Effectiveness of multi-physics numerical model in simulating accelerated corrosion with spatial and temporal non-uniformity

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Abstract

This study is motivated by the need to develop an efficient numerical model to simulate non-uniform interfacial degradation of reinforcing steel in concrete in an accelerated corrosion setup considering the influence of differential aeration, moisture and conductivity. In this study, a multi-physics finite element (FE) model is presented to simulate spatially and temporally non-uniform surface topography of corroding steel with rust layer, and eliminates the assumption of uniform mass loss and its linear variation with time as per available literature that uses classical approach of Faraday’s law. The model is validated experimentally with accelerated corrosion setup. Unlike previous studies, pore saturation (PS) is continuously monitored and its existing experimental correlations with conductivity and oxygen diffusivity are adopted so that the model can be extended to simulate natural corrosion to enhance the accuracy of service life predictions. These evaluations can be made completely nondestructive and in real-time eliminating the challenges in capturing the influence of environment by the use of alternative parameters such as relative humidity from real climate change predictions. The key findings from the investigation reveal that incorporating local environmental parameters measured in situ allows for the model to naturally evolve with anodic and cathodic locations on steel surface avoiding the need to assume predefined locations. It is envisioned that the developed multi-physics FE model can be used as a reliable substitute to accelerated corrosion experiment which is frequently used for durability studies of corroding reinforced concrete (RC) members. It is shown that the daily and cumulative mass loss evaluated from the degraded surface topography of the corroded rebar using the simulated model are in good agreement with those evaluated experimentally. Further, the maximum pit depth evaluated from the simulated surface is validated that has valuable applications in estimating degraded strength of corroding steel and service life of RC members.

1. Introduction

The effectiveness of service life predictions in reinforced concrete (RC) structures subjected to corrosion induced deterioration can be enhanced with accurate corrosion monitoring and strength degradation evaluation strategies. As a step towards this, numerical studies [1–10], and analytical corrosion models [11–13] coupled with service life prediction models [14–19] were developed. Experimental investigations were also performed to examine the efficacy of the numerical and analytical studies [20, 21]. Researchers [22] have developed a stochastic computational framework to incorporate various sources that result in uncertainties in predicting the performance of structures. However, integration of these models with real-time investigations specific to local exposure by considering the non-uniform nature of influencing parameters was not attempted.

Only few investigations had considered real-time corrosion monitoring incorporating nondestructive
evaluations [23–29], but are limited to monitoring corrosion initiation and propagation assuming uniform mass loss and linear rate of corrosion with no possibility of obtaining the non-uniform degraded surface topography. These idealizations stem from the challenges involved in incorporating coupled interactions between structure and its local environment on a space-time frame in a 3D domain. Researchers [30] envisioned that the next generation strategies to maintain RC structures will combine multi-physics numerical simulation having multi-scale capabilities with in situ monitoring, allowing continuous updating of what is called as 4D simulation of structural performance. This forms the basis of present research work.

Recently, a 2D numerical model simulating non-uniform corrosion incorporating the influence of temperature and relative humidity (T-RH) from real climate with temporal variations was presented in [31, 32]. These studies concluded that, sampling methods of real climate data to simplify the real variability, affect the corrosion initiation and propagation rate showing higher corroded depth in case of daily variations in comparison with weekly and monthly variation schemes. It is evident from these observations that the uncertainties associated with real climate data can seriously affect corrosion rate predictions because of fluctuations in T-RH, which was also identified in [33]. Therefore, the researchers [33] have adopted a probabilistic approach to account for these uncertainties, but the real-time local exposure and the environment of members were ignored in their investigation. Thus, the present study proposes a real time data-based model to arrive at conductivity characteristics, oxygen diffusivity and moisture (pore saturation) which directly influences the corrosion current rather than using T-RH from climate data [34–38] to ensure that the findings of this study are not affected.

While modelling capabilities of COMSOL Multi-physics® were explored by few researchers [39, 40], in the present study a fully coupled model with coupling between chemical species transport and the electrochemical cell representing corrosion in an accelerated corrosion environment is developed and the surface topography of corroding steel is simulated. The accelerated corrosion experiment [44] consisted of an RC beam partly immersed in NaCl solution with a constant voltage of 25 V applied across the terminals of the steel to accelerate partial corrosion. The environment of experimental setup [44] that influences corrosion such as differential aeration, oxygen diffusion, concrete conductivity and PS for concrete immersed in NaCl solution are considered as time dependent parameters in the numerical model. The constant voltage applied externally to accelerate corrosion is defined as a boundary condition. Local corrosion current densities are evaluated on the steel surface in order to obtain degradation profiles of the reinforcing bars after suitably modifying the mathematical model for electrode deposition or dissolution proposed in [41–43].

Surface topography of corroded steel with rust layer is simulated at the end of each day of corrosion and variation of maximum pit depth are presented. The mass loss evaluated from the degraded profile at the end of each day for the corroding steel simulated using the mass loss evaluated from experiment [44] for validation.

