical analysis is required where, for instance, autogenous strains and the exothermic reaction of the cement paste must be considered, e.g. [1]. Moreover, as the mechanical characteristics evolve with hydration, the reversible part of the stress-strain relationship is of the hypo-elastic type, i.e. incremental elasticity, see for example [2,3] among the abundant literature on early-age concrete. Within the assumption of small perturbations, the constitutive relation is of the form,

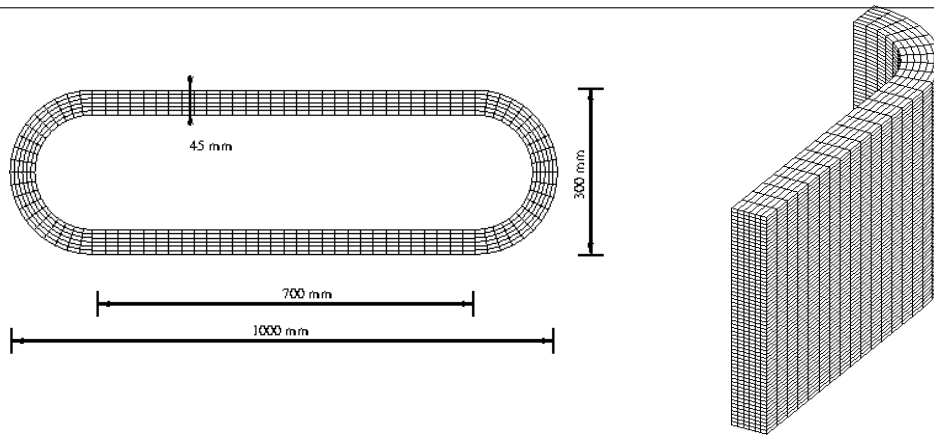
$$\Delta\boldsymbol{\sigma} = \mathbf{H}(\xi(t)) : \Delta\boldsymbol{\varepsilon} \equiv \mathbf{H}(t) : \Delta\boldsymbol{\varepsilon}, \quad (1)$$

where  $\Delta\boldsymbol{\sigma}$  and  $\Delta\boldsymbol{\varepsilon}$  are the increments of stress and strain tensors, respectively,  $\mathbf{H}$  and is the time-dependent elasticity tensor due to the hydration evolution  $\xi(t)$ . Eq. (1) should not be confused with the direct form  $\boldsymbol{\sigma} = \mathbf{H}(\xi(t)) : \boldsymbol{\varepsilon}$ . They could become identical only for fixed elastic parameters, which is not the case for an ageing concrete.

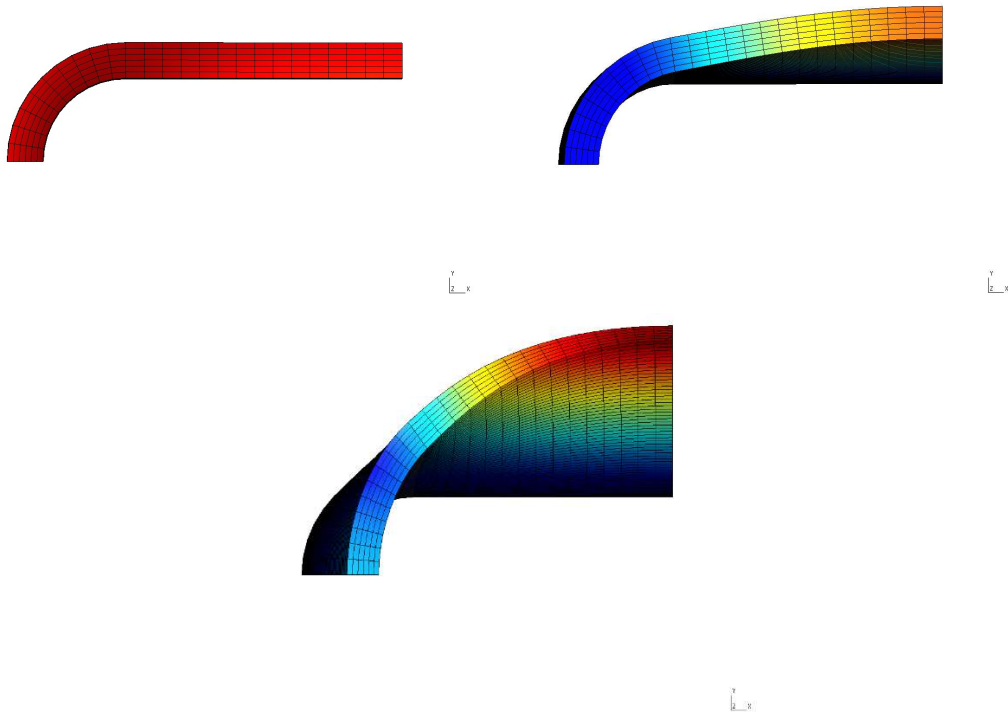
Nowadays, the challenging 3D concrete printing is receiving considerable attention in civil engineering; the ‘Construction 4.0’ as termed in [4]. In general, a concrete mixing is pumped into a pipe connected to a nozzle, and with the help of a robotic mechanism, precise positioning control and deposition path can be achieved. After several layers have been deposited onto each other, the fresh (early-age) concrete must be able to retain its shape due to the lack of confining formworks, i.e. the fresh concrete must carry its self-weight. As the mechanical properties are initially low, possible collapse during the printing process can occur. A predictive theory must then be established within a geometrically nonlinear framework to be able to predict such instabilities. Hence, the above hypo-elastic form, Eq. (1), should be extended toward the finite strain range. On the one hand, the mechanical equilibrium equation is rewritten in an adequate form because of in this case the stress is given in rate (evolutive) form and, on the other hand, the gravity cannot be incremented since it is imposed all at once. These peculiarities have been derived in [5] together with an adequate kinematical choice. For this latter, use has been made of a multiplicative decomposition of the actual deformation gradient  $\mathbf{F}_t$  at time  $t$ , into its known part  $\mathbf{F}_n$  at an earlier time, say at time  $t_n$ , and the relative deformation gradient  $\mathbf{f}_t$  with respect to the configuration at that time:  $\mathbf{F}_t = \mathbf{f}_t \mathbf{F}_n$ . This gives rise to an intermediate configuration on which incremental constitutive relations for stresses and evolution equations for early-age creep can be well defined. Herein, a Lagrangian formulation is adopted: the chosen incremental constitutive relations are then pull-back from the known intermediate configuration toward the reference (initial) configuration. We have shown that the above kinematics is well suited for this transport procedure.

Modeling examples are proposed that are inspired from nowadays well-known models widely used in the literature, such like a Saint-Venant- and a compressible neoHooke-like models [5]. For early-age creep, the concept of internal variables is adopted the evolution of which is motivated by the generalized Maxwell rheological model [6]. The stress-like internal variables consist on over-stresses that have the same structure as the thermodynamically equilibrated second Piola-Kirchhoff stress tensor increments. So far, focus is made on purely mechanical aspects. Topics of thermo-hydric couplings, and more, will soon be addressed in future contributions.

