

Computer based FEM stabilization of oxygen transport model for material and energy simulation in corroding reinforced concrete

Raja Rizwan Hussain*

Department of Civil Engineering, College of Engineering at King Saud University, Riyadh, Saudi Arabia

(Received May 19, 2012, Revised May 4, 2013, Accepted July 30, 2013)

Abstract. This paper unveils a new computer based stabilization methodology for automated modeling analysis and its experimental verification for corrosion in reinforced concrete structures under the effect of varying oxygen concentration. Various corrosion cells with different concrete compositions under four different environmental conditions (air dry, submerged, 95% R.H and alternate wetting-drying) have been investigated under controlled laboratory conditions. The results of these laboratory tests were utilized with an automated computer-aided simulation model. This model based on mass and energy stabilization through the porous media for the corrosion process was coupled with modified stabilization methodology. By this coupling, it was possible to predict, maintain and transfer the influence of oxygen concentration on the corrosion rate of the reinforcement in concrete under various defined conditions satisfactorily. The variation in oxygen concentration available for corrosion reaction has been taken into account simulating the actual field conditions such as by varying concrete cover depth, relative humidity, water-cement ratio etc. The modeling task has been incorporated by the use of a computer based durability model as a finite element computational approach for stabilizing the effect of oxygen on corrosion of reinforced concrete structures.

Keywords: oxygen; corrosion; stabilization; material modeling; computers; concrete

1. Introduction

Reinforced concrete construction corrodes under the effect of various environmental actions such as chloride, carbonation, temperature etc. However, these environmental loadings can cause corrosion only if enough amount of oxygen is available in vicinity of corroding reinforcement bar in concrete construction. Therefore, it is necessary to understand and predict the automated effect of oxygen concentration variation on corrosion of RC construction. Researchers have investigated the effect of oxygen on corrosion of RC construction in the past (Hussain 2011a, Hussain 2011b, Hussain and Ishida 2011a, Kurahashi and Oshita 2010, Raupach 1996). In this research, qualitative as well as quantitative (for which the previous research data is limited) deep investigations have been carried out in order to clarify the involved mechanisms of corrosion under varying oxygen conditions by incorporating realistic and automated mass balance computer-aided modeling as well as multi variable laboratory controlled experimentation. The analysis of oxygen model itself had

*Corresponding author, Assistant Professor, E-mail: raja386@hotmail.com

defined stability problems which needed to be fixed in the first place before comparing with the experiment results. Once the model itself started working properly, then in the next step it was compared with the experiment results to check the reliability of the model. Thus, the objective of this research was to stabilize the oxygen model by comparing the old and new methodologies and then verifying by experiment results, so that the stabilized model can be used for corrosion estimation with full confidence.

1.1 Fem computational modeling measurement approach:

The methodology adopted in this research is based on a 3D finite element model (Hussain and Ishida 2011b, Hussain and Ishida 2010b, Ishida and Maekawa 1999, Ishida 1999, Maekawa *et al.* 1999a, Maekawa *et al.* 1999b). It is a computational program for the evaluation of various durability aspects of concrete such as concrete hardening (hydration), microstructure formation and several associated phenomena, from casting of concrete to a period of several months or years. As such this tool can be utilized to study the effect of ingredient materials, environmental conditions as well as the size and shape of the structure on the durability of concrete. The term durability considered here takes into account both the fresh concrete problems as well as matured concrete exposed to environment. This tool can be used to analytically trace the evolution of microstructure, strength and temperature with time for any arbitrary initial and boundary conditions with some limitations. Since the main simulation program is based upon finite-element methods, it could be applied to analyze real life concrete structures of any shape, size or configuration. Furthermore, dynamic coupling of several phenomena ensures that the effects of changing environmental conditions are easily integrated into the overall simulation scheme.

1.2 Kinetics of oxygen model

The corrosion model is initially adopted from the previous research (Hussain and Ishida 2011b, Hussain and Ishida 2007, Ishida and Maekawa 2000, Maekawa *et al.* 1999b). In general, when dealing with mass, energy and momentum flows in a control volume, the starting point is to build appropriate balance equations (Welty *et al.* 1969). In other words, the summation of rate of mass efflux from a control volume, the rate of mass flow into the control volume, and the rate of accumulation of mass within the control volume should be zero. In this section, the mass balance