2. Numerical modelling of corrosion propagation phase in accelerated corrosion setup

A multi-physics FE model coupling transport of chemical species with electrochemical reactions of corrosion to simulate accelerated partial corrosion with impressed current technique in RC members is developed. The model also takes into consideration the local environment of experimental setup such as differential aeration, moisture, and conductivity using COMSOL Multi-physics®. However, for real time monitoring of naturally corroding structures the chloride ingress needs to be incorporated as a transport of diluted species physics in modelling. Alternatively, many numerical models are also available from literature [5, 31, 32, 45–49] to arrive at the non-uniform chloride profiles. The threshold chloride concentration is made readily available in accelerated corrosion experimentation and therefore, the model represents the propagation phase of corrosion wherein the incorporation of chloride ingress is not relevant.

2.1. Theoretical background of multi-physics modelling for corrosion

The multi-physics model uses FE Method to solve the partial differential equations representing the oxygen diffusion with corrosion propagation phase. The chemical species transport physics (nomenclature used in COMSOL Multi-physics®) is used to model the diffusion of oxygen, and the coefficient form PDE in mathematics section of COMSOL Multi-physics® is adopted to simulate the Nernst plank secondary current distribution governing the conductivity and potential of electrode, and electrolyte surrounding the rebar which is the concrete itself. The model automatically predicts the anodic and cathodic locations that are developed due to differential aeration [50], and their distributions over time.

2.1.1. Corrosion reaction kinetics

In non-uniform wet corrosion, which is the most common type of chloride induced corrosion, an electrochemical cell is set forming anode and cathode on the corroding section. Many reactions are possible during corrosion, and are mainly categorized as oxidation at anode and oxygen reduction at cathode. The reactions in an impressed current setup are considered from [4].

In corrosion propagation phase, especially in case of chloride induced corrosion macro-cells are formed [31]. The macro-cells may also form because of
heterogeneous steel-concrete interface and may also arise from the differences in electrode potentials resulting from differential aeration. Micro-cell results in uniform corrosion without any net flow of current through electrolyte [50].

\[ i_{mac,a} = i_a - i_c \]  
\[ i_{mac,c} = -i_c \]  
\[ i_{mac,a} = -i_c \]  
\[ i_{corr} = i_{mac,a} + i_{mic,a} \]

where \( i_{mac,a} \) and \( i_{mac,c} \) are macro-cell current densities at anode and cathode respectively (A m\(^{-2}\)), \( i_{mic,a} \) is micro-cell current density at anode (A m\(^{-2}\)), \( i_{corr} \) is the total corrosion current density (A m\(^{-2}\)), which in the absence of micro-cell corrosion, becomes \( i_{mac,a} \).

### 2.1.2. Modelling oxygen transport

The diffusion process is simulated using Fick’s first law. The corrosion current at cathode depends on rate of corrosion at cathode, which is governed by availability of oxygen at cathodic surface. On the other hand, the concentration of oxygen at cathodic surface depends on the molar flux from the corroding concrete. This gives rise to a cyclic coupling and is addressed in the modelling.

\[ \frac{\partial C_{O_2}}{\partial t} = \nabla \cdot (D_{O_2} \nabla C_{O_2}) \]  

where \( D_{O_2} \) is effective diffusion coefficient of oxygen in concrete (m\(^2\) s\(^{-1}\)), \( C_{O_2} \) is the concentration of oxygen in concrete (mol m\(^{-3}\)).

The boundary condition at cathodic surface is obtained by using Faraday’s law of electrolysis on equating oxygen flux to cathodic current density as shown in equation (6).

\[ \frac{i_{O_2}}{F z} = -D_{O_2} (n \nabla C_{O_2}) \]

where \( i_{O_2} \) is the cathodic current density; F (96485.3365 C mol\(^{-1}\)) is Faraday’s constant; \( z \) is electrons involved in reaction.

An initial constant concentration of \( C_{O_2}^{ref} \) which is the average atmospheric concentration of oxygen equal to 8.6 mol m\(^{-3}\) is considered on all exposed concrete surfaces.

Zero flux boundary condition is adopted on all other surfaces as shown in equation (7).

\[ n \cdot (D_{O_2} \nabla C_{O_2}) = 0 \]

### 2.1.3. Modelling charge transport

In the presence of an electric field, the ions dissolved in pore solution serve as charge carriers, the difference in electric potential \( \phi \) (corrosion potential) in concrete generates the electric field. As the process of corrosion is electrochemical in nature, charge transport in concrete needs to be considered. The governing equation for charge transport at steady state is given by equation (8).

\[ \nabla \cdot (\frac{1}{\rho} \nabla \phi) = 0 \]

Here \( \rho \) is electrical resistivity of concrete (Ω·m), the reciprocal of which gives electrical conductivity \( \sigma \) (s m\(^{-1}\)). \( \rho \) is used to simplify the phenomenon of complex ionic transport and can be obtained experimentally or by relating with PS [34]. At steel-concrete interface both anodic and cathodic reactions are specified with corresponding current densities on the entire rebar surface. This macro-cell current \( i_{mac} \) is equated to electrolyte potential flux, thus defining boundary conditions at anodic and cathodic sites on full length of rebar embedded in concrete. Even though the entire surface of rebar is specified with anodic and cathodic reactions, the differential aeration specified automatically facilitates the anodic and cathodic sites to evolve naturally.

