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Analyze and modelingofdamage behavior of a $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ HLE Steel Solicited in Selected Physicochemical medium

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Abstract
The influence of environment and physical parameters on $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ HLE steel steel corrosion damage behaviour in NaCl solutions was studied using weight loss, pH evolution at 300k to 370k, electro-exchanges, and passivity. Herein, the results show that the corrosion rate changes versus type of thermal treatment and cooling fluid, solution concentration, shape, size and cooling speed of the samples. The resolution of Nernst equation proves that the increase in temperature has a direct effect on hydrogen potential of the solution, current and corrosion potential of the metal. Moreover, the inhibition efficiency was determined by theoretical calculation using mechanical molecular and semi-empirical method. These results guided us to conclude that the inhibitor, which has low electronegativity than $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ Steel has good efficiency.

Keywords: steel, HLE, damage, corrosion rate, polymer, oil, carbon, inhibition, electronegativity

Introduction
Study of the interactionbetween metal and fluid is one of the prevention methods to find reliable solutions of degradation phenomena under aggressive medium .Several equipment in petroleum industry are basically made using HLE steel (high limit elasticity) such as Oil and Gas facilities,production tubing, pipeline of transport, and tubing for cooling, and storage tanks which are solicited by medium acidity, temperature variation and external loads. Thus, the protection of steel structure as API 5LX60 against NS4 Simulated Soil is proved by using polyphosphates [1]. The Sulphide molecules can decrease the corrosion rate of the API 5L X52 steel sample in a CO_2 environment [2].
The poly (4-vinylpyridine) reduce corrosion rate of carbon steel in presence of H_2S0_4 [3]. Reducing cathodic current density and increasing Iron polarization resistance in presence of Sulfuric acidcan be achieved by Poly (4-vinylpyridine poly-3-oxyde ethylene) [4]. Fortunately, new methods were developed for modeling chemical properties such as correlation model established on electrochemical oxidation potentials of several anions reported in [5].In addition to that, the inhibition stability of Quaternized Poly (4-Vinylpyridine)-Graft-Bromodecane in Sulphuric Acid on pure ion is reported in [6].Wherein, the radical of this last and its derivativehave been applied as inhibitor to protect pure metal as iron, copper and zinc [7-8]. The standard testing and expressions for corrosion have been reported in [9-10-11-12].The inhibition corrosion of mild steel in HCl by using P4VP is due of chemisorption phenomena [13].However, the application of protection methods requires to identify and study the behavior of material under chemical, thermal, mechanical stress and geometries design before using interface inhibitors (vapor phase, liquid phase (anodic, cathodic and mixed adsorption)) or environmental conditioners .
The aim of the present work is to make an assessment on rate corrosion of three states of steel $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ affected by thermal choc which simulates heat affected zone (HAZ) in assembly metals structures .The medium acidity variation is introduced using different concentrations of NaCl. Experimental technique is reached by measuring weigh loss of metal after chemical attack during 720 hours divided in 10 stages. The polymer efficiency estimation was determined by physical calculation using two methods: mechanical molecular and semi-empirical method.

2. Materials and methods

2.1. Material Properties

The Chemical composition of steel was identified by using spectrometry analysis; it is shown from histogram in figure 1 (a, b, c and d) .The microstructures were carried out using scanning electron microscopy (SEM), where figure2 shows states of texture.