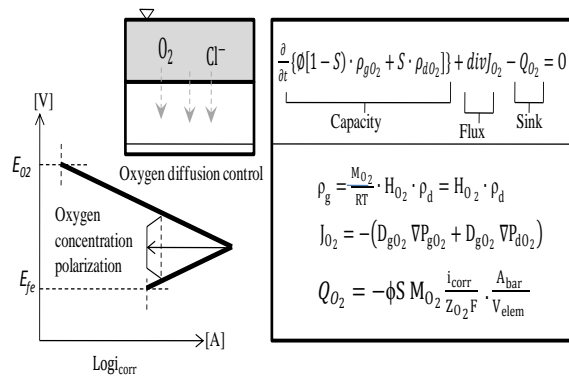
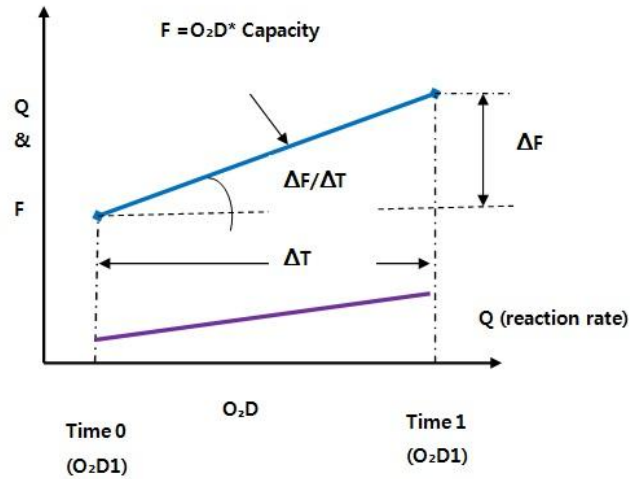
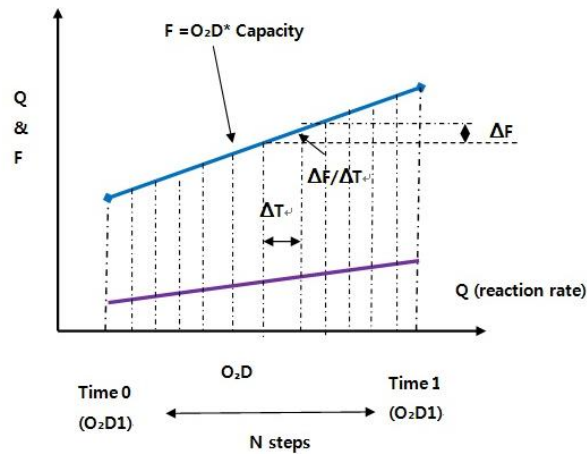


Fig. 1 Limited corrosion current due to oxygen concentration polarization



(a) Large time step



(b) Small time step

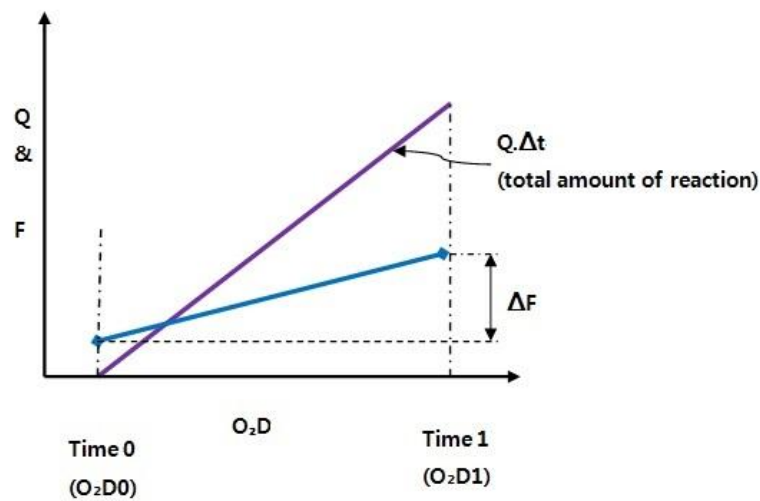
Fig. 2 (a)-(b) – Oxygen capacity and oxygen consumption

conditions for oxygen in a porous medium are formulated. Two phases of oxygen existing in concrete are considered; gaseous oxygen and oxygen dissolved in pore water. By solving the mass balance equation under given initial and boundary conditions, the non-steady state conduction of oxygen is quantified.