For illustrative purposes, we consider the closed wall described in Fig. 1 and manufactured layer-by-layer, each layer with cross-section dimensions of 45 mm width and 10 mm height. In this example we consider low mechanical properties so as to trigger structural buckling. For symmetry reasons, only  $\frac{1}{4}$ -wall is considered for the finite element discretization with adequate boundary conditions. We show in Fig. 2 deformed configurations after 20, 25 and 30 layers. Here the wall is straight in the though-the-layers’ direction at least until 20 layers, then it starts to visibly deviate at around 25 layers. The computed wall after 30 layers shows the very large deformation meaning collapse in bending mode.



**Fig. 1.** Geometry of the closed wall: top view (left), and finite element discretization of  $\frac{1}{4}$ -wall with up to 30 layers (right).



**Fig. 2.** Top views of deformed configurations: after 20 layers (top left), 25 layers (top right), and 30 layers (bottom).

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# Virtual design laboratory for sustainable fiber reinforced concrete structures: From discrete fibers to structural optimization under uncertainty

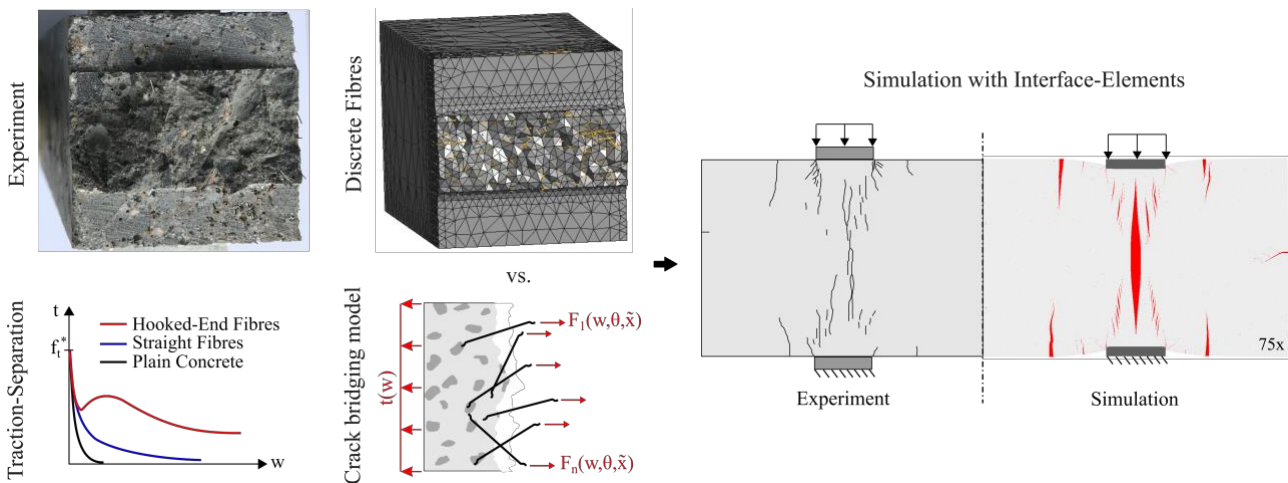
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**Keywords:** SFRC, Interface elements, Discrete crack models, Discrete fibers, Optimization, Uncertainty modeling; Reliability, Segmental tunnel lining.

With ever-rising environmental concerns, designing more sustainable concrete structures is vital. One approach is to improve the methods of designing structures with less material consumption. Steel Fiber Reinforced Concrete (SFRC) in conjunction with high-performance concrete (HPC) shows great potential for material savings, improved durability, and the creation of more slender structures. It is, however, still a challenge to simulate the behavior of such composite material accurately and reliably, especially under complicated loading conditions. In general, the post-cracking response of SFRC is affected by the size, shape, concentration, and orientation of the fibers. Within the frameworks of available guidelines, the residual strength of an SFRC is typically characterized by bending tests. Therefore, the properties mentioned above are not explicitly accounted for in the design [1], resulting in a loss of information regarding critical physical attributes during the structural design and requiring adjustments to the applied safety concept.

In this contribution, a multi-level model for the analysis of SFRC structures is used to assess the influence of a chosen fiber type, content, and orientation on the structural response [2]. Based on the exact fiber geometry, the interface conditions, the material properties, and assumed fiber orientation, a semi-analytical model is used to determine an equivalent uniaxial traction-separation law (Fig. 1, middle). In order to evaluate the post-cracking response of SFRC structures by Finite-Element (FE) analysis, a discrete crack approach using interface-elements [3,4], whose post-cracking behavior is governed by the derived traction-separation law, is used (Fig. 1, middle & right). A systematic validation campaign can be found in [5].



**Fig. 1.** Virtual design lab for fiber reinforced concrete structures. Left: Crack bridging behavior of SFRC based on discrete or semi-analytical models, Right: The multi-level modeling strategy allows assessing the influence of a chosen fiber type, content, and orientation up to the structural response.

The first aim of this work is to compare the crack bridging behavior predictions of a semi-analytical model [2] with a discrete fiber approach (Fig.1, top left). A finite element (FE) model in the context of the cohesive zone theory to model short-fiber-reinforced high-performance concretes is presented. To this end, concrete cracking and crack closure are modeled utilizing zero-thickness cohesive interface elements, and steel fibers are modeled individually via Bernoulli beam elements. Special attention is devoted to bond elements connecting steel fibers and concrete. The bond between fibers and concrete is modeled using an elastoplastic bond-slip law calibrated based on single fiber-pullout experiments.

Displacement-controlled crack opening tests and simulations using both approaches were performed on notched prismatic high-performance concrete specimens reinforced by short steel fibers (~1% vol.).

In the second part of the presentation, the prospects of applying complex FE models in conjunction with methods of optimization to design an SFRC tunnel lining segment are discussed. Nonlinear FE analysis requires special considerations regarding the employed safety concept, which influences the structural design. The objective of the optimization is to minimize the total segment thickness while a constraint ensures that the required safety factor is retained. In the case of a full probabilistic analysis, sensitive uncertain parameters such as the concrete strength and the fiber orientation are quantified by random variables and intervals. The optimized segment designs are discussed and compared to conventional designs. The contribution concludes, how advanced numerical models in conjunction with optimization algorithms may help in reducing material consumption, providing more cost-effective segmental lining designs with reduced environmental impact.

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# Modeling deterioration of RC structures due to extreme environmental conditions

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**Keywords:** Reinforced concrete, Corrosion, Freezing-thawing, Drying creep, Fracture, Simulation, Finite elements, Bridge.

## Introduction

Chloride-induced corrosion of steel reinforcement in concrete, deformations due to creep and shrinkage of concrete, freezing and thawing are some of the major causes for deterioration of reinforced concrete (RC) structures. RC structures exposed to aggressive environmental conditions, such as structures close to the sea or highway bridges and garages exposed to de-icing salts, very often exhibit damage due to corrosion. This damage is usually manifested in the form of cracking and spalling of concrete cover, caused by the expansion of corrosion products around the steel reinforcement bar. The pitting corrosion is even more severe, it is not visible and it can cause strong degradation of reinforcement performance. Furthermore, freezing and thawing causes damage and accelerate corrosion of reinforcement. Moreover, close related to deterioration due to corrosion is also time dependent deformation of concrete structures due to creep and shrinkage (e.g. drying creep). Therefore, to predict durability of RC structure it is important to have a reliable numerical tool, which is able to simulate these processes in order to better understand major phenomena and their consequences for the structural safety.