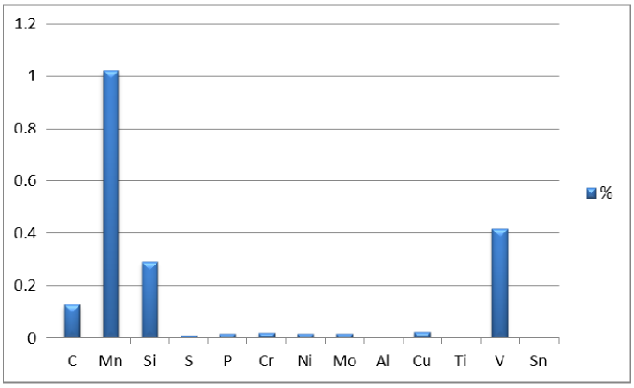
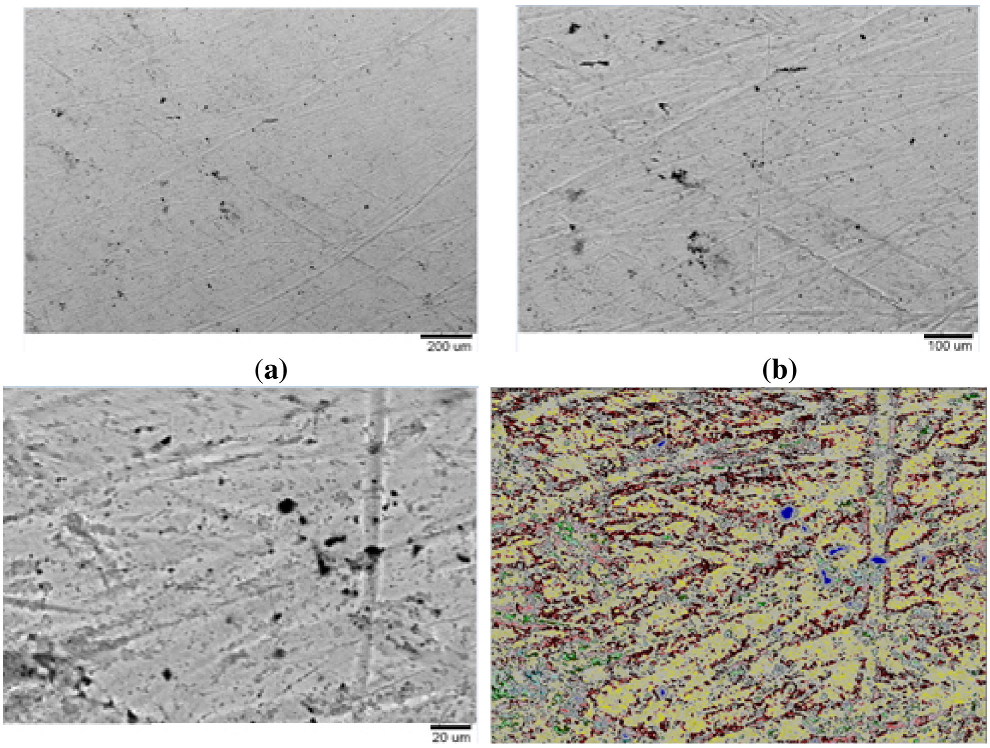


Figure 1 Chemical composition of a $C_{0.12}$% $Mn_{1.02}$%$Si_{0.29\%}$ steel



(**a**) (**b**)

(c) **(d)**

Figure 2 :SEM fractographs of the $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ Steel ,a:200um,b:100um,c:20um,d:map 20um.

2.2 Field condition

An eighteensamples of steel with different geometries and weights are used in this study; the first crew are considered as reference without thermal affect and renamed base metal (BM)). Nevertheless,The two remain crews of samples were affected by heat and cooled by air and multigrade oil respectively .The characteristic of oil was investigated in our laboratory before establishing the thermal choc on samples [14].The selective medium was prepared with different concentration from 0.1M to 0.8 M of NaCl. The rate corrosion is determined by weight loss method. The samples should be cleaned with acetone, bi-distilled water and dried by heated system before each measure. The procedures of preparation of samples, polishing, segmentation, thermal choc, and fluids cooling are shown in figure 3 (a, b, c, d, e, f, g, h and i).

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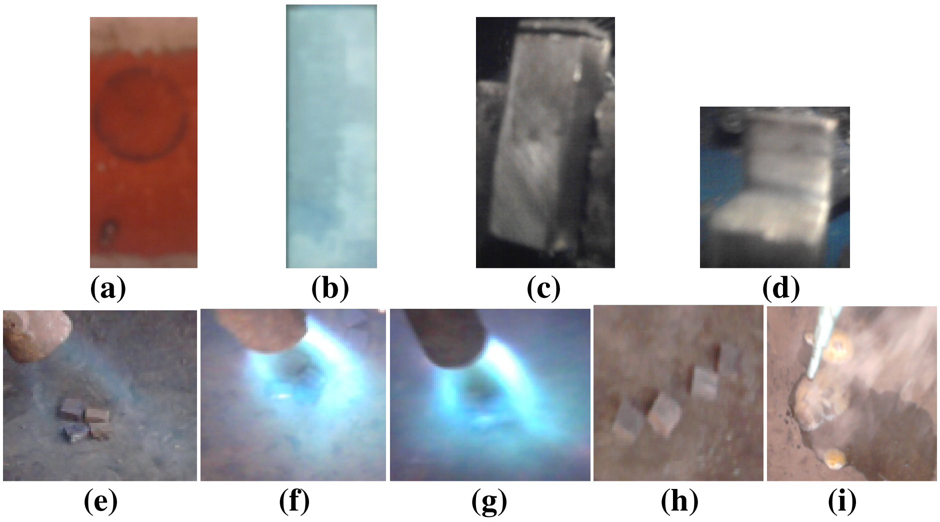

Figure 3 (a) Coupon of steel , (b) sample after polishing, (c,d) segmentation, (e,f,g) thermal choc, (h) air cooling, (i) oil cooling.