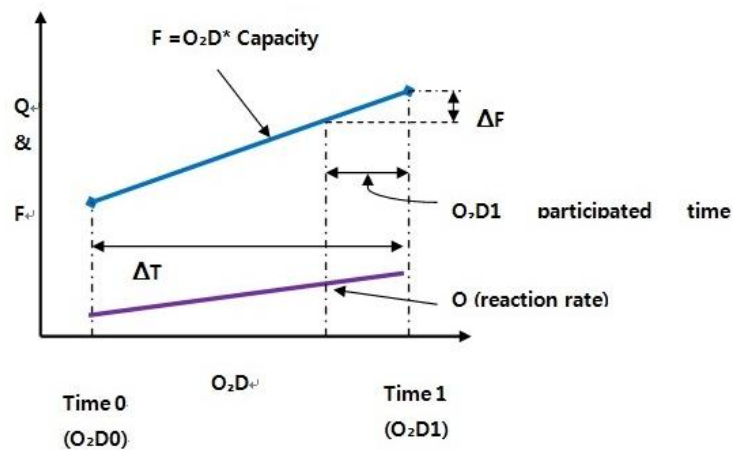
Transport of O_2 is considered for both dissolved and gaseous oxygen phases. The O_2 gas can move through unsaturated pores, whereas dissolved O_2 is transported within pore liquid water. In the model, it is assumed that all pores have a cylindrical shape. In the model, molecular diffusion and Knudsen diffusion are considered, whereas the contribution of surface diffusion is ignored, since surface diffusion takes places when molecules which have been adsorbed are transported along the pore wall, and normally it plays a minor role in diffusion within concrete materials under typical environmental conditions.

When the amount of oxygen supplied to the reaction is not enough, corrosion rate would be controlled by diffusion process of oxygen. By coupling with above oxygen transport model, this phenomenon can be logically simulated. Current density i_{corr} , which is obtained as the intersection of anodic and cathodic polarization curve, corresponds to the corrosion under sufficient availability of oxygen. When oxygen supply shortens, the corrosion current is limited by the slow diffusion of oxygen (Fig. 1). This limited oxygen concentration environment gives rise to the oxygen concentration polarization. A value of current density i_L can be expressed as

$$\frac{i_L}{z_{\text{Fe}} F} = O_2^{\text{sup}} \quad (1)$$



(a) Large time step



(b) Small time step

Fig. 3 (a)-(b) – Influence of length of time step on the amount of reaction

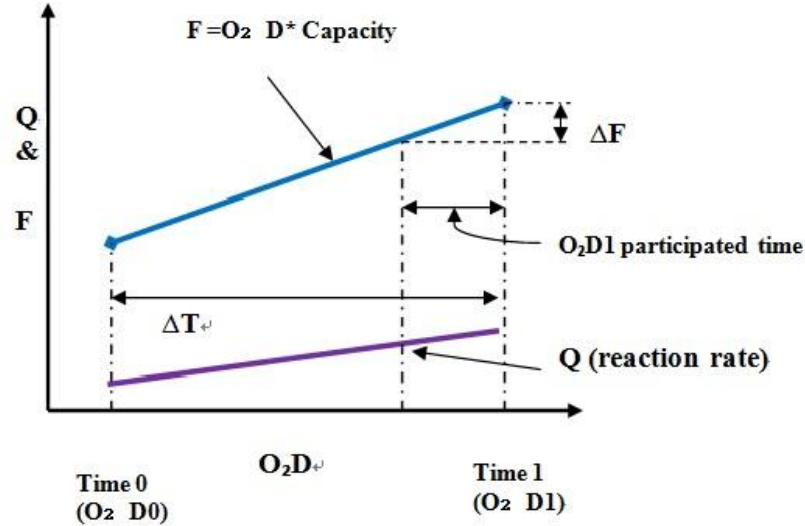


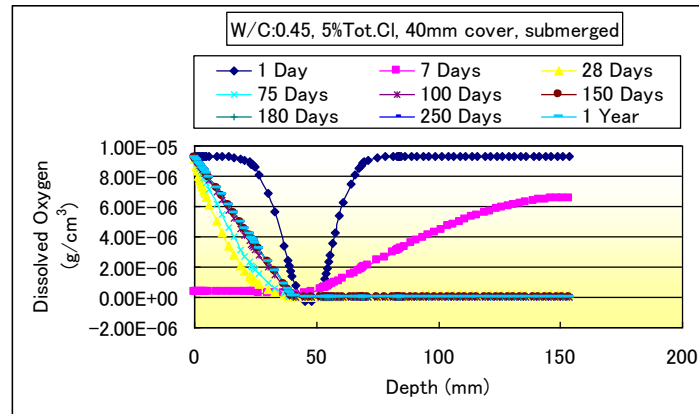
Fig. 4 Computation of minimum required reaction time

