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Multi-scale and multi-physics deterioration modelling for design and assessment of reinforced concrete structures

Mette R. Geiker[a*], Alexander Michel[b], Michel D. Lepech[c], Jie Wu[c], Henrik Stang[b]

[a] Norwegian University of Science and Technology, Department of Structural Engineering, NO-7491 Trondheim, Norway
[b] Technical University of Denmark, Department of Civil Engineering, Brovej, Building 118, DK-2800 Kgs. Lyngby, Denmark
[c] Stanford University, Department of Civil and Environmental Engineering, 473 Via Ortega, Room 314, Stanford, CA 94305

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Abstract

This paper discusses the need for reliable and valid multi-scale and multi-physics prediction models to support the design of new as well as the assessment, maintenance, and repair of existing reinforced concrete structures.
A multi-physics and multi-scale deterioration model for chloride-induced corrosion of reinforced concrete has been established. Ongoing work includes extension of the model to 3D as well as modelling of the impact of the steel-concrete interface characteristics and electrochemical potential on chloride thresholds.
Identified challenges include, among others, the improved understanding and modelling of single- and multi-deterioration mechanisms, environmental exposure, and data for validation.
We envision that next generation maintenance and management of reinforced concrete infrastructure will combine numerical simulations based on multi-scale and multi-physics principles and extensive in-situ monitoring, allowing continuous Bayesian updating of 4D simulations of functional performance.

Keywords: Concrete; Reinforcement corrosion; Multi-scale; Multi-physics

1 Introduction

A well-functioning civil infrastructure form the foundation for quality of life for our society and enable global development and progress. This importance is reflected in the significant investments made annually to our civil infrastructure. In 2016, McKinsey and Company estimated that US$3.3 trillion should be invested globally in infrastructure each year in order to support current growth rates [1]. This annual investment globally is approximately equal to the Gross Domestic Production of Germany (US$3.4 trillion), the world's fourth largest economy [2].

At the same time, several challenges are related to the establishment and maintenance of the infrastructure covering, among others, aspects of sustainability, from environmental impacts over economy to societal impacts as well as climate change calling for reassessment and climate adaptation of existing structures.

Parametric design is seen as a promising approach and it has been found that defined targets facilitate design optimization [3]. However, parametric design requires reliable and valid models and data. These models need to be mechanism based and multi-scale to allow for the use of innovative materials and structural solutions without long-term performance records. Moreover, structural and residual service life assessment of existing structures also requires reliable and valid models and data - similarly to the design of new structures.

Today's infrastructure is to a large extent built from reinforced concrete and there are no expectations that reinforced concrete will play a less important role in the future. However, it is expected that e.g. the type of binders used will increasingly change to low-clinker blends with alternative supplementary materials [4], and depletion of natural sand resources will necessitate the use of local crush aggregates and fines. In addition, increasing use of alternative reinforcement materials and systems is foreseen. Finally, requirements to circular materials economy will enforce recycling at highest level of structures, structural elements, and materials. These changes call for generic mechanism based models to allow for design optimization and later structural assessment of existing structures.

* Corresponding author: Mette R. Geiker, E-mail: mette.geiker@ntnu.no

Initiated by the European projected Duracrete [5] probabilistic performance based service life models for reinforced concrete were introduced in the *fib* Model Code for Service Life Design [6], a decade ago, and subsequently in the *fib* Model Code 2010 [7] and the ISO Standard 16204 [8]. However, as stated in [9] the current service life models and available input parameters are based on several assumptions, and further understanding of mechanisms, model development, and data collection are necessary to improve the reliability and validity of performance prediction. For example, improved modelling of initiation of chloride-induced corrosion in saturated conditions calls for, among others, understanding, and quantification of the time dependency of the surface concentration and chloride diffusion coefficient, the factors causing de-passivation of the reinforcement, and the impact of cracks. For other exposure conditions, modelling and quantification of the environmental exposure becomes an additional important issue. In addition, general international consensus has only been reached for time dependent models for some deterioration mechanisms at the materials level, and only when acting alone.

More importantly, the *fib* Model Code for Service Life Design [6] and the ISO Standard 16204 [8] provide models for prediction of materials performance. They do not support assessment at the structural level of deteriorated structures.

In summary, we see a need for the further development of multi-scale and multi-physics deterioration modelling of reinforced concrete to facilitate design optimization and assessment of reinforced concrete structures. In this context, it should be mentioned that the merger of material science with structural engineering has been suggested earlier, see e.g. [10-14], and that two commercially used models, DuCOM [15, 16] and STADIUM® [17], are based on multi-physics principles.

Reinforced concrete is in most environments a durable construction material. However, both deterioration of the concrete itself and corrosion of the steel reinforcement take place, reinforcement corrosion being by far the main cause of required maintenance and repair investments. Thus, as an example, this paper focusses on prediction of the performance of structures affected by reinforcement corrosion with focus on benefits of using multi-scale and multi-physics based models. The arguments are illustrated using own work.