\[ i_{mac} = \sum_m i_{loc,m} = i_a - i_c \]

\[ i_{mac} = n i_f = n (-\sigma \nabla \phi) \]

Here \( i_a \) and \( i_c \) are anodic and cathodic current densities respectively (A m\(^{-2}\)), \( i_f \) is the current density of electrolyte (A m\(^{-2}\)), \( m \) is tag of electrode reactions defined, \( i_{loc,m} \) is the local current density for a particular reaction \( m \) (A m\(^{-2}\)). Zero flux boundary conditions are enforced on all surfaces other than anodic and cathodic locations.

\[ n \cdot \left(-\frac{1}{\rho} \nabla \phi\right) = 0 \]

\( i_a \) and \( i_c \) the anodic and cathodic current densities (A m\(^{-2}\)) are evaluated using equations (12) and (13) respectively [38]. The polarization experimentation results were adopted from [34].

\[ i_a = \frac{i^0_a}{n_b} \times 10^\frac{\eta_a}{A_{Fe}} \]

\[ i_c = \frac{C_{O_2}^{ref}}{C_{O_2}^{ref}} \times i^0_c \times 10^\frac{\eta_c}{A_{O_2}} \]

Here \( i^0_a \) and \( i^0_c \) are exchange current densities for anodic and cathodic reactions respectively (A m\(^{-2}\)), \( C_{O_2}^{ref} \) is the concentration of oxygen diffused in concrete domain (mol m\(^{-3}\)), \( C_{O_2}^{ref} \) is reference or atmospheric oxygen concentration (8.6 mol m\(^{-3}\)), \( A_{Fe} \) and \( A_{O_2} \) are anodic and cathodic tafel slopes respectively, \( \eta_a \) and \( \eta_c \) are anodic and cathodic over-potentials, respectively and are given by equations (14) and (15).

\[ \eta_a = E_{appl,a} - \phi - E_{O_2}^{ref} \]

\[ \eta_c = E_{appl,c} - \phi - E_{O_2}^{ref} \]
time by solving equation (8), which takes the form of Laplace’s equation. Using the corrosion potential \( \phi \), anodic and cathodic current densities are evaluated, that can further be used in evaluation of micro and micro-cell current densities. From these parameters total current densities at any point on the surface of corroding rebar can be evaluated.

2.1.4. Application of Faraday’s law in evaluating metal dissolution

Faraday’s laws of electrolysis in combined form and its variations are very often used in evaluating weight loss \( w \), and dissolution rate commonly referred to as rate of corrosion.

\[
w = \frac{q_m M}{nF}
\]

Here \( q_m \) is the electric charge (C), responsible for corrosion associated with electrode reaction \( m \), \( M \) is the molar mass (kg mol\(^{-1}\)), \( n \) is the number of electrons transferred and \( F \) is the Faraday’s constant (\( F = 96485.3365 \) C mol\(^{-1}\)).

Electrical charge, \( q \), is the integral of current \( i \) over time for which the charge is passed,

\[
q = \int_{t_1}^{t_2} i dt
\]

and the current density \( j \) is defined as the current per unit electrode area (A m\(^{-2}\)), i.e., the surface area of that portion of electrode participating in electrolysis due to corrosion \[43\]

\[
j = \frac{i}{A}
\]

Therefore

\[
q = \int_{t_1}^{t_2} A j dt
\]

The use of this expression (equation (19)) is preferred than (equation (17)) as the area of corroding surface and \( i \) continue to change with corrosion progress due to dissolution or deposition.

2.2. Non-uniform rate of dissolution using numerical model

The multi-physics model facilitates evaluation of point wise time dependent local current densities responsible for corrosion. Therefore, there is a provision for adding an arbitrary number of dissolving-depositing species. The surface concentration variables of dissolving-depositing species can be used to calculate thickness of dissolution or deposition and the rate of which is used to set the boundary velocity. The velocity of dissolution is expressed as \[41\]

\[
\frac{\partial x}{\partial t} = n \frac{\text{v}_{\text{dis,tot}}}{\text{v}_{\text{dis,tot}}}
\]

Here \( n \) is the total dissolution velocity (m s\(^{-1}\)), defined as the sum of velocity contributions for all species and electrode reactions, and is expressed as:

\[
\text{v}_{\text{dis,tot}} = \sum_i \text{v}_{i,m} \frac{\text{i}_{\text{loc,m}}}{\text{n}_m F}
\]

where \( \text{i}_{\text{loc,m}} \) is the current density of corrosion current density \( j \) at that point where dissolution is intended to be evaluated (A m\(^{-2}\)), \( \text{v}_{i,m} \) is the stoichiometric coefficient of species \( i \) with respect to reaction \( m \), \( \rho_i \) is the density of metal undergoing corrosion, \( n_m \) is the number of electrons transferred.