Where, O_2^{sup} [mol/m².s] is the amount of oxygen supplied to surface of metal, which is obtained by the equilibrium and transport model for oxygen discussed in the above section. In this research, the rate of corrosion under diffusion control of oxygen i_{corr} [A/m²] (A/ft²) is assumed to be as equal to limiting corrosion value calculated by the Fick's Law of diffusion. Fig. 2 shows an outline of oxygen diffusion corrosion model. Finally, using Faraday's law, electric current of corrosion is converted to the rate of steel corrosion. These models derive from mass balance electrochemistry. Further development and improvements are still needed through various verifications of corrosion phenomena in real concrete structures. Fig. 3 summarizes the complete mass balance of oxygen transport-corrosion model (Hussain and Ishida 2011a).

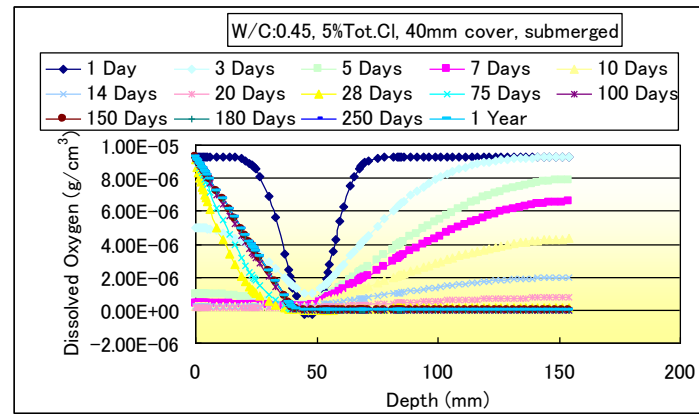
1.3 Computer based stabilization of oxygen model

It was found from the model analysis results that the computation of oxygen model and its convergence highly depended on the time steps. To get stable results, the time step should be very small and in such a situation, the computation time will be very large. The model situation was that even with a time step as small as 0.0002 days, the model still gets unstable and the value of dissolved oxygen becomes negative with a considerably large magnitude on the negative side or sometimes even the analysis collapsed completely. So the final impact was that the total corrosion was much under estimated from the original value. Also using very small time steps means much longer calculation times which is not efficient and is a waste of time (Eymard *et al.* 2000, Eymard *et al.* 2002, Scheiner *et al.* 2009).

Fig. 2 shows oxygen capacity (F) and oxygen consumption rate (Q), for different time steps. Based on this figure, the period of time step has minor effect on the value of (df/dt-Q), only difference may occur due to the influences caused by non- linearity of F or Q in the time step. But,



(a)



(b)

Fig. 5 (a)-(b) – Dissolved Oxygen profile

it should be noted that the concentration of dissolved oxygen (shown as O_2D in Fig. 2) continuously participates in the reaction process. The amount of reaction $Q.Dt$, is highly dependent on the time step and controls the consumption of dissolved oxygen. Concentration of dissolved oxygen (O_2D) during the reaction process is consumed; however it is again replaced from the environment. Consideration of this replacement is the key for stable analysis of oxygen model with regards to the negative value of computed dissolved oxygen.

The influence of length of time step on amount of reaction is shown in Fig. 4. From the figure it is obvious that total amount of reaction at Time1 in the figure ($Q.Dt$) is equal to total amount of reaction at Time1 ($\sum QnDtn$). However in Fig. 5, the concentration of oxygen O_2 participated in reaction process, in each time step, is large enough for reaction or in other words always $Q.Dt$ is less than amount of participated O_2 . At the end of each time step in Fig. 3, concentration of oxygen O_2 again is assumed to replace from the environment (even all amount has been consumed in previous step). But when the time step is large (Fig. 3), this replacement of O_2 , which is continuously done in reality, is ignored. So in order to fix this problem, following methodology is adopted.

2. Stabilization methodology

The minimum reaction time enough for the replacement of oxygen was computed. This was done to ensure that the capacity remains more than the consumption in the oxygen model. Consider the Figure 4 below for further illustration.

