Axial symmetry model of corrosion activities on carbon steel surface in neutral aqueous chloride solution

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ABSTRACT – This paper presents the modelling of corrosion activities of carbon steel when it is immersed in aqueous sodium chloride solution. The bulk solution is taken as neutral, which is pH 7. By using COMSOL Multiphysics as tool, a two-dimensional axial symmetry geometry was constructed to represent a microscale pit. Thermodynamics formula based on Pourbaix diagram of iron were applied in the model and thus, allowing the predictions of active corrosion activities. The corrosion predictions that account for the ionic species being considered suggest the occurrence of active corrosion activities. The results show that metal dissolution occurs when the model is solved for a certain range of time.

1. INTRODUCTION

It has been widely studied that chloride induced corrosion gives a strong impact to a wide range of engineered materials. The presence of this particular halide in the surrounding area can accelerate the rate of any type of corrosion. In principle, corrosion is the destruction of materials due to its reaction with its surroundings. This results in changes to metals which are measurable [1-2]. Serious damage to equipment can occur and its efficiency may be lost if corrosion is not being controlled in a proper way.

Aqueous corrosion is an electrochemical reaction which takes place in the presence of water. American Petroleum Institute Recommended Practice 571 (API RP 571) stated that moist polluted industrial environments with airborne contaminant are most severe, whereas dry rural environments cause very little corrosion [3][4]. It has been established that during active corrosion, the pH inside a pit shows a drop which is much lower than the bulk solution whilst the polarization curve will show a trend that is common to all corroding activities in steel. It has also been established that there are three stages of corrosion, which are initiation, propagation and stable corroding stage [1, 5-9].

In this investigation, the state being considered is after the initiation state. The geometry represents an inclusion on metal surface and the inner region of the geometry is considered as the bulk solution in which the metal is immersed in. The bulk solution is taken as an aqueous sodium chloride solution of neutral pH, which is 7. The presence of chloride ions, Cl⁻, in the

electrochemical process of corrosion, speeds up the rate of corrosion [1, 10-12]. The objective of this study is to investigate the ability of the model to produce results of corroding activities at pH7. COMSOL Multiphysics version 4.2 is used as tool to run the model for a certain range of potential.

2. RESEARCH METHODOLOGY

A two-dimensional axial symmetry model is developed to look at the propagation of a corroding micropit of steel which is being immersed in aqueous sodium chloride solution with pH7. This study considered ten neutral aqueous chemical species to illustrate the corrosion model (Fe^{2+}, OH^-, H^+, $FeOH^+$, Na^+, Cl^-, $FeCl^+$, H_2, Fe^{3+} and FeO_2^-). These ionic species is being governed by the Nernst-Planck law for the case where electroneutrality is enforced [9, 13-15].

$$\frac{\partial [i]}{\partial t} = D_i \nabla^2 [i] + z_i U_i F \nabla([i] \nabla V) + R_i \quad (1)$$

The model also incorporates the respective currents for metal dissolution and reduction of hydrogen ions, H^+, to counter for the active state of metal. These reactions applied Tafel expression. The metal dissolution rate and the hydrogen ions reduction rate follow Fick's First Law of Diffusion.

Dissolution rate of metal ions Fe^{2+}:

$$J_{diss} = \frac{i_1}{2F} = \frac{0.25 \times i_{01}}{F} \exp\left[a_1 F \frac{(V_m - V)}{RT} \right] \quad (2)$$

Reduction rate of of hydrogen ions H^+:

$$J_{H^+} = -\frac{i_2}{F} = \frac{i_{02} \times [H^+]}{F} \exp\left[a_2 F \frac{(V_m - V)}{RT} \right] \quad (3)$$

where $[H^+]$ is the hydrogen ion concentration, $i_{01} = 2.7 \times 10^{11} \text{ A m}^{-2}$, $i_{02} = 2 \times 10^7 \text{ A m mol}^{-1}$, $a_1 = 1$ and $a_2 = 0.5$.

The model then is solved for potential range of -0.8 until 0.32 volt.