3. Experimental setup and validation of the numerical model

The experimental setup of accelerated corrosion with impressed current proposed by \[44\] for analyzing pitting corrosion of rebar embedded in concrete is considered for inducing partial corrosion. The details of the experimental setup can be found in \[44\]. The concrete mix proportion for RC specimen are presented in table 1 \[44\], and the specimens are wet cured for 3 days after casting and then moist cured for 28 days, the specimens are allowed to dry for 7 days before subjecting to accelerated corrosion \[44\]. In the experimental investigation \[44\], the positive terminal of the power supply is connected to bottom rebar to act as anode and the negative terminal is connected to galvanized wire mesh immersed in NaCl to act as cathode as shown in figure 1(a). Impressed current is applied through a DC power supply with constant voltage of 25 V maintained over a period of 12 days, and the corresponding daily variation of current is measured. The bottom middle RC portion of 150 mm length is immersed in 9% NaCl solution to introduce partial corrosion as shown in figure 1(a). This portion is supplied with NaCl to depassivate the gamma iron oxide layer which allows corrosion to progress. The section immersed in NaCl is deprived of oxygen as it is contained inside a plastic tray filled with NaCl and the remaining faces are freely exposed to atmospheric oxygen as shown in figure 2(d). Both differential aeration and selective immersion in NaCl solution leading to difference in moisture and corresponding conductivity characteristics are responsible for partial corrosion in the experiment. In accelerated corrosion experiments usually the rebars connected to positive terminal acts completely as anode. However, in this experimentation difference in availability of oxygen and moisture along the length of the rebar determines the anodic and cathodic locations that are setup on the

| Material | Water | Cement | Sand | 10 mm Aggregate | 20 mm Aggregate |
|----------|-------|--------|------|----------------|---------------|
| Weight (kg) | 170   | 340    | 756  | 440            | 720           |

Table 1. Concrete mix proportions \[44\].
rebar connected to power supply. The development of passive locations (cathode) adjacent to the portion immersed in NaCl (acting as anode) on the same bottom rebar was also confirmed experimentally [44].

The numerical model simulates this experimental setup of accelerated corrosion with impressed current, considering the effect of differential aeration, moisture and corresponding conductivity characteristics to capture the spatial and temporal non-uniformity in corrosion. The mass loss evaluated from experiment are compared with the mass loss evaluated from the degraded geometry of corroding steel simulated using the numerical model for validation.

**4. Specifications of Multi-physics finite element modelling to simulate accelerated corrosion**

Mesh discritization depends on the type of physics being solved and must ensure convergence. Since the numerical model addresses two physics namely, current distribution using coefficient form PDE under mathematics node and transport of diluted species, each having a different type of meshing requirements. The physics controlled meshing capabilities of COMSOL Multi-physics® is adopted that predominantly uses tetrahedral mesh as shown in figures 5(b), (c) and 6(a).

Mesh convergence study is carried out to finalize the meshing criteria.

**4.1. Input parameters for simulating electrochemistry of corrosion in the numerical model**

The electrochemical parameters adopted for simulating corrosion are listed in table 2 and are adopted from experimental studies presented by researchers [34, 40].

**4.2. Oxygen diffusivity and electrolyte conductivity as a function of pore saturation**

The oxygen diffusivity and concrete resistivity are related to the PS levels of concrete. PS level has its
direct bearing on temperature and humidity. Therefore, if PS is evaluated as a function of time, then empirical relations amongst PS, oxygen diffusivity and concrete resistivity presented in [34–37] can be used to simulate the effect of local environment. However, in natural corrosion PS can be evaluated using nondestructive testing (NDT) as described in [51–53]. Oxygen diffusivity and electrolyte conductivity presented by researchers [34] were deduced by direct interpolation from the experimental investigations of [35–37], and therefore, the oxygen diffusivity as a function of PS for a given water cement ratio and cover thickness can be obtained by interpolation [35, 36] and electrical conductivity from [37]. To evaluate PS variation, three cubes of M25 grade are casted and moist cured for 28 days. The initial condition of RC specimen in the accelerated corrosion experiment [44] was relatively dry, therefore, the cubes are air dried for 7 days after moist curing to maintain similar initial conditions. These cubes are then immersed in 9% NaCl solution to maintain the same concentration used in [44], and daily water absorption is monitored for 10 days to calculate PS as presented in table 3. However, because of the first crack in concrete on 11th day, there was a spike in water ingress as evident from impressed current variations [44]. Therefore, a PS of 0.7 is assumed on 11th and 12th day based on the similarities in trend of variation of PS and impressed current [44]. It is assumed that the PS in experimentation followed a similar profile presented in table 3.

The water cement ratio and cover thickness considered in the present model are similar to those presented in [34], therefore, the relation among PS, electrolyte conductivity and oxygen diffusivity are adopted from [34] in the present work and are listed in table 3.

The PS, oxygen diffusivity and concrete conductivity are adopted as bulk properties for defined sections of concrete as shown in figure 2 to simplify the complex phenomenon of ionic transport [34–36]. Adopting bulk properties also facilitates their nondestructive evaluations at regular intervals or for continuous monitoring to update the simulation.