The reaction time (Dt_{Reac}) is calculated by the total oxygen and oxygen consumption rate (the time in which all oxygen is consumed = total oxygen / oxygen consumption rate under plenty of oxygen supply). If the time step is larger than this period the reaction cannot continue. The reaction process is continuously occurred during reaction process, independent on period of time step. If the reaction time is more than the time in which all oxygen is consumed then the corrosion is calculated by the limiting corrosion value (Scheiner and Hellmich 2007). Corrosion is re-computed based on the total amount of reaction during reaction time. Mass balance equation is checked for current step during the participated time of O_2 $D1$ (Dt_{ParO}) as shown in Fig. 4.

2.1 Scrutiny of analytical results using the stabilized model

The oxygen model stability modification was checked for proper functionality. A typical case for the following conditions was considered for checking:

0.45 percent W/C, 5 percent total chloride content by mass of binder, 40 mm clear cover to concrete, curing conditions: the specimen was typically cured under sealed conditions for 28 days and then submerged under water for a period of 1 year, Maximum time step: 5 days.

The output file was checked and documented at several time intervals. The oxygen model has much improved by above modification. Just looking at the negative values in the Table 1 below, one may feel that the dissolved oxygen is becoming negative all the time from day 1 up to the 365 days, as there are negative values at almost all days in the Table 1. But, it is not important how many times the value of dissolved oxygen becomes negative. The more important thing is how much negative it becomes in magnitude. It can be seen that the magnitude of negative values is very small and can be neglected considering the numerical calculation limitations. Details are provided in the following pages.

From the Fig. 5 it can be seen that although the value of dissolved oxygen becomes negative but its magnitude on the negative side is very less as compared to the magnitude of dissolved oxygen on the positive side. This is in contrast to previous model results shown in Fig. 6.

Therefore, it can be said that the oxygen model has much stabilized by the proposed time step modification and works good. One more thing which was noticed was that the results of 7 days look a bit strange as compared to the other results as the amount of dissolved oxygen at the surface seems to be almost zero in just seven days. In order to check this behavior dissolved oxygen profiles at several times intervals from Day 1 to Day 28 were plotted as shown in the Fig. 5(b).

In the Fig. 5(b) it can be seen that the oxygen actually gradually reduces from both sides (0mm and 200 mm in the modeled concrete specimen; see previous sections for details) from Day 1 until the sealed curing of 28 days ends. And then right after 28 days when the specimen is submerged into water it goes back to the original dissolved oxygen concentration at the surface and remains almost zero in the inner side. This is much clear and makes sense, except that the rate of decrease of dissolved oxygen seems a bit faster than normal. Overall, the results look nice.

Fig. 6 shows the previous model analysis without installing the oxygen stability model under discussion. It can be clearly seen that the modified model shows much reduction in the magnitude of negative dissolved oxygen as compared to the previous model. Similar time step independency

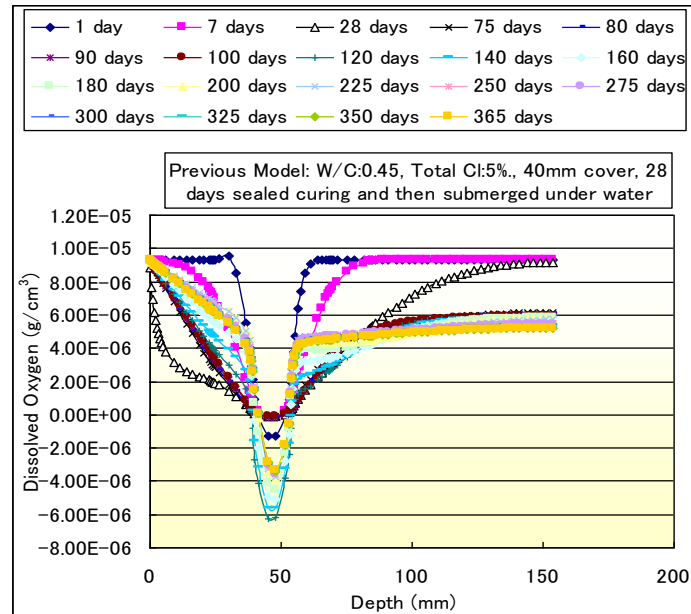
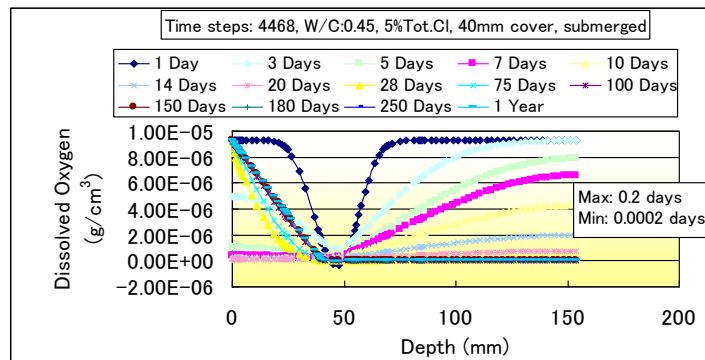
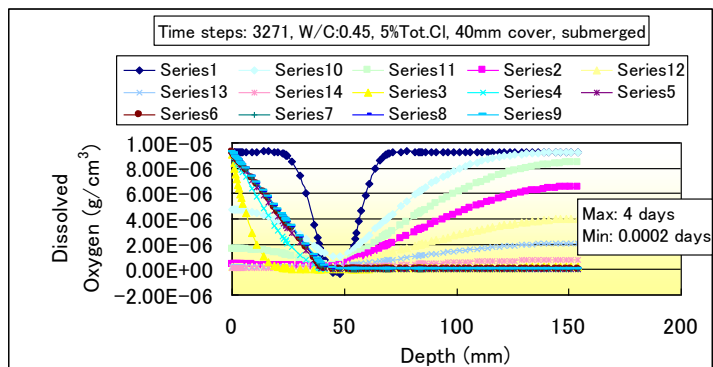