3. RESULTS AND DISCUSSION

Figure 3.1 shows the axial symmetry geometry applied in the model. Point 1-4 are points located in the active region whereas Point 5 is located at the meeting point between active (anode) and inactive (cathode) region. The model is solved for potential range -0.8 until 0.1 volt.
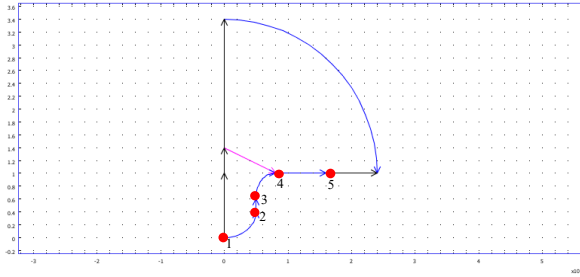

Figure 3.1 The axial symmetry geometry with five points of referral

The polarization curve is shown in Figure 3.2. At lower potential, the limiting current density which is about 1×10^{-7} A m^{-2}, can be plotted, with corrosion potential around -0.74 volt. This is where anodic polarization occurs. The current density is seen increasing gradually, which shows that active corrosion activities occur [13].
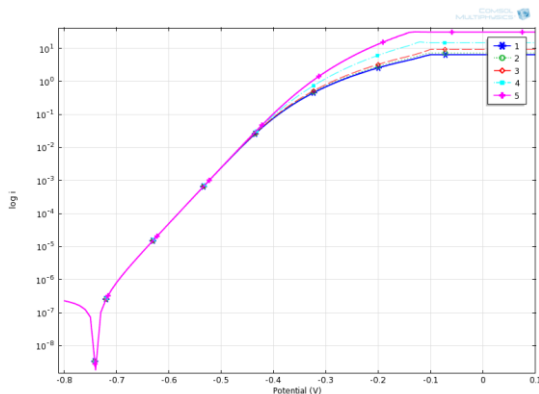

Figure 3.2 Polarization curve at all active points

Due to the active corroding activities, metal ions Fe^{2+} are diffused into the bulk solution. More metal loss occurs and metal ion concentration increases as shown in Figure 3.3. On the other hand, hydrolysis of water results in the formation of ions H$^+$ and OH$^-$, and causes Fe^{2+} t hydrolyse, producing FeOH$^+$ and H$^+$. This causes the pH to drop. Increasing the potential results in an increase in the current density and also increasing the drop in pH. This can be shown in Figure 3.4 where the pH at the bottom of the pit reduces until pH4.8 [13].
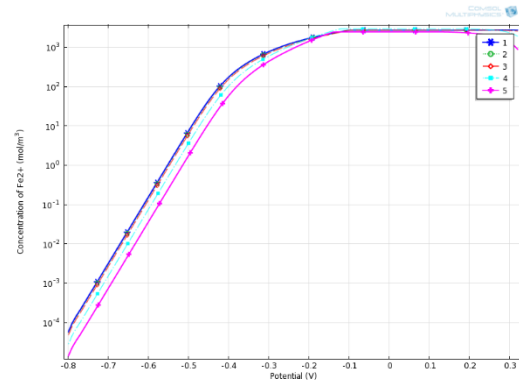

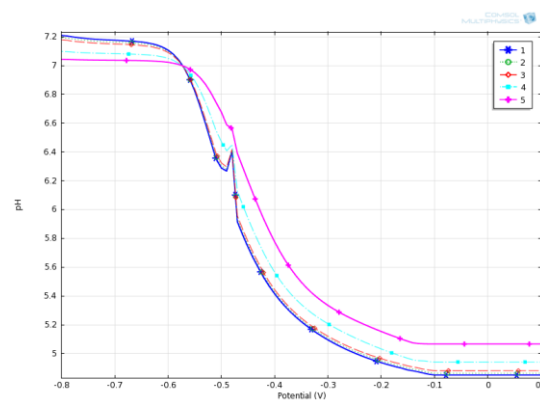Figure 3.3 Concentration of Fe^{2+} at all active points

Figure 3.4 pH at all active points

4. CONCLUSION

The basic results during active corrosion can be produced, in particular the increasing trend in current densities, the increasing level of metal ion concentration which indicates metal dissolution and also the change in pH inside the pit. Hence, it can be concluded that the model is able to integrate all involved corrosion reactions and can show that corrosion occurs in neutral pH condition.

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