ON THE NUMERICAL SOLUTION OF LAPLACE'S EQUATION WITH NONLINEAR BOUNDARY CONDITIONS FOR CORROSION OF STEEL IN CONCRETE

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ABSTRACT

A comprehensive finite element model for predicting the rate of steel corrosion in concrete structures has been developed. The model consists of the solution of Laplace's equation for electric potentials with nonlinear boundary conditions imposed by the polarization of the steel surface. Since current density is a function of potential distribution, the boundary conditions depend on the potential distribution within the medium; hence, the problem is nonlinear. The degree of nonlinearity depends on the geometry of the domain and the boundary conditions, i.e. reinforcement detailing, and whether boundary conditions are defined using simplified or detailed polarization equations. Authors have been working on new methods to improve convergence of the nonlinear solution of Laplace's equation, which can be, at times, difficult to achieve. In this paper, authors will demonstrate the issues associated with the nonlinear solution of Laplace's equation to calculate the corrosion rates in reinforced concrete members. Two methods for the solution of the corrosion problem will be introduced. The results and the convergence rates of the nonlinear solutions obtained from these two methods will be compared.

KEY WORDS

steel corrosion, concrete, polarization, nonlinear solution, Laplace's equation, convergence.

INTRODUCTION

The corrosion of steel in concrete is a result of the dissolution of iron in pore water which can be represented by the following half-cell reaction (Broomfield 1997):

[1] $Fe \rightarrow Fe^{2+} + 2e^-$
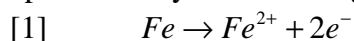
The electrons that are produced in this anodic reaction must be consumed at the cathodic sites on the steel surface to preserve electrical neutrality. The cathodic reaction in which these free electrons are consumed is the oxygen reduction given by:

[2] $\frac{1}{4}O_2 + \frac{1}{2}H_2O + e^- \rightarrow OH^-$

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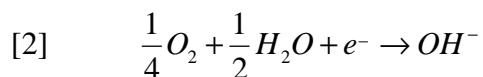
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The corrosion rate at any point on the surface of steel in concrete is related to the current density, which can be predicted if the electrochemical potential (abbreviated henceforth as "potential") distribution around that point is known. Once the potential distribution along the reinforcement is known, the current density at any point can be calculated by (Munn 1982):

$$[3] \qquad i = -\frac{1}{r}\frac{\partial \phi}{\partial n}$$

where i [A/cm^2] is the current density, ϕ [volts] is the potential, r [Ω-cm (ohm-cm)] is the resistivity of the pore solution and n is the direction normal to the bar surface. The rate of rust production at the anodic regions on the steel surface can be calculated by Faraday's law. Therefore, once the current densities on the steel surface are calculated, the determination of the rate and amount of corrosion becomes a straightforward task. The main difficulty in this process is the calculation of current densities on the steel surface. As it can be observed from Eq. 3, the calculation of current densities requires knowledge of the potential distribution around the reinforcement.

GOVERNING EQUATION

The equation governing the potential distribution can be derived from first principles (Munn 1982). If the domain is assumed to be homogeneous, i.e. resistivity of the medium is assumed to be constant within the domain, the potential distribution is governed by the Laplace's equation (Munn 1982):

$$[4] \qquad \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

where x and y are planar Cartesian coordinates.

Calculation of the potential distribution around the surface of the steel involves the solution of Eq. 4 subject to prescribed boundary conditions. These boundary conditions comprise the relationship between potential and current density for the anodic and cathodic regions as well as prescribed current densities. For the anodic and cathodic regions of the steel surface, as illustrated in Fig. 1, the boundary conditions can be defined as (Uhlig 1985):

$$[5] \qquad \phi_a = \phi_{Fe} + \beta_a \log \frac{i_a}{i_{oa}}$$

$$[6] \qquad \phi_c = \phi_{O_2} + \beta_c \log \frac{i_c}{i_{oc}} - \frac{2.303RT}{zF} \log \frac{i_L}{i_L - i_c}$$