## 1 Chemo-Hygro-Thermo-Mechanical model

### 1.1 Theoretical background

To predict the rate of rust production and related effects, it is necessary to simulate the following physical, electrochemical and mechanical processes: (1) Transport of capillary water, oxygen and chloride through the concrete cover; (2) Immobilization of chloride in the concrete; (3) Crystallization and dissolution of free chloride as a consequence of drying and wetting of concrete as well as hysteretic property of concrete; (4) Transport of OH<sup>-</sup> ions through electrolyte in concrete pores; (5) Cathodic and anodic polarization; (6) Transport of corrosion products in concrete and cracks; (7) Creep and shrinkage of concrete; (8) Freezing and thawing of water in concrete with computation of water pore pressure and ice pressure and (9) Damage of concrete due to mechanical and non-mechanical actions. The recently developed coupled 3D chemo-hygro-thermo-mechanical (CHTM) model for concrete [1] [2] will be presented. The model is aimed to simulate the above mentioned complex non-mechanical and mechanical processes before and after depassivation of steel reinforcement.

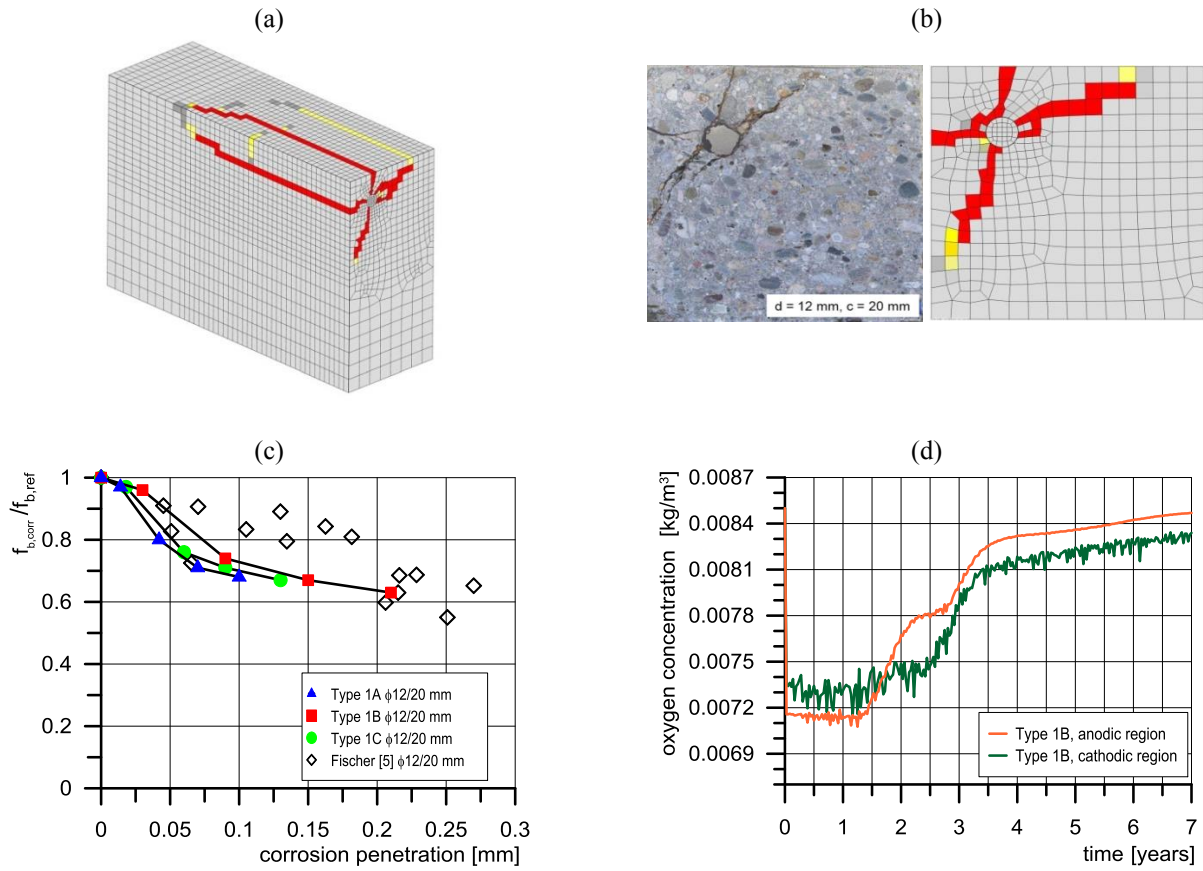
### 1.2 Case studies

The CHTM was implemented into a 3D FE code and its application and performance will be illustrated through several numerical examples. The differences between accelerated corrosion, usually used in the experimental tests, and natural corrosion will be pointed out. It will be demonstrated that the maximum entropy production related to the corrosion of steel reinforcement leads to maximum corrosion induced damage of concrete. Figure 1 illustrates an example of the application of the CHTM model on the study of the pull-out resistance of corroded reinforced bar from the beam-end specimen.

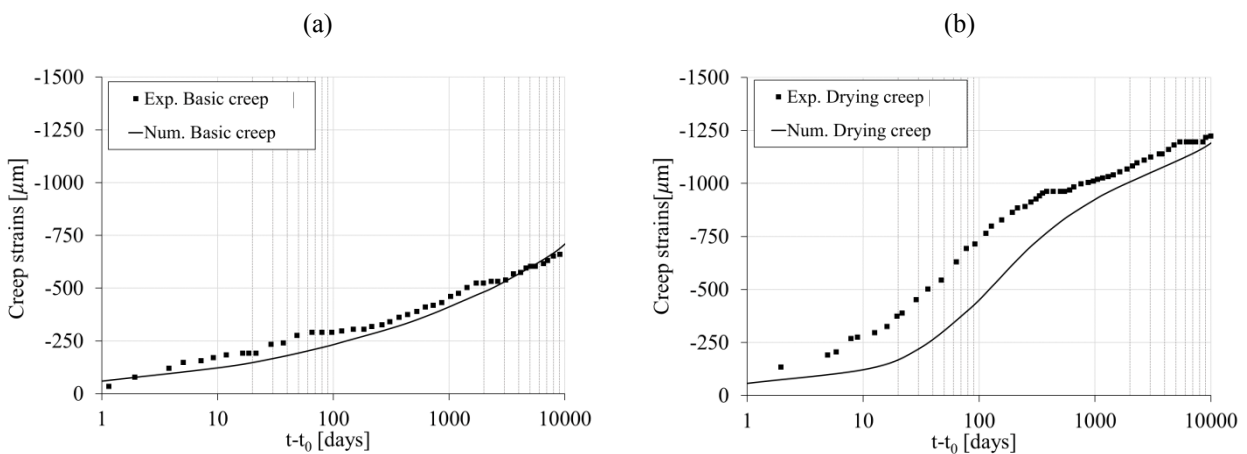
To demonstrate the effect of freezing and thawing, concrete specimen exposed to cyclic freezing-thawing cycles will be simulated. The distribution of pore water pressure and ice pressure will be calculated and resulting damage compared with the experimental data.

To investigate the interaction between damage and non-elastic strains in concrete (drying shrinkage and basic creep) the hygro-mechanical transient 3D FE analysis using two-phase meso-scale model will be performed on concrete cylinder loaded in compression and tension. It will be shown that as a consequence of concrete inhomogeneity there is a strong

interaction between drying shrinkage and damage of hardened cement past (mortar). This seems to be the major reason for drying creep and for the reduction of mechanical properties of concrete, especially in case of tension. In Fig. 2 is shown the model prediction and the test data for basic creep and drying creep. It is interesting to observe that the meso-scale model is able to nicely replicate the long-term experimental tests for drying creep without need for any additional viscos kind of mortar strains due to drying of cement paste.