2 Multi-scale and multi-physics modelling of reinforcement corrosion

To quantify the structural performance of reinforced concrete elements affected by chloride-induced reinforcement corrosion, a multi-physics and multi-scale model is being developed. Presently, the model includes coupled physical, chemical, electrochemical, and fracture-mechanical phenomena at the material level, which are further coupled with mechanical deterioration models at the structural/component level. [18] Selected features of the multi-physics and multi-scale model are briefly presented in the following; including the impact of exposure conditions on chloride ingress, impact of cracks on moisture ingress, and influence of cracks on the initiation of reinforcement corrosion.

2.1 Impact of exposure on predicted chloride ingress

Flint et al. [19] investigated the importance of exposure data, i.e. temperature and relative humidity, on chloride ingress modelling. Results of the study are presented in Fig. 1, illustrating predictions of chloride concentrations at a depth of 30 mm using either detailed meteorological data with a 3 h interval or averaged seasonal data (for further details on data averaging, see [19]). Modelling results indicate that the use of averaged seasonal data as boundary conditions leads to reduced predicted ingress rates compared to the detailed meteorological data. This may be explained by the impact of occasional high moisture contents being neglected (smoothed out) when using averaged seasonal data.

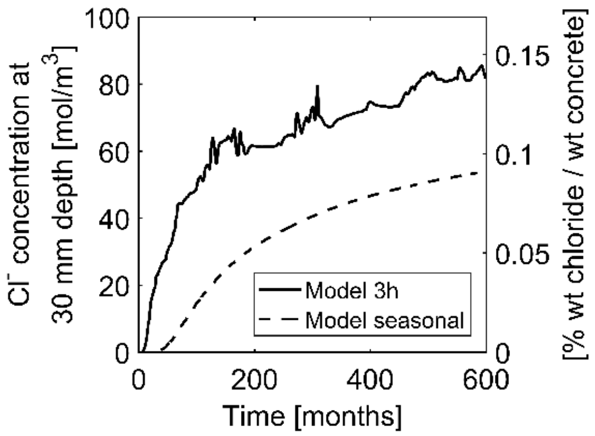

Figure 1. Prediction of chloride concentration at 30 mm depth over 50 years using a coupled heat and mass transport model applying detailed meteorological data (per 3 h) or averaged seasonal data. After [19].

2.2 Impact of multi-ion transport on chloride ingress

Marine exposure of concrete causes elemental zonation [20] and may lead in some concretes to substantial leaching [21]. Leaching affects the binding capacity and chloride ingress rate of the cement paste. Moreover, leaching will also affect the pH of the pore solution and thus the chloride threshold for corrosion initiation. Changes in the pore solution composition can be modelled, among others, coupling mass transport as dependent upon conduction due to heat, concentration gradients, and moisture gradients with mass balance models, see e.g. [22-24]. The predicted development of chloride and hydroxyl ion concentration is illustrated in Fig. 2a, while the $[Cl^-]/[OH^-]$ is given in Fig. 2b. Results are presented for a concrete (ordinary Portland cement (94 %) and silica fume (6 %)) assuming a water-to-binder ratio of 0.4 and using updated experimentally based coefficients for chloride binding. For the present case, the predicted depth of depletion in hydroxyl ion concentration is comparable to the depth of chloride ingress. This calls for reassessment of the chloride threshold for corrosion initiation.

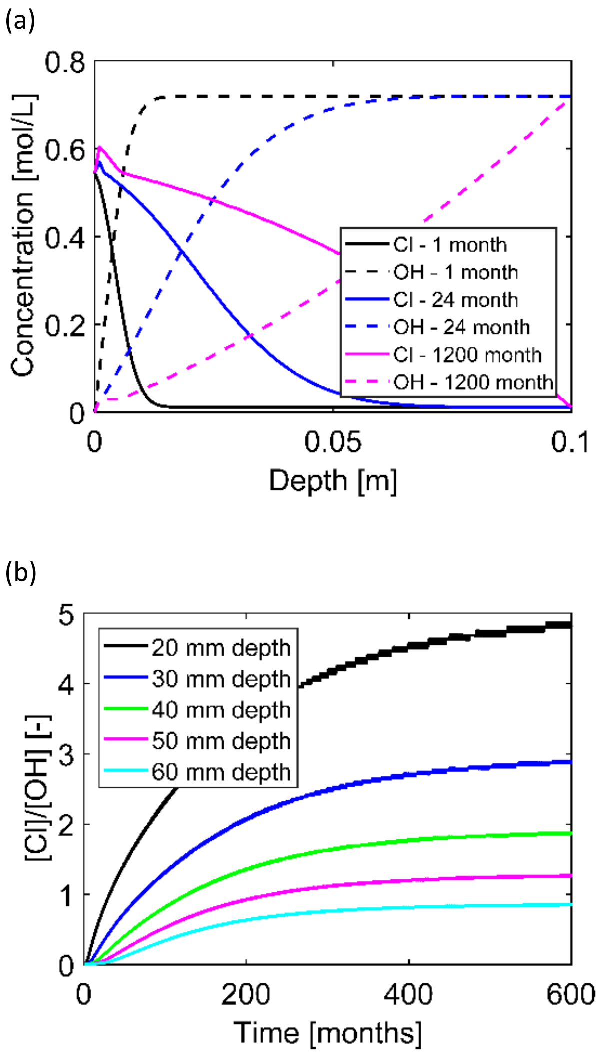

Figure 2. Predicted (a) chloride ion (Cl^-) and hydroxyl (OH^-) ion concentration as a function of depth from exposed surface after 1, 24 and 1200 month marine exposure, and (b) $[Cl^-]/[OH^-]$ in pore solution for selected depths over time.