where ϕ_{Fe} and ϕ_{O_2} are non-standard equilibrium potentials, β_a is the Tafel slope of the anodic reaction, β_c is the Tafel slope of the cathodic reaction, i_a and i_c are anodic and cathodic current densities, respectively, i_{oa} is the exchange current density of the anodic reaction, i_{oc} is the exchange current density of the cathodic reaction, R is the universal gas constant, T is the temperature, and i_L is the limiting current density. In Eq. 5, the polarization is due to activation, and in Eq. 6, it is in the form of activation and concentration polarization. It can be observed that the cathodic polarization imposes more nonlinearity than the anodic polarization.
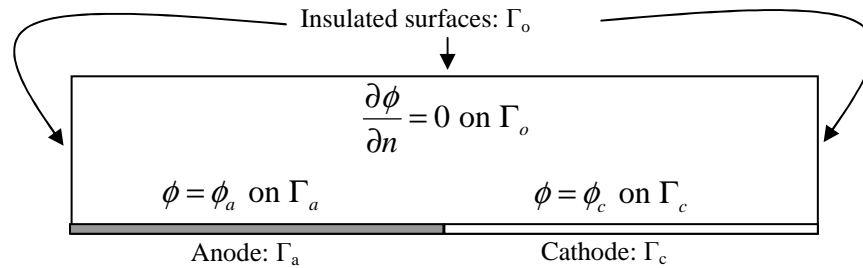
Insulated surfaces: Γ_o

$$\frac{\partial \phi}{\partial n} = 0 \text{ on } \Gamma_o$$

$\phi = \phi_a$ on Γ_a

$\phi = \phi_c$ on Γ_c

Anode: Γ_a

Cathode: Γ_c

Figure 1: Boundary conditions of a typical rebar corrosion problem type

SOLUTION BY DIRECT ITERATION METHOD

One of the methods that can be used to solve the nonlinear boundary value problem for the calculation of corrosion rates is the direct iteration method (DIM). With the reference to Fig. 2, the DIM consists of constructing a series of solutions $\{\phi^0\}, \{\phi^1\}, \cdots, \{\phi^k\}$, where $\{\phi^k\}$ is calculated from the previous value $\{\phi^{k-1}\}$, where the superscript, k, represents the iteration number. The solution starts with the assumption of values for all potentials on the steel surface, $\{\phi^0\}$. These initial potentials can be calculated by substituting small values of current densities, i_a and i_c in Eqs. 5 and 6, respectively. The solution of Eq. 4 with imposed values of the initial potentials at the cathodic and anodic surface of the steel rebars yields a potential distribution within the domain. The potential gradients at the steel concrete interface that are obtained form this distribution are used to calculate new current densities by using Eq. 3, and then the calculated current densities, i_a and i_c, are respectively substituted in Eqs. 5 and 6 to update the new potentials on the steel surface. With these new boundary conditions, Eq. 4 can be solved again to obtain a new set of potentials in the domain. At the end of each solution, the calculated nodal values of the potential are compared with the corresponding values in the previous iteration to check for convergence. Iterations are terminated when a user-defined convergence norm is satisfied.

It should be noted that Fig. 2 shows an ideal case where the solution converges to the expected result with successive iterations. Even though the DIM is easy to implement, it has significant limitations, and for complex problems such as reinforcement corrosion in concrete structures, it generally fails to provide converged and accurate results. One of the main reasons why the DIM does not provide converged and accurate solutions is that it is not based on an analytical nonlinear solution algorithm. Iterations are based on the conditions that are valid at a given iteration and do not include any information from previous iterations. In other words, there is a randomness associated with the DIM, hence to achieve accurate results, large number of iterations may be necessary.

Another limitation of the DIM is the fact that it can violate the limitation imposed in the polarization of the cathodic reactions by the limiting current density. During any iteration, the current density calculated from the solution of the Laplace's equation can be larger than the limiting current density. When this happens, the solution will not converge, as illustrated

in Fig. 3. This problem is more significant when the limiting current density is small, a situation that can be observed in concrete structures where the oxygen supply around the reinforcement is limited. It is also obvious from Fig. 3 that initial assumption of the current densities can make a significant difference in the convergence of the solution (Path A-B vs. path C-D).