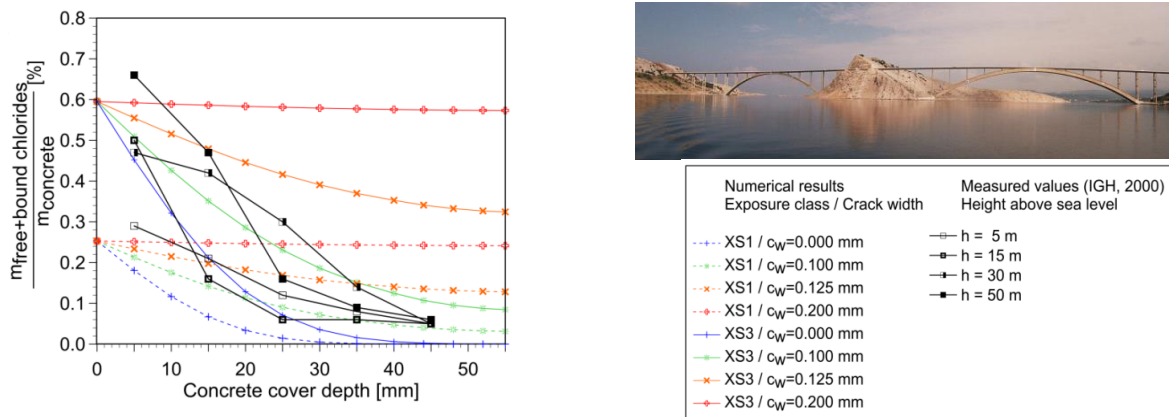
**Fig. 1.** Beam end specimen exposed to 7 years natural corrosion: (a) Crack pattern due to corrosion induced damage; (b) Crack pattern – experimental vs. numerical; (c) Reduction of the pull-out capacity due to corrosion induced damage and (d) Oxygen distribution at anodic and cathodic region after depassivation [2]



**Fig. 2.** Comparison between experimental tests (compression, stress 30% of compressive strength) [3] and two-phase meso-scale FE prediction for: (a) basic creep (creep factor  $\phi_{lin} = 4$ ) and (b) drying creep

## 2 Model prediction vs. measurement on the bridge structure

Although durability mechanics models have been significantly improved in the last four decades, their application on real-life structures is still a challenging task. For their reliable application the verification is required on a real structure accounting for different exposure time and micro-climate conditions.



**Fig. 3.** Total (free and bound) chlorides content in concrete after 20 years of sea exposure – comparison of the numerical results and results obtained on the pier P-20 of the Krk II Bridge at different heights and on surfaces towards South-West [4]

A brief overview of in-service performance of the Krk Bridge on the Croatian Adriatic coast (Fig. 3) [4] will be provided, where combination of aggressive maritime environment, inadequate durability design and poor construction quality has led to rapid deterioration of the structure caused by corrosion of steel reinforcement in concrete. Measured values of chloride content in concrete for different structural elements and micro-climate conditions after 14 and 20 years of exposure to sea (Fig. 3) are presented and discussed. Chloride content in concrete is compared with the results of numerical simulation of transport of chlorides through concrete cover using recently developed 3D CHTM model. The numerical results are in good agreement with the data measured on the bridge. This leads to the conclusion that the model is able to realistically predict service life of reinforced concrete structures exposed to chlorides and mechanical damages. It is shown that the micro-climate parameters, such as wind direction and speed, and cracks in concrete significantly affect the chloride content in concrete.

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# Deterioration mechanism of dam concrete caused by alkali-aggregate reaction: a numerical investigation based on meso-scale modeling

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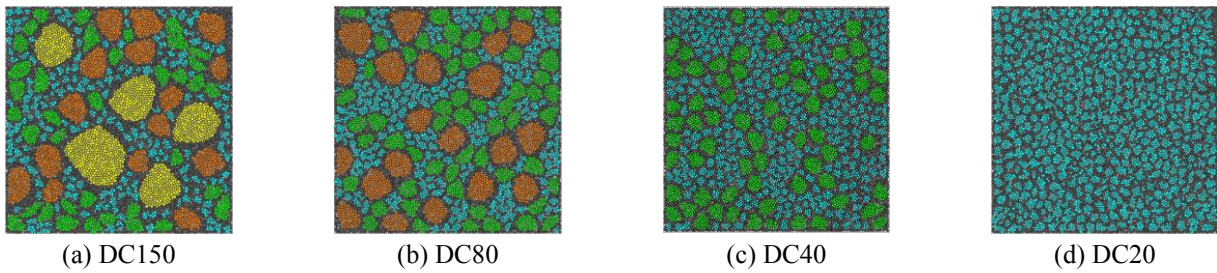
**Keywords:** Alkali-aggregate reaction, Dam concrete, Deterioration, Meso-scale modeling.

Alkali-aggregate reaction (AAR) is one of the main causes of deterioration of concrete, and it significantly reduces the durability of concrete structures. Hundreds of concrete dams have been suffering from AAR all over the world. The understanding in deterioration of mechanism of dam concrete due to AAR could help to mitigate AAR in the material preparation for concrete structures. Furthermore, it can also promote effective measures for rehabilitation and strengthening of existing AAR-affected concrete structures.

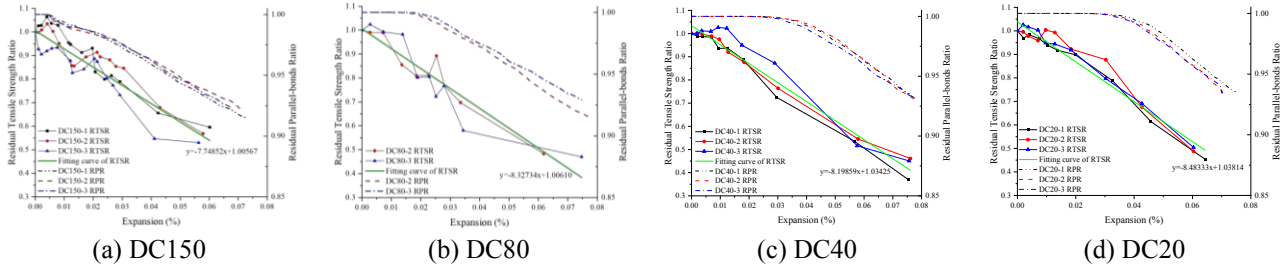
Aggregate size significantly affects the AAR process and deterioration of concrete. Pessimism effect methods based on fracture mechanics were proposed to explain the effect of aggregate size on AAR expansion [2, 3]. The pessimism size causes the maximum expansion of the test concrete, and the decrease or increase in aggregate size will result in decreasing levels of expansion [4-6]. Many studies have conducted to examine the degradation of mechanical properties of AAR-affected concrete. However, there is still a lack of a quantitative relationship between AAR expansion and the degradation of mechanical properties [1]. Moreover, these studies focused on fine aggregates with a diameter less than 25 mm, the findings may not be appropriate for the concrete with large aggregates, such as dam concrete containing aggregates up to 150 mm. The influence of aggregate size on deterioration of concrete due to AAR needs deeply understanding.