3. Results and discussions

The effect of medium aggressiveness on three states metal corrosion with different concentrations of NaCl at various weights and shapes are shown in figures (4, 5, 6, 7 and 8).

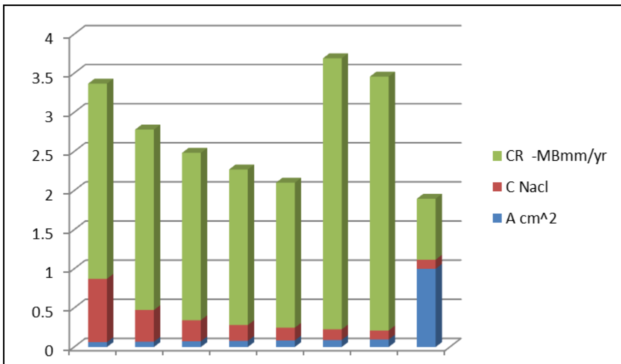

Figure 4 Corrosion rate of base metal (MB) vsNaCl concentration and sample area

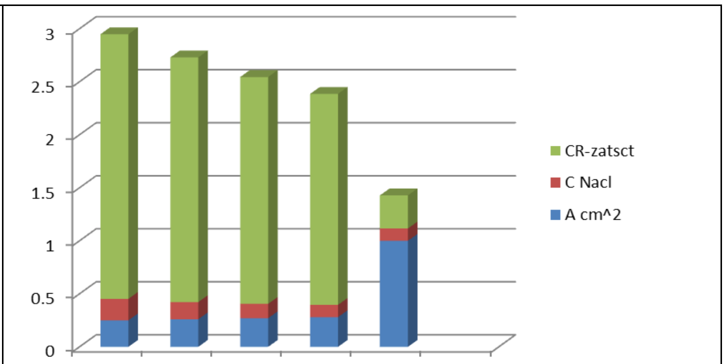

Figure 5 Corrosion rate of samples affected by heat and cooled by air (ZATsct) vsNaCl concentration and sample area

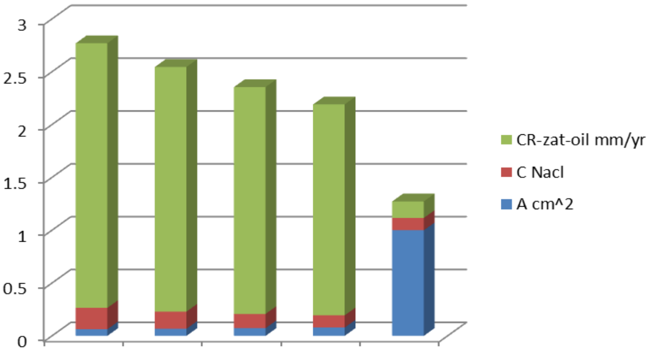

Figure 6 Corrosion rate of samples affected by heat and cooled by multigrade oil (ZATH) vsNaCl concentration and sample area

Wherein, it is noticeable that Corrosion rates of $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ Steel increases with halite concentrations. The increase in geometry or simples size has direct effect on corrosion rate, it can be explained by contact between atomic plan of metal and halite (NaCl).The corrosion rate has significant values for first crew of samples (MB), it reaches 0.376% for 0.135M NaCl. The second crew of samples (ZATsct) affected by heat and cooled by air, has lower corrosion rate values than the base metal, the corrosion rate grows until 0.214% for

0.135 M NaCl .This variation is justified by vicinity of cooling established by air and recrystallization of metal under standard condition .The third crew of samples(ZATH) affected by heat and cooled by multigrade oil has lower corrosion rate values at 0.135M NaCl than base metal and greater values than samples cooled by air .This variation is justified by atomic carbon deposit on metal surface for third state .We notice that the relationship between corrosion rate, sample area, medium concentration, thermal choc and fluids cooling type on corrosion rate are nonlinear.