SOLUTION BY MODIFIED DIRECT ITERATION METHOD

Modified direct iteration method (MDIM) is a generalized version of the DIM. The MDIM uses the same approach as the DIM, albeit with a relaxation factor, ξ. Therefore, it is still subject to some of the issues that were described for the DIM. In the MDIM, the boundary conditions on the steel surface, assuming Dirichlet-type definition, are determined as:

[7] $$\phi^{k+1} = (1-\xi)\phi^k + \xi f(i^k)$$

where ξ is a factor between 0 and 1. The new boundary condition ϕ^{k+1} is calculated as a weighted average of the boundary condition of the previous iteration and the boundary condition provided by the polarization equation, $f(i^k)$. The MDIM has an inherent measure of trust that the new iterate is moving towards a converged solution. It should be noted that when $\xi = 1$, the MDIM is the same as the DIM.

As illustrated in Fig. 4, the MDIM can provide a converged solution when the DIM method is not successful. In addition, due to the reasons that are obvious in Fig. 4, the convergence of the solution is generally faster in the MDIM. However, the success and rate of convergence of the MDIM is function of the value of ξ.
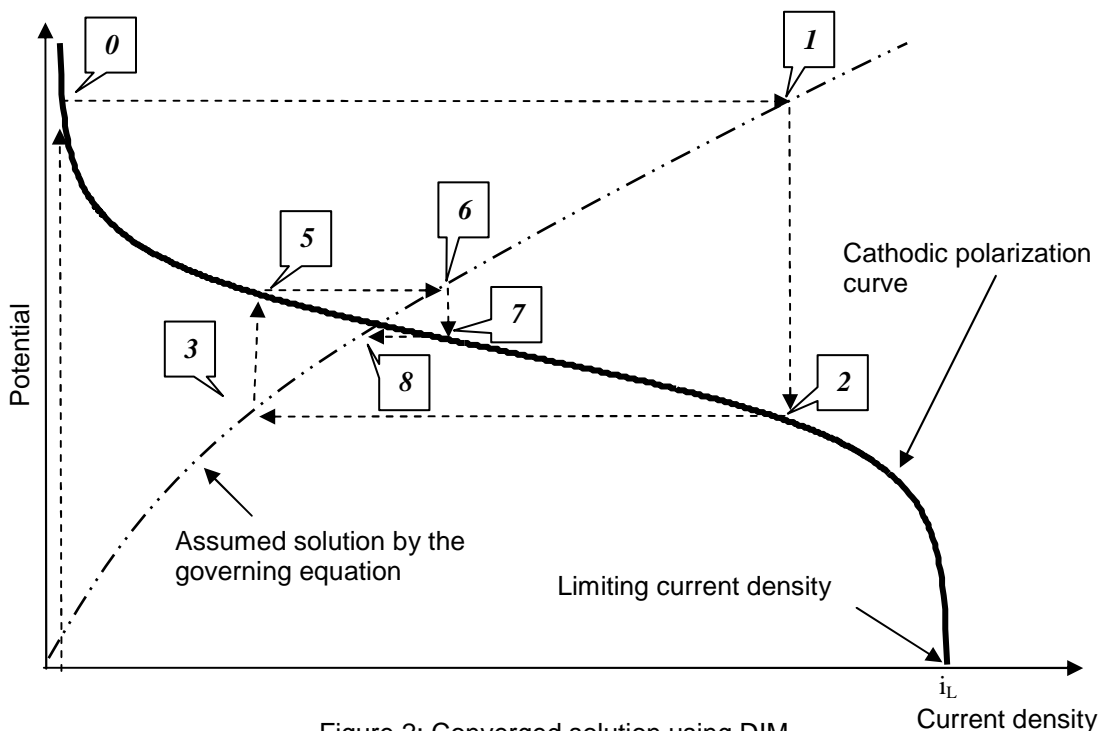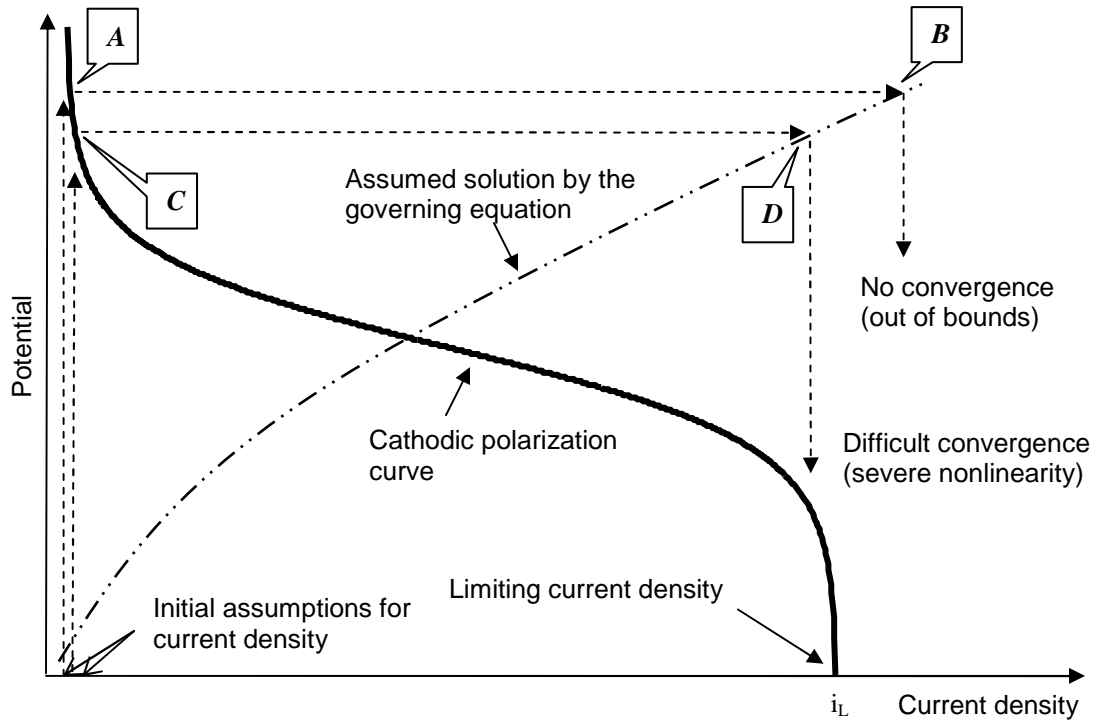