2.3 Cracks and ingress

Studies concerning the impact of cracks on moisture ingress in cement-based materials have generally concluded that cracks facilitate rapid ingress of moisture, see e.g. [25-28] as well as aggressive substances, such as carbon dioxide and chlorides, see e.g. [29].

Among others, Pease [30] investigated the short-term impact of cracks on the ingress of liquid water in partially saturated wedge split test (WST) specimens by means of x-ray attenuation measurements, see also [31, 32]. The applicability of the multi-physics model to simulate the moisture ingress in loaded/cracked WST specimens is illustrated in Fig. 3 comparing experimental observations and numerical predictions. Results of numerical simulations for WST specimens with different load levels and CMOD clearly show that moisture ingress occurs more rapidly, see Fig. 4. In particular, increase in moisture ingress in the y-direction (vertical direction) is observed for peak load and cracked WST specimens compared to specimens with 70 % and 90 % of peak load. Furthermore, numerical results indicate that the lateral ingress, however, appears to be unaffected by loading/cracking of the WST specimens.

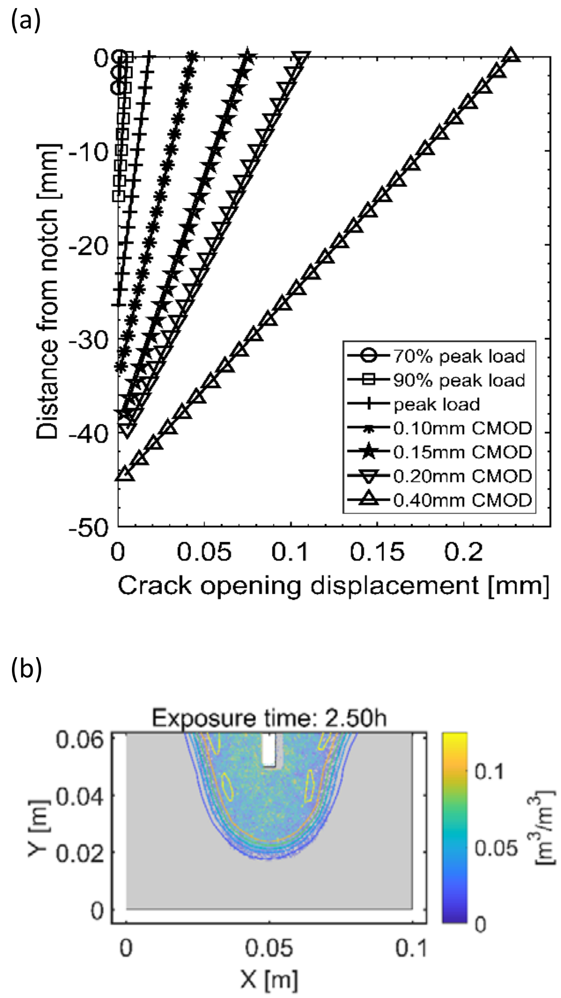

Figure 3. (a) Estimated crack profiles using cracked hinge model [33-35] for WST specimens investigated in [30] and (b) experimental and modelled ingress results for 0.1 mm CMOD WST specimen after exposure to liquid water. Please note: color bar indicates (measured and modelled) moisture content in m^3/m^3. After [31].

2.4 Cracks and corrosion

Numerous investigations on the impact of cracks on the ingress of corrosion initiating substances and reinforcement corrosion have generally concluded that cracks facilitate rapid ingress and subsequently reduce the time to corrosion initiation, see e.g. recent reviews [30, 36, 37] and references therein.

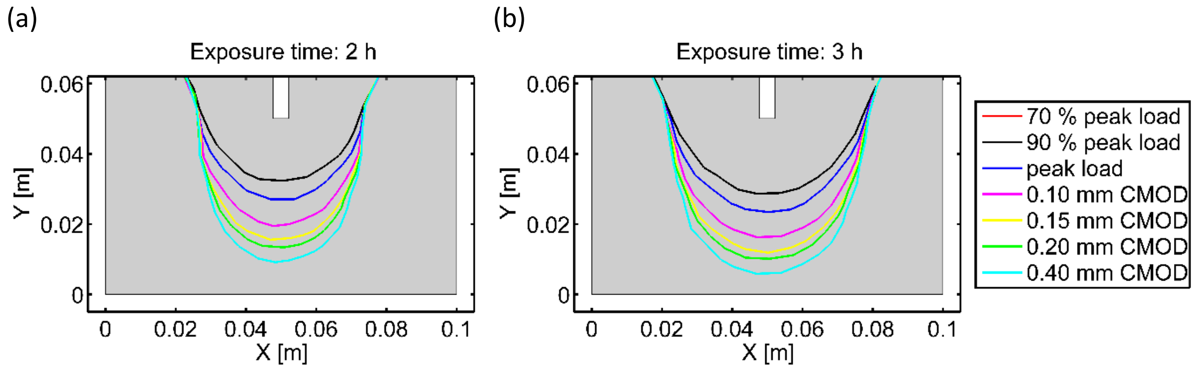

Figure 4. Numerical predictions of extend of moisture ingress for loaded/cracked WST specimens at selected times after exposure to liquid water. Estimated crack lengths can be deduced from Fig. 3a as the distance from notch to where COD=0. After [31].