In this paper, a mesoscale particle model of concrete was presented to simulate the AAR process and mechanical testing of AAR-affected concrete. Four types of concrete with different sizes of coarse aggregates were considered. The experimental AAR expansion of dam concrete containing aggregates up to 150 mm was used to validate the mesoscale model. The numerical simulation results show that the coarse aggregate size significantly affects the AAR expansion and the degradation of mechanical properties. Dam concrete with 150 mm aggregates exhibits smaller expansion but earlier cracks than general concrete with small coarse aggregates. The degradation of tensile strength was evaluated in terms of the residual tensile strength ratio (RTSR), which was defined as the ratio of the tensile splitting strength of the AAR-affected specimen to the strength of the specimen without AAR. The decreasing trend is similar in the four types of concrete, and the RTSR approximately linearly decreases with an increase in AAR expansion. The splitting tensile strength is reduced more in concrete with larger aggregates at the same AAR expansion. This indicates that the maximum aggregate size significantly affects the AAR-induced degradation of mechanical properties. The traditional evaluation index based on general concrete, in which the aggregate size is smaller than 20 mm, is not approximate for dam concrete, and it would lead to the safety risk of the structures.





**Fig. 1.** Mesoscale particle model of concrete specimens with different gradations. DC150: concrete with maximum aggregate up to 150 mm; DC80: concrete with maximum aggregate up to 80 mm; DC40: concrete with maximum aggregate up to 40 mm; DC20: concrete with maximum aggregate up to 20 mm.



**Fig. 2.** Variation in the residual tensile strength ratio and residual parallel bond ratio with AAR expansion of the four types of concrete.

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# Development of a thermo-hydro-mechanical model of the containment vessel Vercors to study its aging and leak tightness, based on specimen tests and in situ measurements

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**Keywords:** Ageing phenomena in concrete structures, delayed strains, damage and cracking of reinforced and prestressed concrete structures, air transport in concrete.

## Purpose

An important function of a reactor containment vessel is to provide sufficient leakage tightness during normal operation and severe accident condition. The purpose of this paper is to present a set of numerical models along with a study methodology to understand the mechanisms most responsible for aging and leakage tightness degradation of prestressed reinforced concrete containment vessels without liner. The solution proposed here is adapted to the study of full-size buildings while most research work dealing with this matter offers sophisticated modeling techniques mostly suitable for local studies.

The methodology is applied to study the thermo-hydro-mechanical behavior of Vercors mock-up [1]. Vercors is an experimental mock-up of a reactor containment building at 1/3 scale (with diameter of 7.7 m, height of 20 m and thickness of 0.4 m) built at EDF Lab "Les Renardières" near Paris in 2015 to analyze the possibility of the life extensions of French Nuclear Power Plants. The mock-up is finely instrumented, and its behavior is monitored from the beginning of the construction. In the numerical application of our modelling methodology to Vercors mock-up the thermo-hydro-mechanical models are all calibrated by considering first the material test specimen and then the in-situ measurements to have a representative digital clone of the mock-up. All necessary models and resolution strategy are implemented in Code Aster® (EDF) finite elements program (Mozayan [4]).

## 1 Mechanical model

The computations of the thermo hydro mechanical model are partially coupled. First, thermo-hydric analyses are performed to determine the saturation degrees of concrete. Then, total strains are calculated, as the sum of elastic strains, thermal strains, desiccation shrinkage and clean and desiccation creeps. Creeps are represented by Burger constitutive law [5].

All the parameters of those behaviors are calibrated separately on the laboratory tests done on Vercors' concrete specimen and their values are discussed based on literature. Once a satisfying set of parameters is encountered, a global calculation on Vercors model is performed. Then, reduced models are extracted, and mechanical parameters are optimized so that they fit more to the in-situ measures. This allows to get an even more representative clone of the mockup, and a picture of the variability of the concrete within the building. Finally, the cracking state is calculated based on the strains, using Mazars 'model [2].

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## 2 Hydraulic model

In the methodology proposed by this work, the gas flow across concrete walls is classified in two parts. First, transport through the unsaturated sound concrete, micro-cracked concrete and reclosed cracks which is calculated by Darcy's law. The gas permeability in these different zones is defined by the hydric state of concrete (degree of saturation) and either intrinsic porosity or mechanical state (damage). Then, transport through open cracks is calculated with Poiseuille-flow equation, corrected by a coefficient proposed by Mivelaz [3], to consider the crack tortuosity depending on crack opening and concrete formulation.

The gas transfer equations are solved by analogy to non-linear heat equations. Flow parameters are estimated based on in situ measurement during pressurization tests. Various sensitivity studies have been performed to discuss the validity of the measures and their impact on the results.

## 3 Conclusions

A partially coupled thermo-hydro-mechanical model adapted to study the long-term behavior of large-scale structures is developed. Different parameters of the model are calibrated with the Vercors laboratory tests, and then optimized with in-situ measures. The reasonable computation time, the stability of the numerical model and the quality of results, which follow the in-situ measures of strains, global and local leakage, constitute the assets of this tool and methodology to perform industrial studies.

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# Modeling of the behavior of concrete specimens under uniaxial tensile stresses through the use of a 3D probabilistic semi-explicit model

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**Keywords:** numerical modeling, probabilistic cracking model, scale effects, uniaxial tensile test, finite element method.

In this article the numerical modeling of plain concrete specimens subjected to uniaxial tensile stresses is presented. The simulations are performed by using a three-dimensional macroscopic probabilistic model for semi-explicit concrete cracking. As it is well known, concrete structures are largely related to the scale effects phenomenon or, in other words, to the dependence of its global structural response to its size or volume. This phenomenon can be attributed, among other reasons, to the heterogeneous nature of the material, and it is extremely important when dealing with the modeling of the concrete cracking. Therefore, the model used herein, which is developed in the framework of the finite element method, takes into account the material heterogeneity by means of the assumption that each finite element represents a volume of heterogeneous material, with mechanical properties of tensile strength and fracture energy being randomly distributed over the mesh. These properties are distributed in the finite element mesh according to the Weibull and lognormal distributions, respectively. In the model formulation, the cracks are created within the concrete with different energy dissipation depending on the spatial distribution of the material constituents and initial defects, according to an isotropic damage law. Considering that a probabilistic model is used, the results are obtained through the use of Monte Carlo procedures, in order to obtain coherent statistical responses. In addition, with aim to develop a numerical model capable to perform 3D simulations in a viable computational time, a parallelization strategy is employed in the implementation of the Monte Carlo method using OpenMP. With the purpose of modeling the uniaxial tensile test and verifying the prediction of the scale effects, simulations of three prismatic plain concrete specimens with different sizes are performed.

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# The influence of autogenous shrinkage and creep on the risk of early age cracking

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**Keywords:** Early Age Cracking, Autogenous shrinkage, Creep, Concrete.

## Abstract

The study aims to investigate the mechanism of early-age cracks in different massive concrete structures (i.e. tunnels, bridge foundations and underground parking garages), with the objective of answering the following three specific questions:

- 1) How do the parameters of concrete proportion mix (e.g. w/c ratio, cementitious materials, aggregates, etc.) influence the formation of autogenous shrinkage and creep, especially at early age with the focus on the first 24 hours?
- 2) How to build theoretical and numerical model for the process of early-age crack formation and then quantify the damage status of concrete materials?
- 3) How to link the results derived from material scale to structural scale, and provide useful reference for practical engineering projects?