Figure 2: Converged solution using DIM

Figure 3: The effect of limiting current density on the convergence of DIM
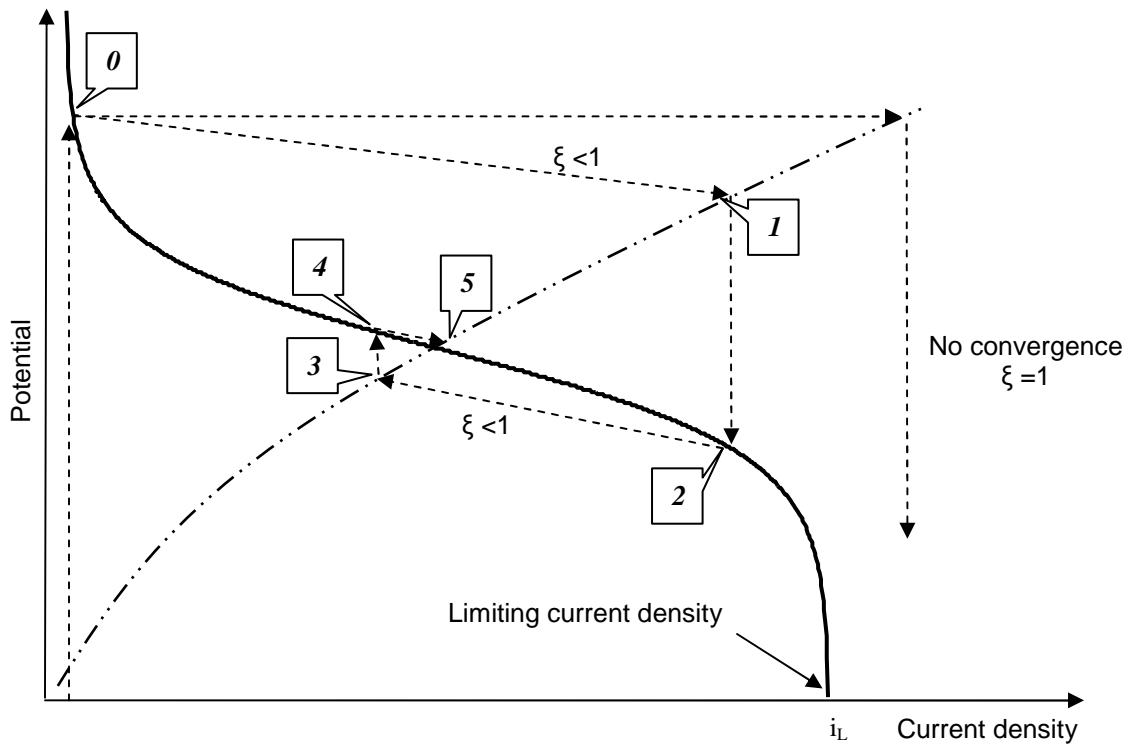