PS is assumed to be constant in the top portion as shown in figure 2(a) and bottom portions adjacent to corroding unit as shown in figure 2(b) and corresponding oxygen diffusivity and concrete conductivity are adopted, the bottom middle portion of concrete immersed in NaCl is the corroding unit and therefore, PS, oxygen diffusivity and concrete conductivity are adopted as function of time from table 3 as shown in figure 2(c). The corroding unit immersed in NaCl is deprived of oxygen and the remaining surfaces are freely exposed to atmosphere as shown in figure 2(d) inducing differential aeration which is incorporated in the model. Both anodic and cathodic reactions are specified on the full length of bottom corroding rebar, however, due to the differential aeration oxygen is available only at the adjacent units of concrete highlighted in figure 2(b) thus passivates the rebar portion embedded in these sections. The rebar embedded in the corroding unit is deprived of oxygen and therefore the cathodic equation defined in equation (13) becomes zero and only anodic reactions prevail.

| Notation | Value | Units | Description |
|----------|-------|-------|-------------|
| $A_{Fe}$ | 0.41  | V     | Tafel slope in iron oxidation |
| $A_{O2}$ | −0.18 | V     | Tafel slope in oxygen reduction |
| $E_{Fe}^0$ | −0.76 | V     | Iron oxidation equilibrium potential |
| $E_{O2}^0$ | 0.189 | V     | Oxygen reduction equilibrium potential |
| $i_0^o$ | 7.1E-5 A m$^{-2}$ | | Iron oxidation exchange current density |
| $i_0^c$ | 7.7E-7 A m$^{-2}$ | | Oxygen reduction exchange current density |
| $E_{app, O2}$ | 25 | V | Applied potential to rebar |
| $i_{app, mesh}$ | 1E-7 A m$^{-2}$ | | Oxidation exchange current density on mesh |
| $i_{app, mesh}$ | 1E-4 A m$^{-2}$ | | Oxygen reduction exchange current density on mesh |
| $E_{O2, mesh}$ | −0.44 | V | Mesh oxidation equilibrium potential |
| $E_{Fe, mesh}$ | 0.189 | V | Oxygen reduction equilibrium potential |
| $A_{O2, mesh}$ | −0.25 | V | Oxygen reduction tafel slope on mesh |
| $A_{Fe, mesh}$ | 0.12 | V | Mesh oxidation tafel slope |
| $E_{app}$ | 0 | V | Applied potential to mesh |

### Table 3. Electrolyte conductivity and oxygen diffusivity as a function of PS [34].

| PS Days | Electrolyte conductivity ($\sigma$, 5 m$^{-1}$) | Effective diffusivity of $O_2$, ($D_{O2}$ m$^2$s$^{-1}$) |
|---------|-----------------------------------------------|-------------------------------------------------|
| 0.200   | 1.75E-04                                      | 1.52E-08                                        |
| 0.449   | 3.42E-05                                      | 6.62E-09                                        |
| 0.606   | 7.16E-03                                      | 2.70E-09                                        |
| 0.700   | 9.82E-03                                      | 1.50E-09                                        |
| 0.699   | 9.77E-03                                      | 1.51E-09                                        |
| 0.688   | 9.38E-03                                      | 1.62E-09                                        |
| 0.658   | 8.29E-03                                      | 1.92E-09                                        |
| 0.626   | 7.53E-03                                      | 2.39E-09                                        |
| 0.621   | 7.44E-03                                      | 2.47E-09                                        |
| 0.607   | 7.17E-03                                      | 2.69E-09                                        |
| 0.605   | 7.14E-03                                      | 2.72E-09                                        |
| 0.700   | 9.80E-03                                      | 1.50E-09                                        |
| 0.700   | 9.80E-03                                      | 1.50E-09                                        |
therefore the model automatically creates time dependant anodic and cathodic locations on bottom rebar to facilitate nonuniform corrosion simulation.

The model can be extended to simulate naturally corroding structures by adopting the PS and electrolyte conductivity data obtained by scheduled monitoring using concrete moisture meter and four probe resistivity meter, respectively, and oxygen diffusivity as a function of PS can be obtained using experimental relationship presented in [35, 36]. Also, the ingress of chloride can be modelled as transport of diluted species in multi-physics modelling environment. Extending the application to model natural corrosion will form the scope of future investigations and is briefly mentioned in the present study as one of the applications and adaptability of the proposed model.

5. Methodology to quantify metal dissolution

The methodology adopted in evaluating weight loss from the experiment is shown in figure 3. Note that in the experimental study [44] a constant voltage of 25 V is applied, as a result current varies as a function of time due to various factors of reaction kinetics and the environment of experimental setup. The mass loss using Faraday’s law may be calculated on a daily basis by monitoring the daily variation of current in accelerated corrosion experiment and cumulative weight loss can be evaluated, but the weight loss cannot be predicted beforehand to plan the experiment. However, in the proposed numerical model local current density evaluated point wise is used to obtain non-uniform pointwise corrosion rate (dissolution velocity). The pointwise dissolution is then evaluated by multiplying dissolution velocity with a small time interval dt for which the dissolution velocity is assumed to be constant. Finally, the coordinate points representing pointwise dissolution is used in modelling deformed rebar geometry to calculate weight loss as depicted in figure 4.