To study the basic mechanism a research program is performed in which different mixes are tested in a Temperature and Stress Testing Machine (TSTM). Since investigating the stresses that built up in the first hours after casting in such a TSTM is rather difficult, we designed a new version of the TSTM machine in which dogbone specimens are tested vertically in a Universal Testing Machine (Instron). The results indicate that the combined shrinkage (or expansion and the relaxation (or creep) during the first hours of hydration have a huge influence on the stresses that develop later and with that are important to determine the risk of cracking in massive concrete structures.

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# Relevance of behaviour laws of homogenized reinforced concrete in the context of finite elements of different sizes

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**Keywords:** Finite Element, phase fields, reinforced concrete, statistical scale effect, rebars sliding.

Despite the increase in computational power, the accurate modelling of crack openings in reinforced concrete remains an open problem for structural elements of complex shapes. Since the national CEOS.fr project dedicated to the control of cracking for large structures, it is accepted that the statistical scaling effect on the tensile strength of concrete and the realism of the concrete steel slip law are two essential ingredients to achieve a good level of accuracy in the prediction of crack spacing and openings. The implementation of these two aspects in finite element codes faces two problems: on the one hand, the statistical scaling effect depends on the dimension of the tensioned zone, which varies with cracking, and on the other hand, the steel-concrete slip is generally longer than the size of the finite elements. In this context, proposing homogenized reinforced concrete finite elements is problematic. The most common methods consist in using random mechanical property fields to integrate the statistical aspect of the tensile strength, and the slip is explicitly modelled by joint elements, preventing the use of homogenized elements. However, it is possible to avoid both random draws and explicit modelling of concrete-steel interfaces. The proposed method generalizes the notion of phase fields to address both problems simultaneously. A first phase field integrates the scale effect, and another one the steel-concrete slip. The FE code Castem (CEA) has been modified to allow such generalizations. After having given the theoretical bases of the methods used, we will illustrate their interest via a case study.

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# Design Optimization of Concrete Railway Tracks by Using Non-Linear Finite Element Analysis

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**Keywords:** Railway Track, Slab, FRC, Numerical model, Cracking, Design Optimisation

Between 2007 and 2014, UGE, Alstom and other industrial partners developed a new concept of railway track called New Ballastless Track (NBT). The concept was validated under 10 million fatigue cycles on a real-size mock-up at UGE. A first numerical study using a non-linear model was performed to evaluate the possibility of replacing the original reinforced concrete layer of the track slab with Steel Fibre Reinforced Concrete. The objective is to simplify the NBT track's construction and take advantage of the redistribution of mechanical stresses on a hyper-static structure. This study led to the conclusion that this replacement was very relevant.

This paper is on optimizing this Fibre Reinforced Concrete (FRC) solution by using the same non-linear numerical model. It is shown that this optimization procedure leads to a significant reduction of CO<sub>2</sub> emissions compared with the initial one. This document is a guide for MS Word users.

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# Numerical and Experimental Evaluation of Multi-Ion Kinetics Associated with Macro-Cell Corrosion by Pseudo-Concrete

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**Keywords:** Macro-cell Corrosion, Multi-ion Kinetics, Pseudo-Concrete, Pore Solution.

## 1 Introduction

As one of the deterioration factors of structural concrete, steel corrosion causes loss of reinforcement and cracking of concrete. Macro-cell corrosion is a typical steel corrosion which relates to not only the electric field but also the chemical substances of polarized metal and electrolytes such as concrete matrix. This study presents a numerical evaluation of the multi-ion kinetics induced by macro-cell corrosion as well as the experimental validation with pseudo-concrete electrolyte. In general, the ion profiles could be well explained by three dominant mechanisms: Nernst-Plank theory, chemical and electro-chemical reaction, and ionization. Specially for calcium ion which is a key species of cementing material, its distribution under macro-cell circuit is found closely relevant to the initial saturation of calcium hydroxide and supply of carbon dioxide. The framework of this paper follows the order of introduction, numerical platform and simulation, experiment with pseudo concrete, discussions, and conclusions.

## 2 Numerical Analysis

In this chapter, the numerical analysis will be introduced in details. To solve the coupled electrical and chemical fields, the governing theories including continuity equations (both ion and electron), Nernst-Plank-Poisson equations, polarization equations and geo-chemical equilibrium are calculated with overlapped elements methodology [1-3]. The smeared concrete-steel elements with shared DOFs allow the calculation of polarization in the 3D spatial domain instead of 2D interface, which has consistency with the 3D smeared crack models of structure for mechanical analysis [4]. Simulation is conducted on model with specific pore structure and pore solution by applying external charge. The corrosion location/magnitude as well as the ion concentration profiles are captured dynamically.

## 3 Experiment

In order to validate the numerical platform and to perform the parametric study, laboratory experiment is conducted with several types of pseudo concrete materials [3, 5]. Pseudo concrete has the advantages of measuring the ion-profiles dynamically without causing much damage to the electrolyte, which is different from the typical destructive measurement methods with concrete. In addition, the polarization products at both anode and cathode can be observed which show strong proof to verify the simulation results. From comparing the experimental data with simulation in terms of ion profiles of several species and corrosion products, the reliability of numerical platform is demonstrated.

## 4 Discussions

As a key novelty of current study, the profile of cation calcium ion with positive charge is found to gather around anode instead of cathode in certain occasions, which is unlike the common sense. In fact, the initial saturation of calcium hydroxide and the supply of carbon dioxide are proved to have huge impacts on the ion profiles of  $\text{Ca}^{2+}$ . Three conditions are generally categorized with different dominant mechanisms to explain the varying  $\text{Ca}^{2+}$  profiles, see Fig. 1.

## 5 Conclusions

Finally, some conclusions are drawn from the accomplished numerical and experimental studies.