Figure 4: Solution using MDIM

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COMPARISON OF THE SOLUTION METHODS

A typical test case, as shown in Fig. 5, is used to compare the solution algorithms described above. The sensitivity of the results and convergence of the solution as a result of the changes in the following parameters is investigated: (1) element size, (2) anode-to-cathode ratio, (3) resistivity of the concrete pore solution.
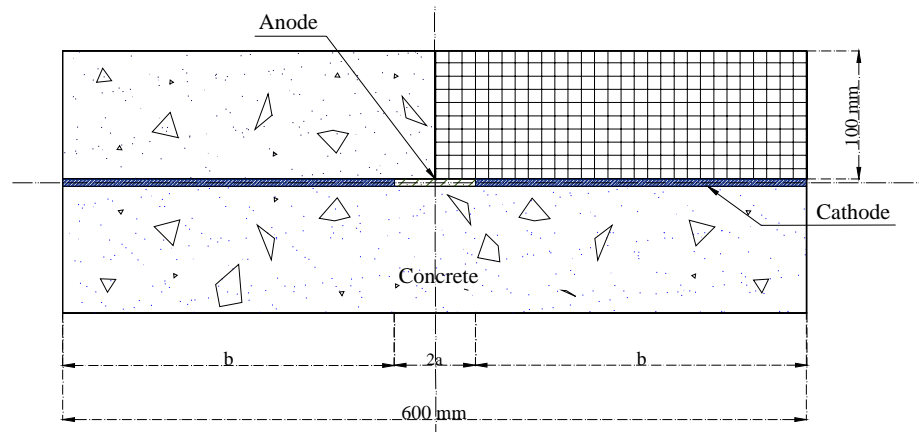

Figure 5: Model used in the comparison of the solution algorithms

As illustrated in Fig. 5, using symmetry, only half of the upper-right quarter of the member is modeled. To simplify the problem, the concrete is treated as a homogenous medium with uniform resistivity. In order to eliminate the possible convergence problems that may originate from the limiting current density, it is assumed that adequate amount of oxygen is present around the reinforcement. Therefore the limiting current density used in the analysis is selected as 1×10^{-6} A/mm^2, which is large enough to ensure that the convergence issues will not be as a result of the limiting current density. Table 1 provides the input parameters and constants that are used in the analyses presented here.

EFFECT OF ELEMENT SIZE

The effect of element size on the convergence of the nonlinear finite element solution of the corrosion problem defined Fig. 5 is studied. Nonlinear solution algorithms described in the previous sections are used to solve the problem with varying element size. The anode-to-cathode ratio is kept constant as 0.111, with an anode length of 60 mm (cathode length = 540 mm). Table 2 shows a comparison of the solution algorithms based on the element size. It can be observed from this table that the DIM method does not converge to a solution even after 10,000 iterations for small element sizes of 0.5 mm, 1 m and 2 mm. For larger elements, the convergence can only be achieved if the maximum convergence norm, i.e. the maximum difference between the potentials of the two successive iterations at a node, is kept large. If this difference is interpreted as an error, the error in the DIM varies between 58.2 mV to 91.1 mV, which is not within the acceptable range. In order to reduce the error within the DIM, the number of iterations need to be increased. However, due to the random nature of the DIM, increasing the number of iterations does not guarantee a better convergence. It may be

necessary to carry out millions of iterations in order to achieve an acceptable level of convergence. The randomness of the DIM is illustrated in Fig. 6 in which the error term in successive iterations carried out by the DIM is plotted for a mesh created by 5 mm elements.