6. Results and discussion

The results are evaluated at half section of length 75 mm of the total corroding portion of length
150 mm using symmetry in the model shown in figure 1. This portion of 75 mm length is divided into four typical cross sections namely CSA, CSB, CSC, and CSD. CSA and CSD segments are of length 12.5 mm, whereas CSB and CSD segments are of length 25 mm. The results are evaluated at 10° angular spacing on the circumference of each cross section and is assumed to be constant over the length of that particular segment for evaluating deformation profile and weight loss as shown in figure 5. However, the model can evaluate all these parameters at any point. The evaluated electrolyte potential and the corresponding total electrolyte current density shown in figure 6 (b) represents the the locations where corrosion is severe, and can be seen in further results of degraded geometry. These observations are in concurrence with the experimental observations [44]. It may be noted that as the central portion of rebar is deprived of oxygen, this location develops into anodic site and adjacent location on the same rebar which has relatively larger supply of oxygen acts as cathodic site. This development of anodic and cathodic macro cells on the same rebar surface is completely ignored in estimating mass loss using Faraday’s law from accelerated corrosion experiment, based on the assumption that the entire rebar subjected to impressed current.
will act as anode. The electrode and electrolyte current density in figure 6(c), follow similar trend that are evaluated from corresponding potentials. Figure 6(d) represents the diffusion of oxygen governing the formation of anodic and cathodic sites, which is not taken for consideration in evaluating weight loss location using conventional approach of Faraday’s law in an impressed current setup. This could be one of the reasons for the differences between predicted weight loss and experimental results as observed in previous studies [54, 55], which suggested the need for further investigation to identify the cause for deviation. But the consideration of diffusion of oxygen would help in reducing the deviation that can be further seen in weight loss comparisons. In modeling, the oxygen diffusivity is allowed through exposed portions of concrete surface with an equilibrium concentration of 8.6 mol m$^{-3}$, which is the concentration of oxygen in air. Also the portion that is immersed in NaCl is deprived of oxygen exposure. It can be clearly seen from figure 6(d) that the adjacent portions to the left and right side of middle corroding portion of rebar is consuming oxygen, therefore, embedded rebar here is potentially acting as cathode.

6.1. Local current density
At every 10° intervals on CSA, CSB, CSC, and CSD sections the point wise corrosion current density is obtained from the numerical model as an average daily data for 12 days of corrosion. The daily data is taken as an average over 24 h. The simulation was carried out for 12 days as the crack started appearing on the 11th day in accelerated corrosion experiment as observed in [44]. The trend of local current density shown in Figure 7 is along similar lines with the electrolyte potential and total current densities, and shows that maximum local current density is at the bottom portion of the rebar. The possible reason for this could be the closest proximity of this portion with the galvanised wire mesh resulting in quicker transaction of ions. Another reason that can be found from the experimental setup is that this corroding portion of rebar recieves NaCl at a much faster rate than other sections due to lesser cover thickness needed to be travelled for NaCl. Further, it can be observed that at CSA as in figure 7(a), the maximum current density is at 180°. But in CSB, CSC and CSD, in figures 7(b)–(d) respectively, the maximum occurs not exactly at 180° but adjacent to it. This is possibly because of their locations, which are within the corroding unit immersed in NaCl whereas, CSA is at the junction of corroding and non corroding unit and is subject to diffusion of oxygen from left unit of concrete exposed to surface. Also, at CSB, CSC and CSD, the sections from 0° to 90° and 270° to 0° are belonging to the unit of concrete exposed to oxygen and not immersed in NaCl. But, the remaining portion of the rebar is not exposed to oxygen and immersed in NaCl. Thus, for CSB, CSC and CSD, the 90° and 270° locations have oxygen availability faster than 180° location, but 180°
location has faster supply of NaCl solution, but no or very less oxygen supply. Thus, the locations that are between 90° and 180° as well as between 180° and 270° has a better availability of combination of NaCl solution and Oxygen diffusion.

6.2. Surface topography of corroded rebar and rust layer

Point wise degraded geometry is evaluated at 1 mm spacing in the direction of length on the corroding steel surface using local current densities. The profile of degraded geometry follows the profile of local current density, and the lower section of rebar towards NaCl solution gets corroded the most following the same reasoning as provided in section 6.1. This approach can effectively simulate non-uniformity of corrosion and resulting degraded surface topography as presented in figures 8–13. The volume of rust depends on the type of corrosion products formed and is assumed to be 3 times of the volume of metal dissolved \([4, 16, 31]\). The local free expansion of rust from degraded steel surface is a function of of dissolution \(x\) normal to the steel boundary as defined in equation (20) and the coordinates for the topography of top surface of rust is evaluated using equation (22) \([31]\).

\[
\nabla b(r, \theta, z, t) = (\beta - 1)x(r, \theta, z, t) \quad (22)
\]

where \(\nabla b(r, \theta, z, t)\) is the coordinates for the topography of top surface of rust and \(\beta\) is 3. Using equation (22) spatially and temporally non-uniform rust layer is modelled as dipicted in figures 9, 10 and 13(c). Figure 9 represents sample cross sections at the end of 12 days of corrosion showing the degraded profile and rust layer at the steel concrete interface (SCI). Figure 10 dipicts the longitudinal section showing the nonuniformity of corroded steel surface and thickness of rust at 12th day of corrosion.