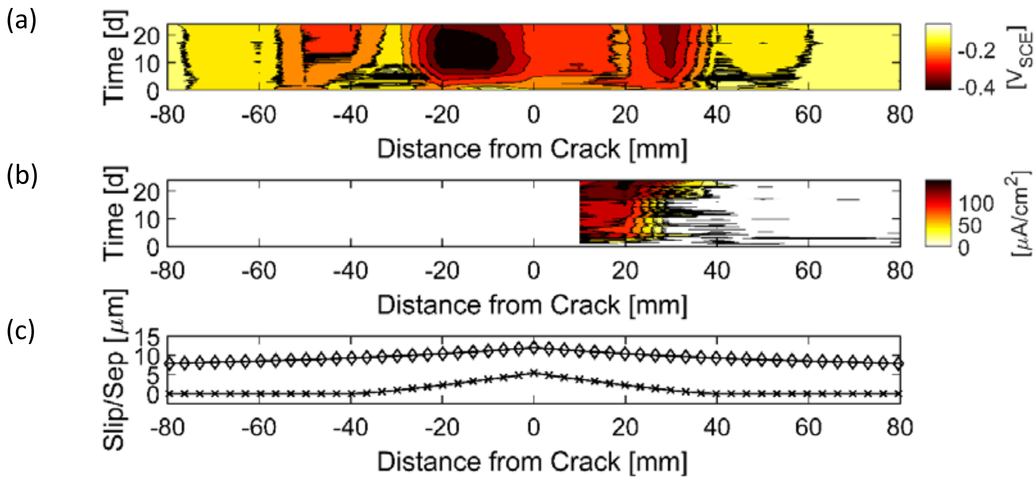

Figure 5. Location and time-dependent (a) open circuit potential, (b) corrosion current density (bottom), and (c) interfacial damage for specimen with crack width of 0.07 mm. After [39].

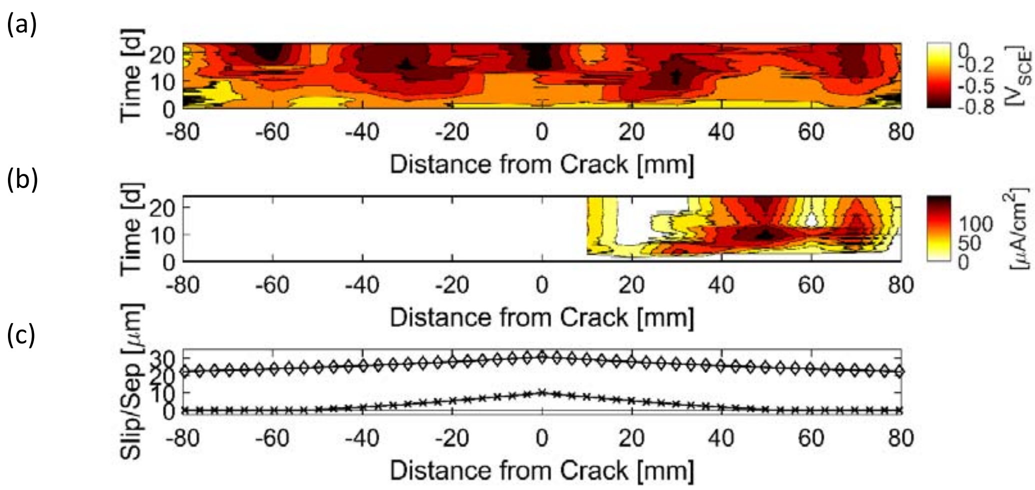

Figure 6. Location and time-dependent (a) open circuit potential, (b) corrosion current density (bottom), and (c) interfacial damage for specimen with crack width of 0.14 mm. After [39].

The effect of cracks on the time to corrosion initiation was investigated, among others, by Pease et al. [38] and Michel et al. [39] using so-called instrumented rebars. They investigated the relation between macroscopic damage at the concrete-steel interface and corrosion initiation of reinforcement embedded in plain and fiber reinforced concrete. Comparisons of experimental and numerical results are given in Figs. 5 and 6 for fiber reinforced concrete beams. The results presented include predicted interfacial damage, i.e. slip and separation, along the reinforcement, open circuit potential (OCP) measurements in a region between -80 mm and 80 mm, and macrocell current density measurements between 10 mm and 80 mm from the main bending crack. Comparisons between the extent of interfacial damage, in particular the separation between concrete and reinforcement, correlate very well with the extent of measured active corrosion, indicating a strong correlation between corrosion initiation and interfacial condition. Both, electrochemically measured active corrosion and simulated separation are seen in a region between -70 mm and 70 mm from the main transverse crack.

3 Ongoing work

Ongoing work includes a) extension of the model to 3D modelling, b) integration with BIM to help with design and management of structures, and c) improved modelling of mechanism, e.g. the modelling of the impact of the steel/concrete interface characteristics and electrochemical potential on chloride thresholds.