The solution of the same cases using the MDIM (with $\xi = 0.2$) provides better results. Although the convergence is still not achieved for small element sizes of 0.5 mm and 1 mm, for larger elements, the results are promising. For a mesh created with 5 mm elements, the maximum error (the maximum difference between two successive iterations for a node) is 1.6 mV after 28 iterations. Although this can still be considered as a large difference, it is within the acceptable range of results. As illustrated in Fig. 6, the convergence of MDIM does not have a random nature as observed in DIM for this specific case. It should be noted that the results of the MDIM is highly dependent on the selection of ξ, however, the discussion of the is not within the scope of this paper.

Table 1: Input parameters and constants for the comparison of the solution methods

Parameter	Value
Length, a+b (mm)	300
Height (mm)	100
Standard half cell potential of *Fe* (mV ~SCE)	-780
Tafel slope of the anode, β_a (mV)	60
Anodic exchange current density, i_{oa} (A/mm^2)	300×10^{-10}
Standard half cell potential of oxygen (mV ~SCE)	-160
Tafel slope of the cathode, β_c (mV)	160
Cathodic exchange current density, i_{oc} (A/mm^2)	10×10^{-10}
Limiting current density, i_L (A/mm^2)	1×10^{-6}
Temperature, T (K)	298

Table 2: The comparison of the solution algorithms based on element size

Element size (mm)	A/C ratio	DIM ($\xi = 1.0$)		MDIM ($\xi = 0.2$)	
		Error (mV)	# Iterations	Error (mV)	# Iterations
0.5		N/C	> 10,000	N/C	> 10,000
1		N/C	> 10,000	N/C	> 10,000
2		N/C	> 10,000	2.7	3096
3	0.111	91.1	2552	1.9	1574
5		87.1	3127	1.6	28
6		78.6	786	1.3	29
10		71.7	1440	1.7	22
15		58.2	2640	1.6	22

The problem associated with the DIM can also be observed in Fig. 7. Although anodic potentials calculated by both methods are quite stable, the cathodic potentials from the DIM show significant fluctuations. On the other hand, MDIM provide the expected smooth

potential distribution along the cathode for most element sizes. The fluctuations in the MDIM start at the far end of the cathode, and as the element size get smaller, the convergence becomes difficult to achieve.
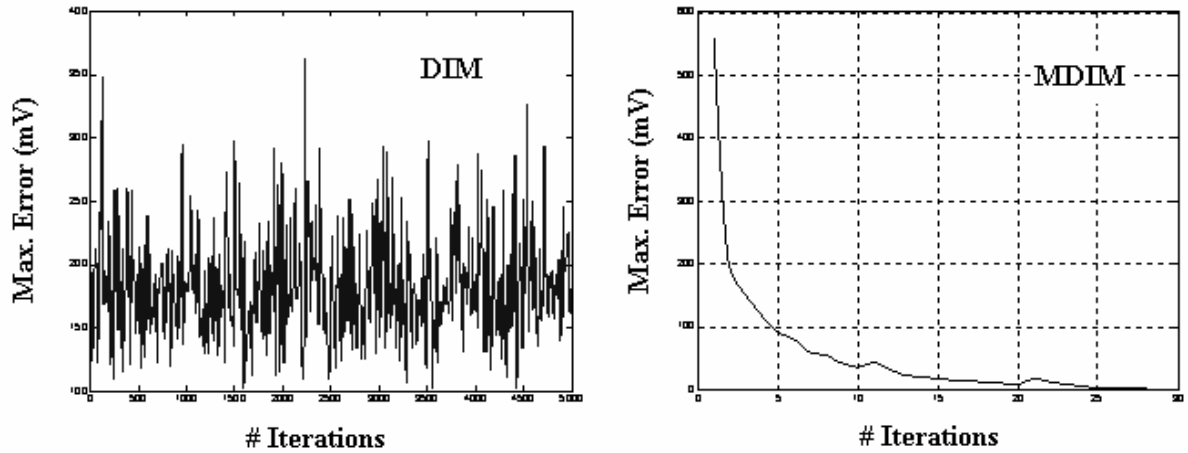