To facilitate 3D modelling of corroded steel with non-uniform corrosion pits, 3d coordinate points representing the non-uniform surface topography of corroding steel is evaluated for segments CSA, CSB, CSC and CSD as shown in figure 11. The coordinate points are connected by curves at every section spaced at 1 mm as dipicted in figure 12 to facilitate modelling of the surface topography of corroding steel. Figures 13(a)–(d) represents the sequential steps in building 3D model of corroded steel with rust layer. Figure 13(d) clearly dipicts that the simulated model can capture spatial and temporal non-uniformity of corrosion pits on corroding steel surface. The modelling approach presented in this section can be used in accurately modelling the steel-concrete interface, characteristics of pits, degraded strength of corroded steel and interfacial pressure due to formation of rust. Modelling the surface topography of corroded steel with pit characterisation has great applications in accurately predicting service life of corroding RC structures \([16, 18, 55]\).

6.3. Evaluation of mass loss from experimental investigation

A much better way of using Faraday’s law in evaluating mass loss from experiment is to use varying impressed
current $I_I$, and use trapezoidal rule to evaluate the total charge flow (area under the curve in figure 14) in Faraday’s law of electrolysis for each time interval that is considered (24 h) from figure 14 [44]. Table 4 shows the mass loss evaluated using average current $I_a$, considering $I$ to be constant for 24 h.

Figure 9. Typical cross sections of corroded rebar with rust on 12th day at (a) CSA, (b) CSB, (c) CSC and (d) CSD.

Figure 10. Typical longitudinal section of corroded rebar with rust layer on 12th day of corrosion showing non-uniform degradation of both corroded steel surface and surface of rust.
6.4. Evaluation of mass loss from numerical model

The 3D deformed geometry is modelled in CAD, to obtain volume of corroded rebar and multiplying it with density of steel gives weight loss and is depicted in table 5. The daily and cumulative mass loss evaluated from the degraded profile generated using numerical model is in good agreement with the corresponding values evaluated from experimentation [44] as shown in figure 15. The predicted mass loss by numerical model is on the lower side from mass loss evaluated by varying current in the experiment, and similar observations were made by [54, 55].

This validates the numerical model for simulating corrosion in an accelerated corrosion setup with impressed current method. However, relatively larger deviation of mass loss evaluated by the numerical model is observed on 11th and 12th day, which is because of visible cracks on 11th day of accelerated corrosion [44], and was evident by the spike in corrosion current shown in figure 8. As the PS used in numerical model is evaluated from experimentation on cubes, and cannot reflect the PS levels at the onset of crack, therefore, the model deviates from the experimental result. Further investigation is needed to incorporate the effect of crack on PS variation. Thus, it can be established that the proposed numerical model not only predicts the mass loss with desirable accuracy but also predicts the degradation profile of corroded rebar as a nonlinear time dependent parameter, because of the fact that the mass loss evaluated using numerical model is based on corroded profile of degraded rebar geometry.

Table 4. Mass loss evaluated from experimental investigation.

| V (Volts) | I (A) | L (A) | Mass loss per day (g) | Cumulative mass Loss (g) |
|----------|-------|-------|----------------------|-------------------------|
| 0        | 0     | 0     | 0.00                 | 0.00                    |
| 25       | 0.16  | 0.16  | 4.00                 | 4.00                    |
| 25       | 0.3   | 0.23  | 5.75                 | 9.75                    |
| 25       | 0.48  | 0.39  | 9.75                 | 19.50                   |
| 25       | 0.5   | 0.49  | 12.25                | 31.75                   |
| 25       | 0.49  | 0.495 | 12.38                | 44.13                   |
| 25       | 0.6   | 0.545 | 13.63                | 57.75                   |
| 25       | 0.4   | 0.5   | 12.50                | 70.25                   |
| 25       | 0.4   | 0.4   | 10.00                | 80.25                   |
| 25       | 0.4   | 0.4   | 10.00                | 90.25                   |
| 25       | 0.36  | 0.38  | 9.50                 | 99.75                   |
| 25       | 1     | 0.68  | 17.00                | 116.75                  |
| 25       | 0.7   | 0.85  | 21.25                | 138.00                  |

Figure 11. Coordinate points representing degraded surface topography of corroded steel on 12th day for segments (a) CSA, (b) CSB, (c) CSC and (d) CSD.
The validated numerical model is used in evaluating the maximum pit depth at each day of corrosion using the coordinate points of corroded steel surface and is presented in Figure 16. Accurate prediction of the maximum pit depth and its location enhances the accuracy of service life estimation and the assessment of remaining strength of corroding structures [18].