Fig. 6 Analysis by previous oxygen model

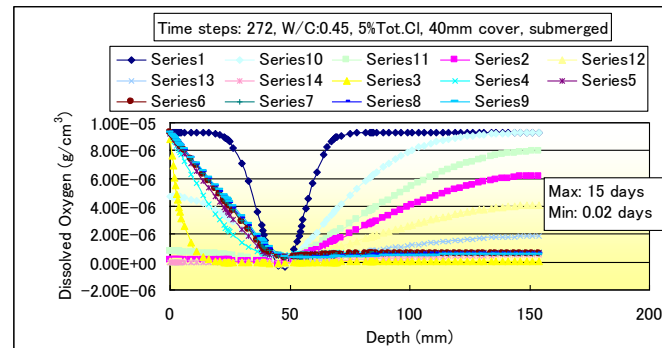


(a)



(b)

Fig. 7 (a)-(c) –Time step independency and stability of modified model



(c)

Fig. 7 Continued

Table 1 Dissolved Oxygen (g/cm^3)

Depth/Time	1	7	28	75	100	150	180	250	365
45.1	-2.45E-07	1.67E-07	1.67E-09	1.09E-08	7.77E-09	1.61E-09	-1.51E-09	-1.01E-08	-2.25E-08
47.9	-2.85E-07	-5.47E-09	-5.47E-09	5.08E-09	-2.36E-09	-1.19E-08	-1.56E-08	-2.42E-08	-3.72E-08
51.6	6.74E-07	2.32E-09	2.32E-09	8.65E-09	4.59E-09	2.60E-09	1.31E-09	1.79E-10	-2.83E-09

(W/C: 0.45, concrete cover: 40mm, Tot. Cl: 5%, submerged condition)

of the modified model can be seen in the Fig. 7. Concluding the above discussion, the modification works well and this small negative value of dissolved oxygen can be accepted as numerical calculation limitation.

2.2 Experimental validation of stabilized oxygen model

Deformed round carbon steel bars 13 mm in diameter were used as reinforcing material in the experiment specimens. Ordinary Portland cement (OPC) as per ASTM specifications was used. Natural river sand passed through sieve No. 4 (4.75 - mm openings), was used as fine aggregate for all concrete mixes. Its density and water absorption were $2.65 \text{ g}/\text{cm}^3$ ($165.43 \text{ lb}/\text{ft}^3$) and 2.21%, respectively. Crushed sandstone with a maximum size of 20 mm was used as coarse aggregate with density of $2.70 \text{ g}/\text{cm}^3$ ($168.55 \text{ lb}/\text{ft}^3$) and water absorption 0.59%. The air content was kept around $3.5 \pm 1\%$.