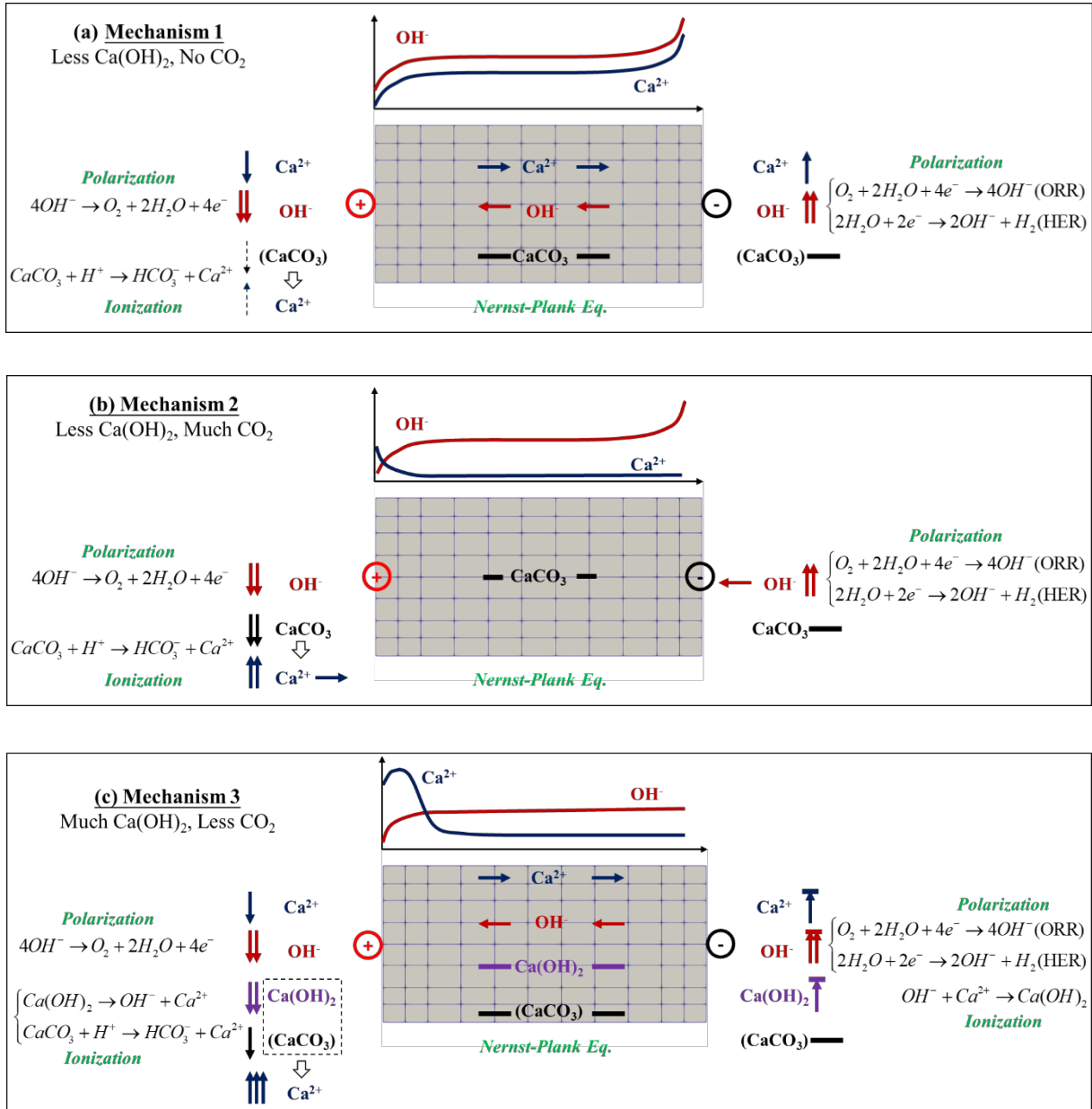


Fig. 1. Summary of the three governing mechanisms.

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# Discrete Models of Structural Concrete

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**Keywords:** Structural Concrete, Discrete Models, Fracture, Reinforcement.

## 1 Introduction

The cracking of structural concrete is a prime factor determining its safety and serviceability. The conditions that promote cracking are myriad, ranging from early-age phenomena (e.g., volumetric instabilities due to hygral and thermal actions [1,2]) to a variety of in-service loadings. Susceptibility to cracking is strongly related to concrete materials design and the methods of production. Computer modeling offers a precisely controlled environment for investigating such relationships between material composition and structural performance, accounting for the relevant mechanical and environmental boundary conditions. Such modeling complements the knowledge acquired through laboratory testing and monitoring of field performance. Via computational modeling, variations in the material composition, production processes, and exposure conditions (as well as the effects of such variations on life-cycle behavior) can be simulated for large intervals on the length and time scales.

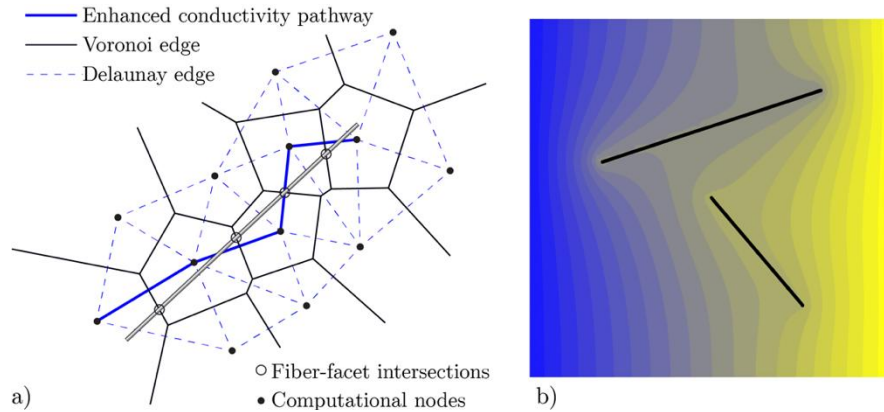
The choice of model depends on the nature of the problem and objectives of analysis. The literature covers an array of approaches to modeling structural concrete, each with its strengths and weaknesses. According to one classification scheme [3], models are based on either discrete or continuum representations of the relevant field variables (e.g., capillary pressure, temperature or displacement). In the former class, the field variable is typically represented along primitive 1D elements that compose the model (i.e., the field variable is not continuously represented within the model domain). Compared to continuum models, the discrete approaches often rely on simpler formulations. Furthermore, the representation of local behavior via 1D elements readily accommodates cracking and other types of displacement discontinuity. Such capabilities are advantageous for life-cycle analyses, where accurate estimations of crack opening and spacing are central to the durability mechanics of structural concrete.

## 2 Methodology

Within the community of developers of discrete models, there are two main veins of thought [3]: 1) the discrete nature of the model (in terms of the 1D elements that interconnect on nodal sites) represents physical features of the material; or 2) the discretization strategy should not have a dominant influence on the analysis results. Advo-

cates of the first vein of thought can argue, with some merit, that the discrete approaches effectively capture the effects of large-scale heterogeneity of concrete. From another viewpoint, however, it is attractive for the models to retain selected qualities of the continuum approaches including, for example, elastic homogeneity under uniform straining.

The research presented herein resides in the second vein. One goal is to provide an unbiased framework without artificial heterogeneity, such that the presence of actual heterogeneity (in the form of phase fractions, interfaces, reinforcing bars, short fibers, etc.) can be explicitly represented. Discrete modeling approaches can also be used to simulate transport processes and their coupling with mechanical behavior [4]. By providing unbiased frameworks for both the mechanical and potential field analyses, the effects of various forms of reinforcement can be precisely analyzed. Considering potential flow through a fiber composite material, for example, the individual and combined effects of conductive fibers can be simulated [5], as shown in Fig. 1. Analogous results will be presented for the response of structural concrete to mechanical loading, where an accurate modeling of the Poisson effect is found to be essential.



**Fig. 1.** a) Semi-discrete modeling of fiber contributions to composite conductivity; b) contours of nodal potential local to conductive fibers [5].

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# A Three-Dimensional Coupled Probabilistic Lattice Model Approach to Corrosion Induced Crack Modelling in Reinforced Concrete to Optimize for Sustainability

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**Keywords:** Concrete, Lattice Model, FEM, Sustainability, Corrosion.

## 1 Abstract

Cement production contributes to 10% of all carbon dioxide emissions and 6% of all greenhouse gas emissions [1]. The primary use for cement is as a binder for concrete, which is used to construct infrastructure and construction projects globally. Alternative binders for concrete are an active area of research. However, concrete is predicted to be a predominant building material for the foreseeable future due to its cheap cost and easy accessibility [1]. Therefore, to minimize cement-related carbon emissions, global concrete use needs to be minimized.