3.1 3D modelling of structural performance and integration with BIM

A central goal of the ongoing modelling efforts is to enable realistic 3D simulations of corrosion-induced deterioration of reinforced concrete elements. This includes the description of phenomena that are not accurately represented by 2D simulations, e.g. location and interaction of anodic and cathodic sites during corrosion in a structural member as well as the quantification of the impact of current design decisions. Integrating the multi-scale and multi-physics deterioration model with BIM will not only assist in design but also the planning of inspection, maintenance, and repair. The architecture of the multi-physics and multi-scale model to predict and assess the deterioration of reinforced concrete structures in an interactive framework using a customized plug-in to connect to BIM GUI is illustrated in Fig. 7.

Within the framework [18], the deterioration analysis in the backend is carried out in Matlab®, at the same time a customized plug-in is providing a user interface to allow for communication between Autodesk's^{TM} Revit® building information modelling (BIM) software suite and Matlab®. This plug-in allows users to import a complete 3D building information model (BIM Level of Development 400) of a reinforced concrete element that has been created by an engineer, steel fabricator, or other design team member. The plug-in automatically preserves all BIM geometries (i.e., element dimensions, reinforcement details and locations, reinforcement connectivity) in a Matlab® matrix format that is readable by other finite element codes, such as COMSOL Multiphysics® software, for computational modelling of transport, phase changes, corrosion evolution, and damage propagation. The plug-in is also capable of exporting the results of deterioration modelling back into a Revit® BIM model using colour changes or element shading.

To improve computational efficiency and allow for parallel processing, the model for coupled transport of heat and matter and phase changes in the cementitious material is run in Matlab®, while the corrosion model, based on physical laws describing thermodynamics and kinetics of electrochemical processes at the reinforcement surface, is run in COMSOL Multiphysics® software. Corrosion-induced damage is modelled utilizing a coupled lattice and finite element method (FEM) modelling approach within Matlab®.

3.2 Chloride thresholds

Previously, the chloride thresholds for corrosion initiation has been described by a uniform random distribution along the rebar [18]. However, as described by Angst et al. [10] the susceptibility to corrosion varies over the steel surface due to variations in metallurgic and other interface properties. Based on this, they suggested to conceptually consider the chloride threshold as a variable over the length of a rebar. Multi-variate uniform random distributions allow for more realistic elaboration on the potential impact of systematic (e.g. bleeding at the downward side of the rebar) and random characteristics at the steel/concrete interface (SCI). To model chloride thresholds using a multi-variate distribution, the rebar is divided into geometric sections along its length and into four different parts around its circumference. In this way, the chloride thresholds for the top faces of the rebar can be different from the bottom faces of the rebar. All variables are correlated using a matrix, which is a function of distance between each geometric section. Fig. 8 illustrates the impact of assuming a uniform random distribution of chloride threshold along a rebar length versus a multi-variate uniform random distribution.

Future improvements are expected possible based on ongoing work in the technical committee RILEM TC 262-SCI, which recently submitted a state-of-the-art paper on the occurrence of local characteristics at the SCI and their physical and chemical properties [41].

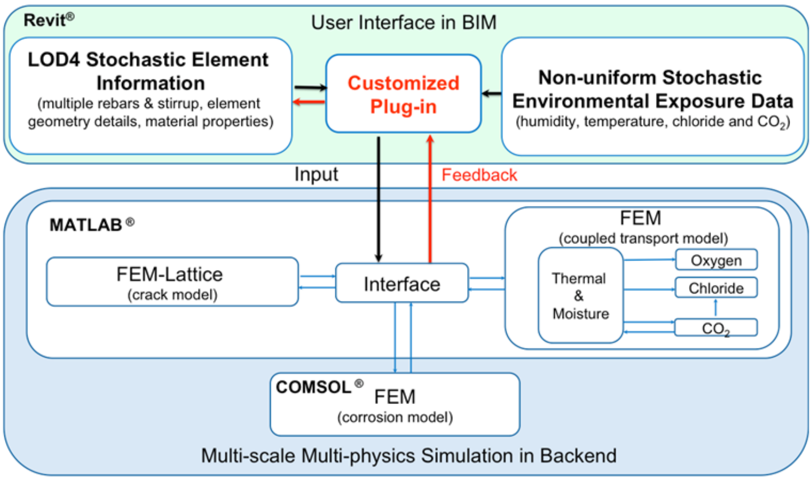

Figure 7. Architecture of the multi-physics and multi-scale model to predict and assess the deterioration of reinforced concrete structures in an interactive framework using a customized plug-in to connect the deterioration model to a user-friendly building information modelling (BIM) interface [40].