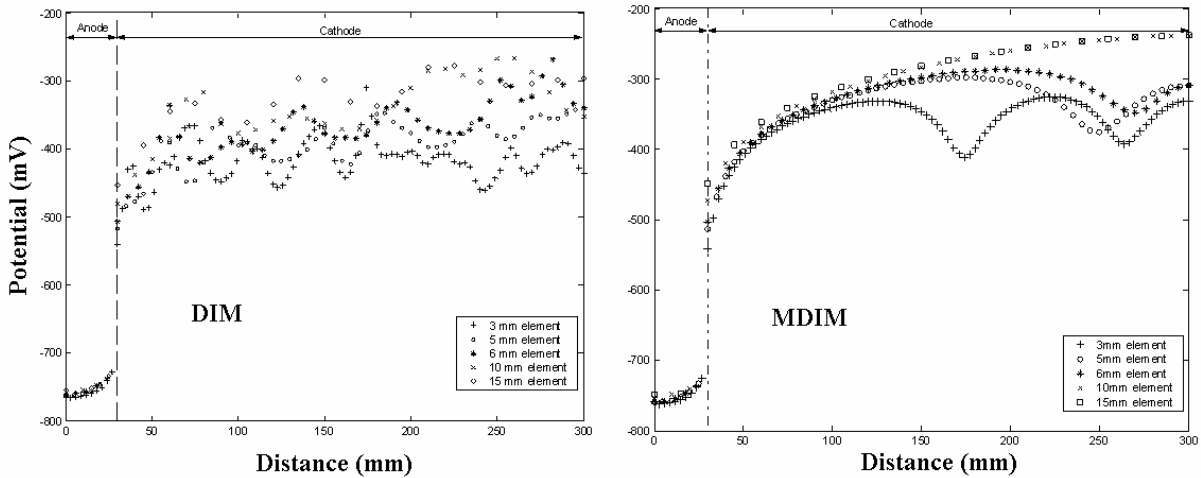Figure 6: Maximum error vs. number of iterations when for a 5 mm elements are used

Figure 7: Surface potentials calculated with DIM and MDIM

EFFECT OF ANODE-TO-CATHODE RATIO

The effect of anode-to-cathode (A/C) ratio on the convergence of the nonlinear finite element solution of the corrosion problem defined Fig. 5 is studied. Nonlinear solution algorithms described in the previous sections are used to solve the problem with varying A/C ratio from 0.001 to 1.0. In all cases, 10-mm elements are used to discretize the domain. The results of the analysis are plotted in Fig. 8 for both methods. As it can be seen from this figure, both methods give very similar (and stable) results for the anode. However, the solution along the cathode anodes show significant fluctuations for all A/C ratios in the DIM. The convergence problems experienced in the DIM can be attributed to these fluctuations along the cathode. In

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the MDIM, the fluctuations does not exist for large A/C ratios; however, as the A/C ratio becomes very small, some disturbance can be observed at the far end of the cathode.
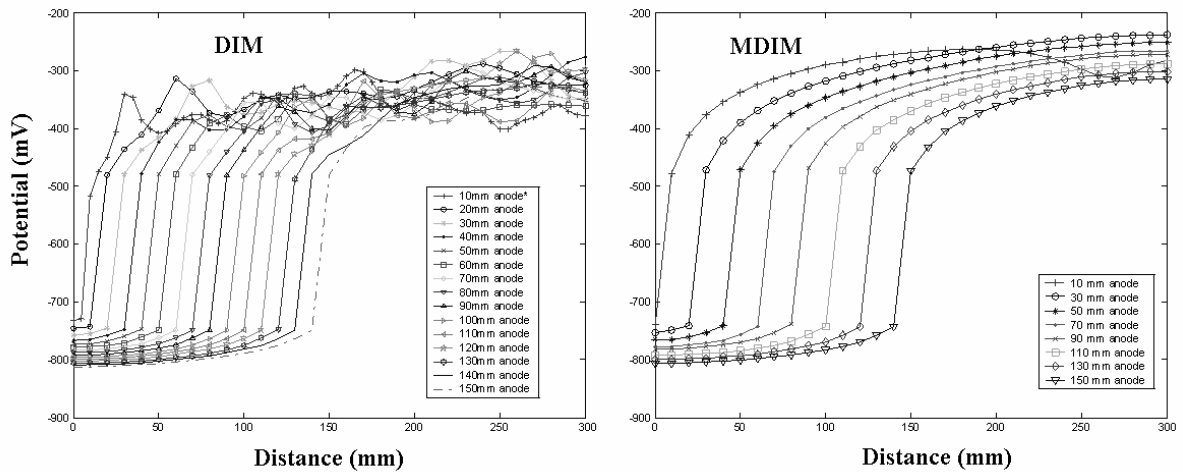