To optimize the use of concrete in infrastructure, the deterioration of reinforced concrete must be well understood [2]. Corrosion-induced cracking is an important deterioration mechanism of reinforced concrete. Current methods to model corrosion-induced damage of reinforced concrete in industry consider a structure to be at end of life when corrosion is initiated [3]. However, in practice, corrosion is allowed to continue, and cracking is often observed before repairs are made. Additionally, current models only consider uniform corrosion, rather than nonuniform corrosion, which is what is typically observed in practice due to varying exposure conditions. Nonuniform corrosion has been shown to cause accelerated crack propagation; therefore, it must be considered when modelling deterioration of reinforced concrete [4]. This research introduces a new method to model corrosion induced cracking in reinforced concrete using a three-dimensional, coupled, probabilistic lattice model.

To create this three-dimensional, coupled, probabilistic lattice model, the two-dimensional, probabilistic lattice model approach proposed by Michel et. al. is adapted [5]. This method creates a random field of points within uniform grid cells, connects the points using basic finite element modelling meshing tools, then separates the elements into two-node, bar elements, and analyzes the mesh as a truss. The mesh is analyzed by applying the corrosion stress in load steps and removing the element with the largest stress to simulate cracking. The mesh is analyzed as a truss rather than typical triangular elements to capture the quasi-brittle nature of concrete. This method is modified to consider three dimensions, allowing for the consideration of the effect of nonuniform corrosion along the axis of the reinforcement. Additionally, the model introduced in this research uses real corrosion patterns by coupling the corrosion induced cracking model with the corrosion model introduced by Wu and Lepech [5]. Wu and Lepech's model allows for environmental exposure data as an input, and outputs a reinforcement corrosion pattern. By coupling this model with the three-dimensional, probabilistic lattice model, only environmental exposure data must be known to determine the extent of cracking in a concrete structure.

To validate the lattice model, the results are compared to experimental results published by Jiang et al. [7]. The results from Jiang et al. are a time series of three-dimensional x-ray CT-scans of the nonuniform corrosion pattern as well as the crack pattern at each time step. Since this experiment is nondestructive and on a single sample, less uncertainty is introduced between time steps. The nonuniform corrosion patterns are used as an input to the lattice model, and the model outputs a plot of crack depth into the concrete matrix, which are then validated using crack patterns obtained from experimental results. Results indicate good agreement between experimental observations and lattice model computational predictions.

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# Modeling C-S-H sorption at the molecular scale: effective interactions, stability and cavitation

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**Keywords:** C-S-H, Adsorption, Grand canonical Monte Carlo simulations, Molecular dynamics, Disjoining pressure, Hydration states.

Calcium silicate hydrate (C-S-H) is the main product of ordinary Portland cement hydration, being the main phase responsible for the mechanical behavior and durability of cement-based materials. C-S-H is the percolating phase that binds the inclusion-like phases (calcium hydroxide, ettringite, AFm, cement particles and even capillary porosity) present in cement systems. Fundamental understanding of C-S-H structure and its behavior is very important since it can reveal the physical origins of the thermomechanical behavior of cement-based materials and provide a methodology to improve the performance of these materials. Unfortunately, knowledge on the structure and the characteristics of C-S-H is still limited by the fact that the structure of C-S-H is very complex due, for instance, to the variable chemical composition (with respect to Ca/Si ratio) [1], possible co-existence of crystalline and glassy phases [2], and multiscale pore size [1].

C-S-H mentioned above, presents a layered structure with nanometer size pores filled with water and ions. It is well known that the properties and the dynamics of water confined in C-S-H interlayer pores differ from the properties and the dynamics of water in larger pores (gel pores for example) [3], in which both differ from bulk water properties and dynamics. Note that, the behavior of confined water molecules in C-S-H has a great influence on various physical and chemical properties of C-S-H gel, which further determine the macroscale behavior of cement-based materials such as creep, shrinkage, cracking and reactivity [4].

Here, we perform Grand Canonical Monte Carlo simulations combined with molecular dynamics to study water sorption and to investigate the stability of nanoconfined water in C-S-H nanopores. For this purpose, we have used Kunhi Mohammed et al. [1] atomistic C-S-H model with Clay-FF interatomic potential [5] to model the interactions between atoms in C-S-H structure. Properties including the confining pressures, sorption isotherms, potential of mean force (PMF), equilibrium basal spacings, meta-stable domains, elastic modulus perpendicular to the pore surface and cavitation of nanoconfined water are analyzed. We evaluate all these properties as a function of basal spacing at various relative humidities ranging from (liquid) saturated (RH=100%) to completely dried (RH=0%) conditions for ambient temperature (300 K). From the PMF profiles, we can identify equilibrium basal spacings as well as meta-stable domains resulting from the transition between hydration states. These meta-stable domains can help understanding the hysteresis observed in water sorption isotherms for cement based materials [6]. We also observe that each relative humidity value is associated with a stable basal spacing and that when we decrease the relative humidity, drying shrinkage of C-S-H layers occurs. All these properties can be useful to explain the physical origins of the thermomechanical behavior of cement-based materials.

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# Numerical and experimental investigation of wall effect in concrete

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**Keywords:** Durability, wall effect, concrete drying, aggregates distribution, transport properties, mechanical properties, ...

One of the main advantages of using concrete is that the material in its fresh state can be poured into formworks and assume the most variable shapes. Nevertheless, the casting is not without effect on concrete. The formwork perturbs the arrangement of aggregates; this effect is known as ‘the wall effect’ and it is generally neglected in both experiments and numerical calculations. So far, there is no validated method to quantify the gradation of transport and mechanical properties induced by the wall effect. The manifestation of the wall effects can be decomposed on the contributions of (i) the particle size distribution per se; and (ii) the interactions with the environment such as drying (which may induce cracks because of drying shrinkage gradient and strain incompatibility between cement paste and aggregates), hydration slows down (due to rapid water evaporation on exposed surfaces), and carbonation in long-term. Altogether, these aspects lead to changes in the properties of a superficial layer, and these changes can be relevant to some applications of cement-based materials and concrete structures potentially affecting their performances.

This study presents a new numerical approach using tools developed to perform a molecular simulation to simulate the wall effect on aggregates and mortar distribution in concrete. Aggregates are represented by spheres interacting via a generalised Lennard-Jones potential (which approximates a hard-sphere potential). This approach allows obtaining the particle profiles according to the reference frame of interest (e.g. the confined directions). The particle-based distributions are transformed into continuum profiles of volume fractions using a convolution. The method is first validated against theoretical data from the literature on monodisperse confined hard spheres. Then, we extend the study to the polydisperse case to model aggregates in concrete using real granulometry. Based on volume fraction profiles, transport or mechanical properties are estimated by the Mori-Tanaka scheme from classical homogenization. This study shows an important interference in both mortar and aggregate distribution in the very first millimetres. When mortar fraction is larger, it is expected a higher porosity, water content, and higher transport properties which means higher drying kinetics and durability issues regarding CO<sub>2</sub> and chloride migration, for instance. An application is tested later on real concrete formula. Results are compared to experimental work. The wall effect on concrete drying is being also investigated by mass loss monitoring. The skin effect on mechanical properties is also evaluated by conducting 3-point bending tests and the irregularity of the surface (poured and non-poured surfaces) is quantified.

The numerical method could be generalised and used for other applications. Perspectives of this study include accounting for aggregate shapes closer to the real ones, and the effect on concrete drying when the wall effect induced gradation is considered on transfer properties.



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