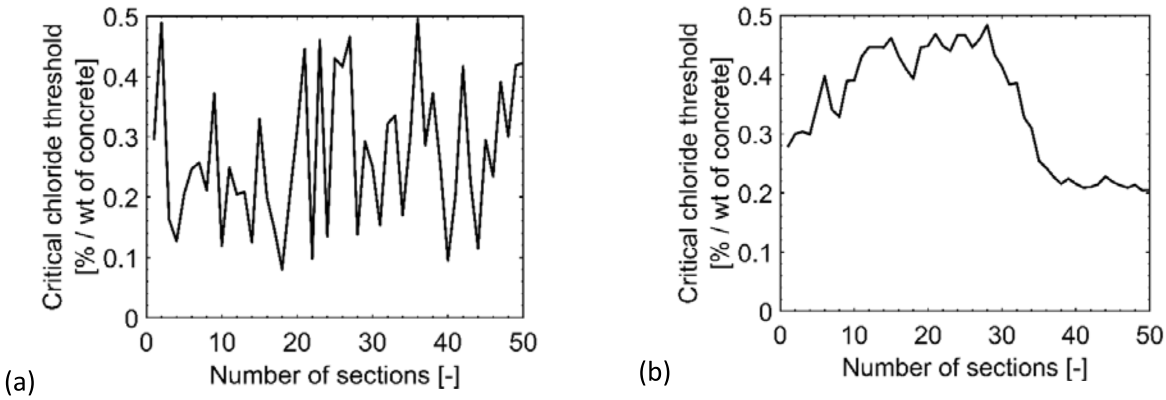

Figure 8. Distribution of initial chloride threshold values along the length of a single rebar. (a) using a random distribution, and (b) using a more realistic, multi-variate uniform random distribution.

Their ongoing work concentrates on the influence of these local characteristics on corrosion initiation. When available the results will be incorporated into the modelling work, both to modify the multi-variate uniform random distribution and to provide statistical data.

Following from this more realistic distribution of initial chloride threshold values, the model recognizes that the electrochemical potential of the reinforcing steel is an essential factor for critical chloride concentration, e.g. [42-45]. The impact of ongoing corrosion on chloride thresholds of cathodic sites is modelled as potential-dependent chloride thresholds according to [43]:

$$C_T = C_{T0} \qquad \text{for } E_S \geq E_{T0} \qquad (1a)$$

$$C_T = C_{T0} 10^{(E_{T0}-E_S)/\beta_{CT}} \qquad \text{for } E_S < E_{T0} \qquad (1b)$$

where C_T is the chloride threshold, C_{T0} is the chloride threshold at E_{T0}, E_S is the polarized passive steel potential with respect to an SCE located in the concrete next to the steel surface, E_{T0} is the baseline potential (chosen to be -0.1 V to represent an undisturbed condition), and β_{CT} is the cathodic prevention slope. This is an inverse slope of the increase of C_T with respect to E_S when plotted in a log$C_T(E_s)$ representation.

4 Examples

To demonstrate the potential of the multi-scale and multi-physics deterioration model two examples are given below.

4.1 Service life prediction

In the first example, the initiation and propagation of reinforcement corrosion in an un-cracked and a cracked beam are simulated in 2D (Fig. 9). When assembled with adjacent 2D models, a 3D damage representation of the beam can be created. Within each 2D simulation, heat and mass transfer is fully coupled with the corrosion modelling and corrosion is initiated when a chloride threshold at the reinforcement surface is reached. Varying climatic boundary conditions are applied (chloride content, relative humidity, and temperature) as shown in Fig. 10, which will, among others, affect the thermodynamics and kinetics of reinforcement corrosion. Chloride thresholds are distributed randomly along the reinforcement surface (Fig. 11a), thus, anodic areas will also form randomly. The remaining model parameters can be found in [46]. Fig. 11 illustrates the predicted chloride ingress, corrosion potentials, and corrosion current along the rebar, and the cross section reduction (maximal rebar diameter reduction, worst case) as a function of time for the un-cracked and the cracked beams. The presented results clearly show the impact of the crack on the chloride ingress. Considerably higher chloride concentrations can be found in the vicinity of the reinforcement due to the presence of the crack, which leads to an earlier accumulation of the assigned chloride thresholds in the vicinity of the crack. As soon as a chloride threshold is reached, corrosion is initiated and a decrease in the corrosion potential is observed. Comparing the uncracked and cracked geometry reveals that corrosion is initiated considerably earlier in the cracked beam. The development of the anodic and cathodic sites in the cracked beam geometry results in localized corrosion attack near the crack, with higher cross sectional reductions of the reinforcement compared to the uncracked beam geometry, see Fig 11 (d). The predicted continuous growth of the pit is based on the description of the corrosion mechanisms used in the present model. To the author's knowledge, data on the long-term effect of cracks are non-conclusive; see e.g. [36], and improved understanding of the mechanisms controlling corrosion initiation and propagation is required. A flattening of the maximal rebar diameter reduction curves towards the end of the simulations is observed for both geometries. This is attributed to the formation of large anodic areas along the reinforcement, rather than distinct anodic and cathodic areas. The corresponding corrosion current density is then considerably lower, corresponding to lower rates of cross sectional reductions.