Uniform chloride content has been used as corrosion initiator considering the corrosion cell as a fused anode cathode system. The oxygen concentration available for corrosion at the surface of rebar embedded in concrete was limited by varying water to cement ratios, cover depths and chloride concentrations. Specimens were allowed to set and harden in mold for 1 day before being de-molded and then cured for the next 28 days in the environment control chamber in sealed condition at 20°C . After that the specimens were epoxy coated on the top face edges of plastic containers in order to avoid any possible oxygen penetration and given the already described four environment exposures for six months and one year durations. Half-cell potentials were measured

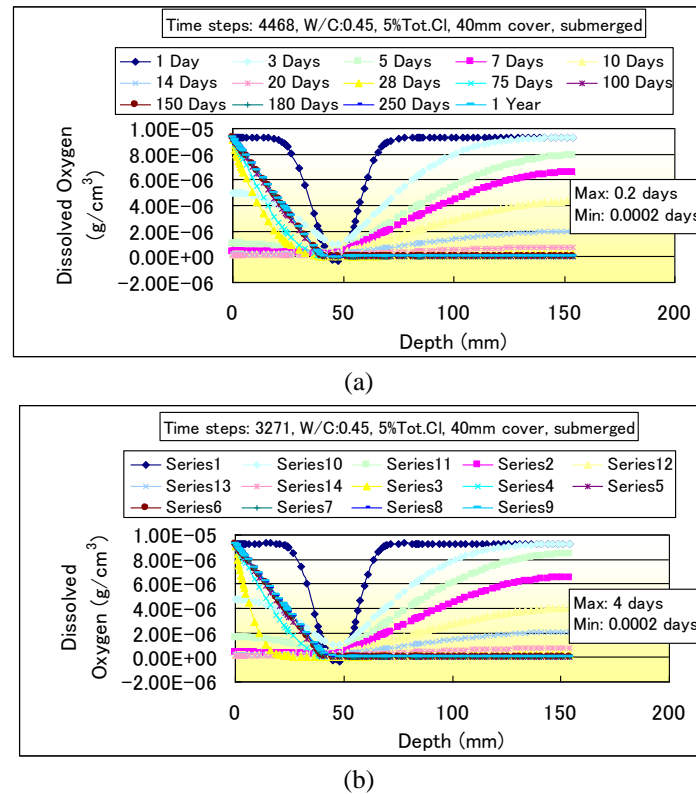


Fig. 8 (a)-(c) –Time step independency and stability of modified model

with two days interval for all specimens using copper-copper sulfate reference electrode (CSE) in accordance with standard specifications which can be found elsewhere (Ishida and Maekawa2000). The complete details can be obtained from the already published research (Hussain and Ishida 2011a, Hussain and Ishida 2010a).

2.3 Comparison of experiment results with previous model and enhanced oxygen model with time step stabilization

In this section a comparison between the experiment results and analysis is given by the previous and modified model for a time period of six months and one year. A typical nominal case as shown in Fig. 8 (Hussain and Ishida 2011a, Hussain and Ishida 2010a) has been selected for this study. The first “EXP” is for 6 months experiment result and second “EXP” is for 1 year experiment results for all the four cases and same is for the model analysis. The “Previous model” means the original model without any modification and “modified model” stands for the oxygen stabilized model after modification for independency of time step. The comparison with experiment results shows improved results by the oxygen stability in the modified model as compared with the previous model. Overall there is much increase in the corrosion rate from previous to modified model for all the four cases as shown in the Fig. 8.

In case of “Air” the model shows same results by previous and modified model which is logical.

Comparison with experiment results also seems reasonable for both 6 months and one year time periods. In submerged case “Sub”, the previous model shows little under estimation while the modified model shows a little over estimation. So, modified approach is better since it gives safer side analysis. In case of 95% R.H case, the modified model shows much higher values as compared to the previous model in comparison to the experiment results. The same impression can be had that previous model under estimates and the modified model over estimates. But again the over estimation comparison is better than the under estimation comparison as far as the safety of structure against failure is concerned. For alternation wetting drying case “W/D”, again much improvement can be seen in case of modified model which shows closer comparison to experiment results as compared to the previous model. But, it still under estimates the experiment results in contrast to the above two cases.

6. Conclusions

It can be concluded that the modified model is good for dry air condition, shows a little over estimation for submerged and 95% R.H and a little under estimation for W/D. Overall, the stabilized model works well and shows much improved results. The research presents the comparison of a simple oxygen model and stabilized oxygen model along with the verification of the results by the use of past experiment data. The comparison of experiment results with the modified stabilized methodology used in automated model simulation shows that the model can effectively predict the influence of oxygen on corrosion on RC construction qualitatively. In this research the effect of oxygen on corrosion of RC construction under various prevailing environments and compositions has been successfully obtained by automated computer-aided, mass balance, transport simulation design and constitutive modeling which is also verified through extensive laboratory experimentation conducted in the past. The comparison of experiment results and automated model simulation shows that the model stabilized in this research can effectively predict the influence of oxygen on corrosion on RC concrete qualitatively and with some limitations quantitatively which needs further enhancement as a scope for future research.