Figure 8: Model used in the comparison of the solution algorithms

EFFECT OF RESISTIVITY

The effect of concrete resistivity on the convergence of the nonlinear finite element solution of the corrosion problem defined Fig. 5 is studied. Nonlinear solution algorithms described in the previous sections are used to solve the problem with varying concrete resistivity from 10,000 to 1,000,000 ohm-mm. In all cases, 10-mm elements are used to discretize the domain. The results of the analysis are plotted in Fig. 9 for both methods. As it can be seen from this figure, both methods give very similar (and stable) results for the anode. However, the solution along the cathode anodes show significant fluctuations for all resistivity in the DIM. The convergence problems experienced in the DIM can be attributed to these fluctuations along the cathode. In the MDIM, the fluctuations are minor, but still exist at the far end of the cathode.
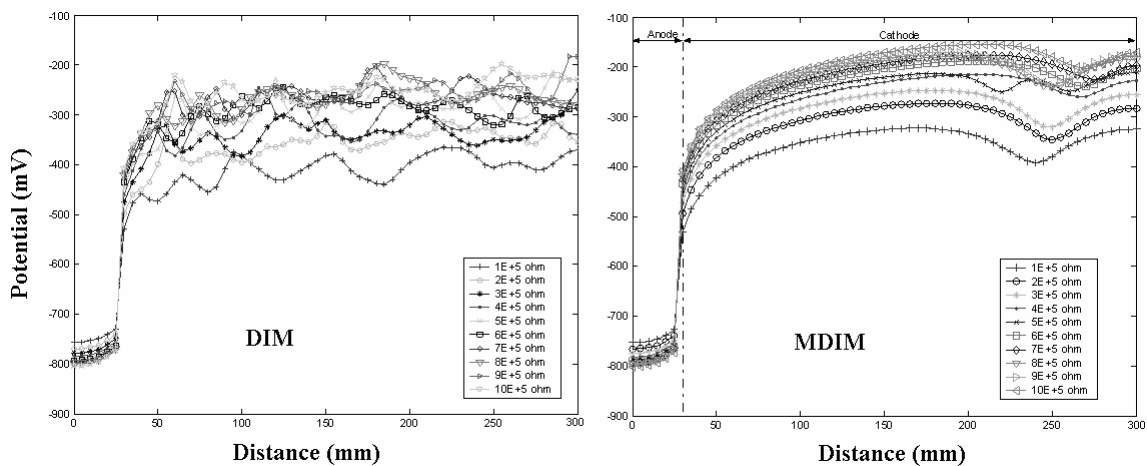

Figure 8: Model used in the comparison of the solution algorithms

CONCLUSIONS

The following conclusions can be drawn from the analyses performed in this study:

1) The nonlinear solution of the Laplace's equation for corrosion of steel in concrete can be difficult due to convergence problems originating from the non-linear polarization boundary conditions.

2) Both methods used in this study gave stable solutions along the anodes, but showed fluctuations along the cathodes. This can be explained by the fact that the non-linearity due to the anodic polarization is not as severe as the non-linearity due to the cathodic polarizations. Unlike the MDIM, the convergence of the DIM showed a random pattern.

3) Fluctuations along the cathodes were more severe in the DIM than the ones in the MDIM. Fluctuations in the MDIM were limited to the far end of the cathode, and were more obvious when small elements were used.

4) The convergence could not be achieved in neither of the methods studied here when small elements were used to discretize the domain.

ACKNOWLEDGMENTS

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