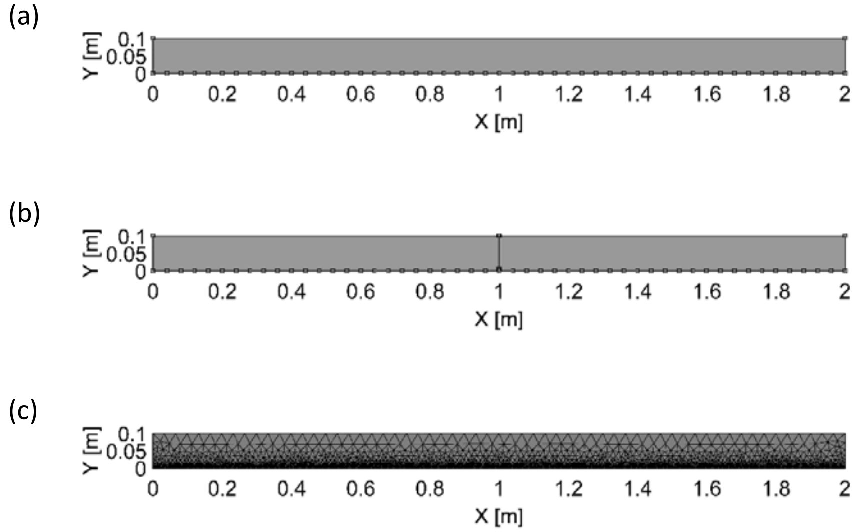

Figure 9. Lattice model geometry for (a) un-cracked beam, (b) cracked beam, and (c) mesh. After [46].

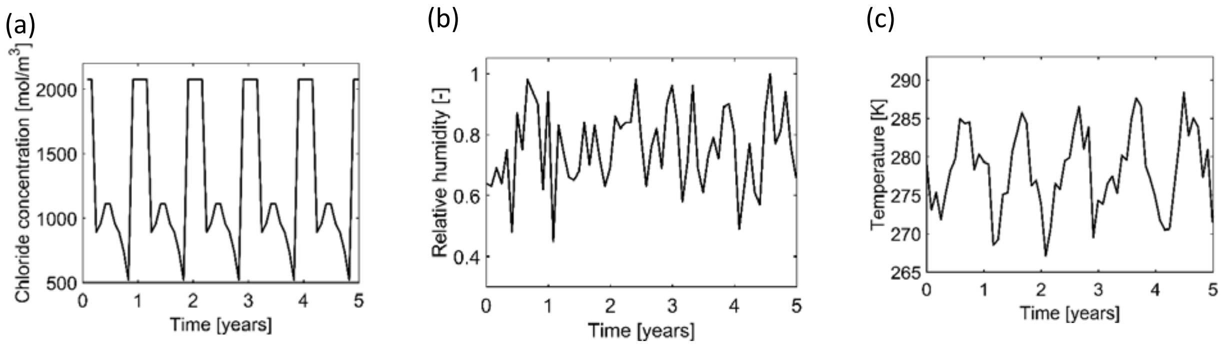

Figure 10. Exposure conditions (a) chloride content, (b) relative humidity, and (c) temperature. Please note: exposure conditions are presented for 5 years only. After [46].