### Table 5. Mass loss evaluated from numerical model.

| Day | CSA (mm²) | CSB (mm²) | CSC (mm²) | CSD (mm²) | Mass loss per day (g) | Cumulative mass loss (g) |
|-----|-----------|-----------|-----------|-----------|----------------------|--------------------------|
| 0   | 314.159   | 314.159   | 314.159   | 314.159   | 0.00                 | 0.00                     |
| 1   | 312.252   | 312.120   | 312.120   | 312.125   | 2.37                 | 2.37                     |
| 2   | 311.370   | 310.840   | 310.861   | 310.861   | 3.80                 | 6.17                     |
| 3   | 309.949   | 308.820   | 308.888   | 308.888   | 6.03                 | 12.20                    |
| 4   | 308.274   | 306.475   | 306.592   | 306.592   | 8.63                 | 20.83                    |
| 5   | 306.602   | 304.139   | 304.304   | 304.304   | 11.23                | 32.06                    |
| 6   | 305.057   | 301.966   | 302.176   | 302.176   | 13.64                | 45.70                    |
| 7   | 303.674   | 300.008   | 300.256   | 300.256   | 15.81                | 61.51                    |
| 8   | 302.407   | 298.204   | 298.487   | 298.487   | 17.81                | 79.32                    |
| 9   | 301.202   | 296.487   | 296.802   | 296.802   | 19.71                | 99.04                    |
| 10  | 299.984   | 294.756   | 295.103   | 295.103   | 21.64                | 120.67                   |
| 11  | 298.529   | 292.719   | 293.106   | 293.106   | 23.90                | 144.57                   |
| 12  | 296.862   | 290.412   | 290.845   | 290.845   | 26.46                | 171.03                   |

### Figure 12. Coordinate points connected with curves representing degraded surface topography of corroded steel on 12th day for segments (a) CSA, (b) CSB, (c) CSC and (d) CSD.

#### 7. Conclusions

The present work pertains to modelling non-uniform time dependent corrosion in 3D domain, analyzing the degraded surface topography of corroded rebar, evaluating mass loss and maximum pit depth and, extending the proposed multi-physics numerical
model as a tool for real-time simulation of spatial and temporal non-uniformity in corrosion induced deterioration to facilitate service life prediction.

The following conclusions can be drawn from the results presented in sections discussed earlier:

1. The multi-physics FE model can be used reliably as a substitute for the accelerated corrosion experiment which is commonly used for durability studies of corroding RC members. The validation shows that the model can predict the non-uniform
time dependent mass loss and maximum pit depth with acceptable accuracy which has valuable applications in estimating current state of degradation and service life prediction.

2. One of the possible reasons for deviation of weight loss predicted by Faraday’s law from experimental results was found to be non-inclusion of nonlinear corrosion current distribution and non-uniform corrosion as a consequence of differential aeration, resulting in cathodic locations on rebar, changing PS, concrete conductivity and temperature. Inclusion of these parameters in the proposed numerical model resulted in a much better prediction of weight loss and its localisation.

3. Time dependant weight loss, local current density (day wise), non-uniform degradation of rebar geometry can be obtained at every point on corroding surface using the numerical model which eliminates the need for simplification by assuming uniform mass loss and corrosion rate. These simplifications are commonly found in literatures pertaining to corrosion rate simulation and accelerated corrosion experiment. As the mass loss evaluated by experiment validates the mass loss evaluated from degraded rebar profile, the degradation profile generated, distribution of pits and maximum pit depth are also validated. This is a significant advancement from the conventional approaches found in literature pertaining to

Figure 15. Mass loss from numerical model compared with experimental results (a) Daywise, and (b) Cumulative.

Figure 16. Maximum pit depth as a function of time.
estimating current state of spatial and temporal degradation and conditions of SCI considering local exposure and environment.

4. Electrolyte conductivity and oxygen diffusivity are taken as function of PS, which are influenced by temperature, humidity, water cement ratio, varying ionic concentration of different chemical species etc. Instead, a single parameter such as PS is used to capture the effect, which intern is a function of time and therefore the model can easily be extended to simulate naturally corroding RC members.

5. Unlike previous studies, where predefined anodic and cathodic locations are assumed on steel surface, in the present model anodic and cathodic locations naturally evolve on corroding steel surface as corrosion progresses because of considering differential aeration corresponding to experimental setup. Differential aeration may arise due to the service conditions or local exposure in case of naturally corroding RC members and the presented modelling approach is best suited for such scenarios.

6. Both continuous and in situ monitoring of PS, concrete resistivity and temperature is possible with embedded sensors and NDT respectively. Therefore, the local environment can be captured on a real time basis, rendering the model free from possible deviations arising in prediction models that are based on climate data such as relative humidity. Also, these predictive models have larger possible deviations for long range predictions and are insensitive to local exposure and usage. It is recommended to switch from prediction models based on T-RH to the multi-physics model combined with NDT data to assess the current state of degradation for better accuracy and minimal deviations from actual conditions.

7. The presented numerical model apart from being able to simulate accelerated and natural corrosion also finds its application in Bayesian updating of predictive models that are based on climate change data such as T-RH.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Authors’ contributions

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