Acknowledgements

The author acknowledges the support by King Saud University, Deanship of Scientific Research, College of Engineering Research Center.

References

- Eymard, R., Gallouet, T. and Herbin, R. (2000), “Handbook of Numerical Analysis”, Finite volume methods, **7**(3), 731-1018.
- Eymard, R., Gallouet, T., Herbin, R. and Michel, A. (2002), Convergence of a finite volume scheme for nonlinear degenerate parabolic equations, *Numer. Math.*, **92**(1), 41-82.
- Hussain, R.R. (2011a), “Enhanced mass balance Tafel slope model for computer based FEM computation of corrosion rate of steel reinforced concrete coupled with CO₂ transport”, *Comput. Concr.*, **8**(2), 177-192
- Hussain, R.R. (2011b), “Effect of moisture variation on oxygen consumption rate of corroding steel in chloride contaminated concrete”, *Cement Concrete Compos.*, **33**(1), 154-161.

- Hussain, R.R. and Ishida, T. (2011a), "Computer-aided oxygen transport model of mass and energy simulation for corrosion of reinforced steel", *Autom. Construct. J.*, **20**(5), 559-570.
- Hussain, R.R. and Ishida, T. (2011b), "Enhanced electro-chemical corrosion model for reinforced concrete under severe coupled environmental action of chloride and temperature", *Construct. Build. Mater. J.*, **25**(3), 1305-1315.
- Hussain, R.R. and Ishida, T. (2010a), "Influence of connectivity of concrete pores and associated diffusion of oxygen on corrosion of steel under high humidity", *Construct. Build Mater.*, **24**(6), 1014-1019.
- Hussain, R.R. and Ishida, T. (2010b), "Development of numerical model for FEM computation of oxygen transport through Porous media coupled with micro-cell corrosion model of steel in concrete structures", *Comput. Struct. J.*, **88**(9-10), 639-647.
- Hussain, R.R. and Ishida, T. (2007), Modeling of corrosion in RC structures under variable chloride environment based on thermodynamic electro-chemical approach, Journal of SSMS, JAPAN, SMS07-106, **3**, 104-113. (Best paper award for the last four years 2005-2009)
- Ishida, T. and Maekawa, K. (2000), "Modeling of pH profile in pore water based on mass transport and chemical equilibrium theory", *Proceedings of JSCE*, No.648/V-47.
- Ishida, T. and Maekawa, K. (1999), "An integrated computational system for mass/energy generation, Transport, and Mech. Mater. Struct.", *Journal of JSCE*, No.627/V-44.
- Ishida, T. (1999), An integrated computational system of mass/energy generation, transport and mechanics of materials and structures, Thesis Ph.D, University of Tokyo, Japan.
- Kurahashi, T. and Oshita, H. (2010), Shape determination of 3-D reinforcement corrosion in concrete based on observed temperature on concrete surface, *Comput. Concr.*, **7**(1), 63-81.
- Maekawa, K., Chaube, R. and Kishi, T. (1999a), Modeling of concrete performance, E & FN Spon, NY.
- Maekawa, K., Chaube, R. and Kishi, T. (1999b), Modeling of Concrete performance, E&FN Spon NY.
- Papadakis, V.G., Vayenas, C.G. and Fardis, M.N. (1991), "Fundamental modeling and experimental investigation of concrete carbonation", *ACI Mater. J.*, **88**(4), 363-373.
- Rui, H. (2008), "A conservative characteristic finite volume method for solution of the advection-diffusion equation", *Comput. Methods Appl. Mech. Engrg.*, **197**(45-48), 3862-3869.
- Raupach, M. (1996.), "Investigations on the influence of oxygen on corrosion of steel in Concrete-Part 1", *Mater. Struct.*, **29**, 174-184.
- Scheiner, S. and Christian, H. (2009), "Finite volume model for diffusion- and activation-controlled pitting corrosion of stainless steel", *Comput. Meth. Appl. Mech. Eng.*, **198**(37-40), 2898-2910.
- Scheiner, S. and Hellmich, C. (2007), "Stable pitting corrosion of stainless steel as diffusion-controlled dissolution process with a sharp moving electrode boundary", *Corrosion Science*, **49**(2), 319-346.
- Welty, J.R., Wicks, C.E. and Wilson, R.E. (1969), Fundamentals of momentum heat and mass transfer, John Wiley & Sons, Inc.