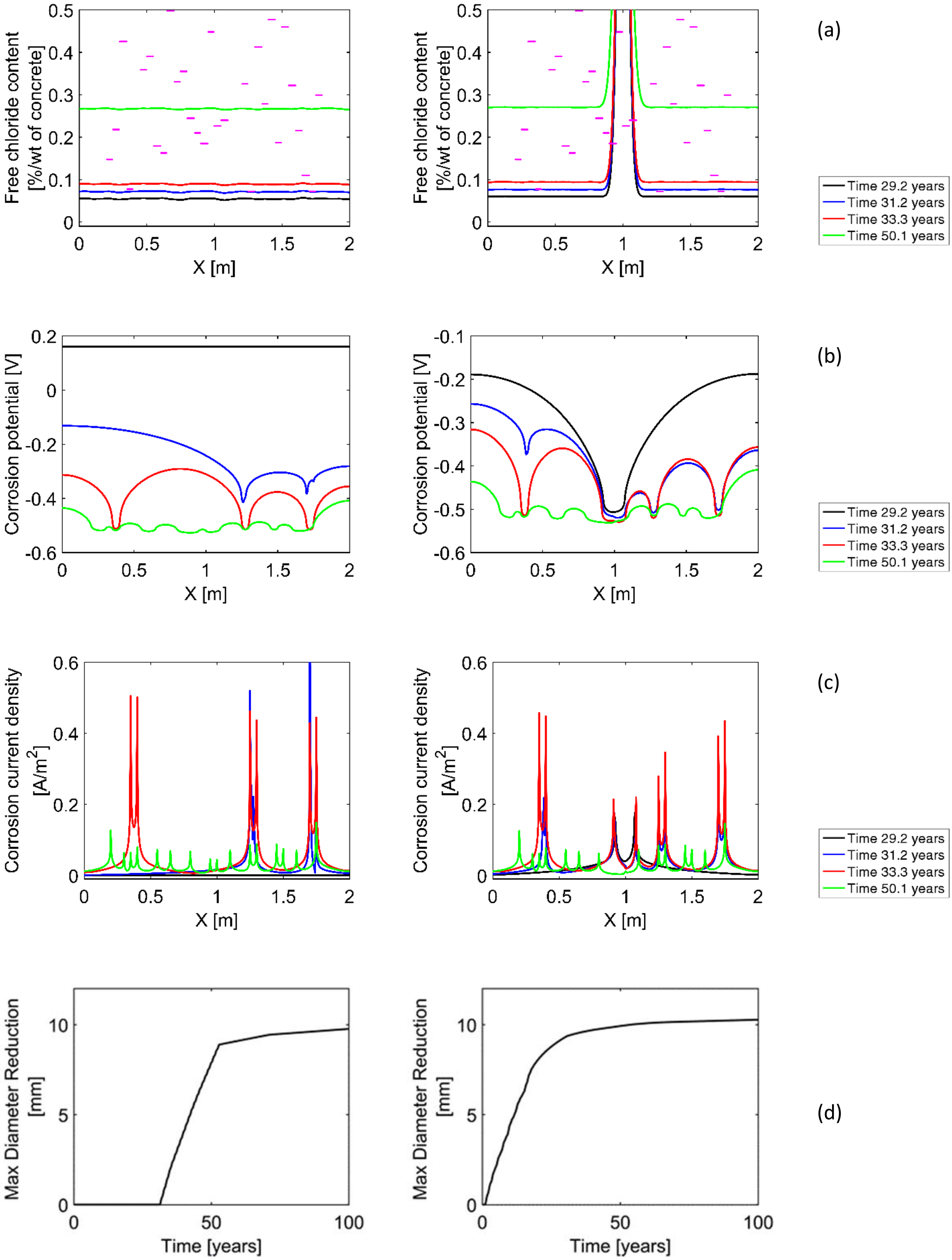

Figure 11. 2D prediction for an un-cracked (left) and a cracked beam (right) with geometry as shown in Fig. 9 of (a) chloride threshold (purple lines) and free chloride concentration at the reinforcement surface, (b) corrosion potential, (c) absolute corrosion current density, and (d) maximal rebar diameter reduction. After [46].

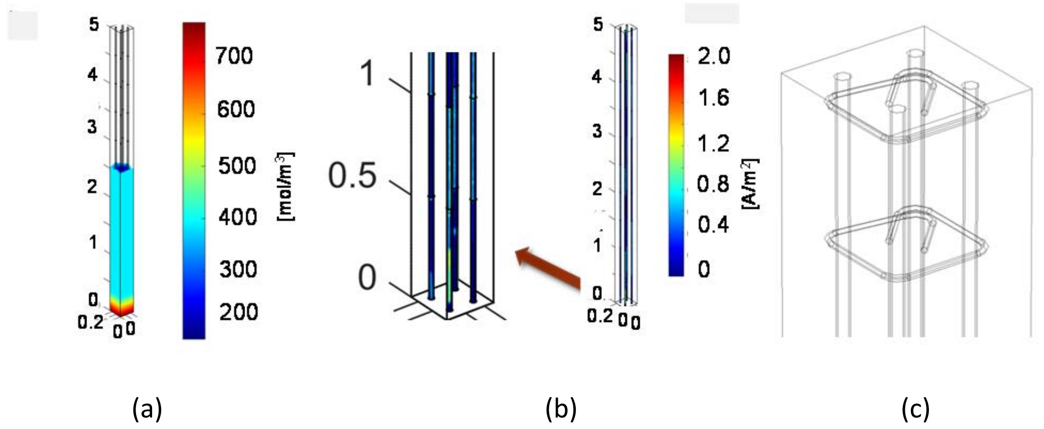

Figure 12. 3D prediction for an un-cracked beam of (a) free chloride concentration at the reinforcement surface, (b) absolute corrosion current density, and (c) rebar cage geometry.

4.2 Preliminary 3D deterioration modelling

In the second example, transport phenomena as well as the initiation and propagation of reinforcement corrosion in an un-cracked beam is simulated in 3D. A preliminary version of the proposed 3D multi-physics deterioration model has been constructed. Within the model, the heat and mass transfer is fully coupled with the corrosion and corrosion-induced damage modelling. The critical chloride concentration is assumed to be distributed using a spatially correlated distribution. Fig. 12 illustrates the predicted chloride ingress and corrosion current density at an arbitrary time step after corrosion initiation. Fig. 12a represents the 3D chloride concentration profile and Fig. 12b shows corrosion current density map at the surface of longitudinal steel. Although the rebar cage geometry has been modelled (Fig. 12c), corrosion of stirrups is not considered, yet. The preliminary version of the 3D multi-physics deterioration model has been modified to be fully interoperable with BIM.

5 Challenges

Models for predicting structural degradation due to reinforcement corrosion are in the focus of the research community; whereas models for other deterioration mechanisms e.g. freeze thaw action and alkali silica reaction, are lacking behind; not to mention coupled models for multiple deterioration mechanisms acting simultaneously.

Despite being in focus of many research efforts, models for the prediction of reinforcement corrosion still need further development. For example, the understanding of the chloride threshold for corrosion initiation, the long-term impact of cracking, and the corrosion process itself is still limited. Reliable and valid service life predictions furthermore require improved models and data for e.g. material and structural changes due to sequential maintenance and repair, and the environmental exposure. Considering these limitations and the limited validation of current service life prediction models, it is proposed to use sensor technology to support verification and updating of service life models and to facilitate proactive maintenance and repair of actual infrastructure.

6 Conclusions and perspectives

To assess potential innovative approaches and to quantify their sustainability the construction industry needs reliable and valid scientifically based performance prediction models. Such models must be mechanism based (multi-physics) to capture the actual degradation mechanism as well as multi-scale to allow for prediction of the structural performance taking into account materials degradation of a suite of concrete compositions.

We envision the next generation maintenance tools to combine numerical simulations based on multi-scale and multi-physics principles and extensive in-situ monitoring, allowing continuous updating of 4D simulations of functional performance.

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