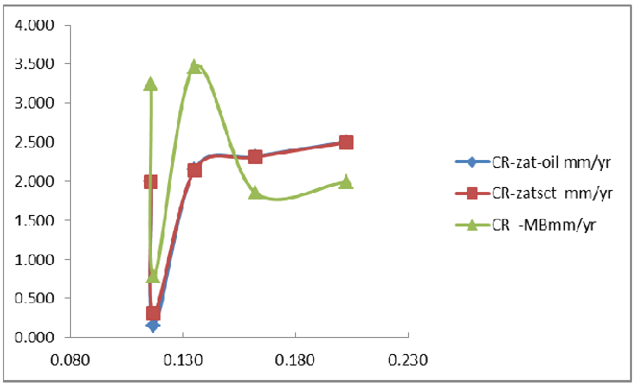

Figure 7 Corrosion rate vsNaCl concentration.

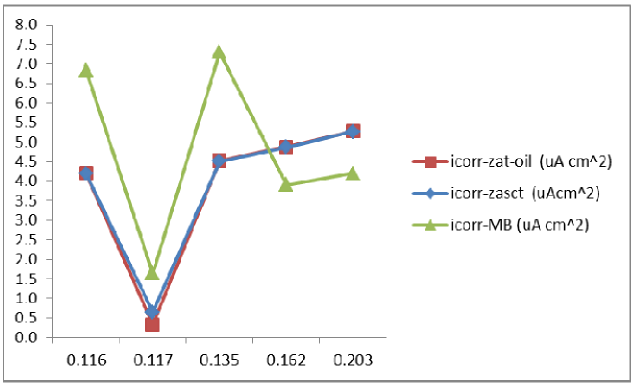

Figure 8 Current density vsNaCl concentration.

Polarization Curve

To obtain polarization curve, we resolved Nernst equation (ion equilibrium potential).Following,spectrometry analysis results obtained, we can noticed that Fe atoms are very amount dominated,it's about 98% which make one of initial condition to get solution of ion equilibrium potential equationand to estimate its' corrosion and current potential with variation temperature and PH. From Figure 9 and 10 its can be seen that the cathodic and anodic slopes changes apparently with the increase of the temperature and variation of medium PH acidity; it is clearly indicated by the existence of the cathodic proton-discharge reaction phenomena, the maximum displacement in E_{corr} and i_{corr} value is -0.45 V, 0.002 mA cm^2 respectively at 370K towards the cathodic region. The corrosion rates as well as current density of studied material extensively increase in aggressive medium simulated by variation of potential hydrogen and number of charge transfer.

The increasing of temperature has direct impact on potential hydrogen as shown in figure 9 which, by consequence, increases acidity of the medium and current density.

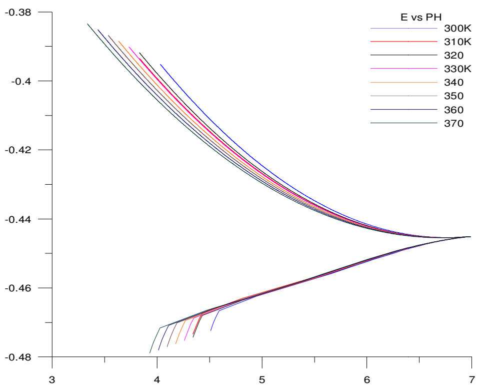

Figure 9 Effect of temperature on potential Hydrogen and potential corrosion

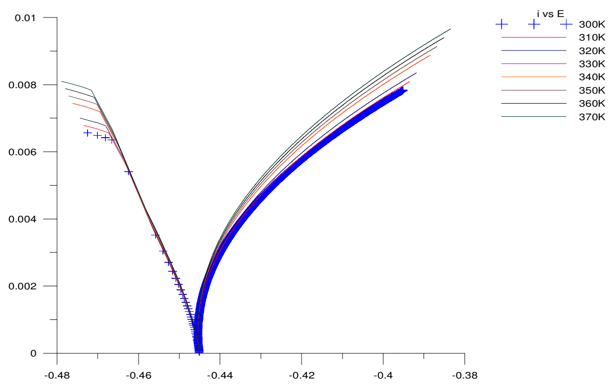

Figure 10 Effect of temperature on polarization curves

Figures 9 and 10 shows the effect of thermal agitation by increasing the temperature on polarization cutoff for 1M NaCl , after establishing slope line the corrosion potential of studied material is about -0.449 V for $2*10^{-3}$ (mA cm^2) (which is indicated in figure11). The degradation rate evaluation is important in technical engineering field. Figure 12 shows corrosion rate (CR or R); it increases quickly with temperature increase of medium until it reaches 0.701 mm/yr at 370K. After establishing the regression method, we found an equation of five degree with 99.55% certitude which can be make relationship between corrosion rate and temperature, we note that this equation is reliable just in next temperature range of [300k, 370k] at standard concentration:

$$\mathbf{CR = 10^{-8}*T^5 - 2*10^{-5}*T^4 + 0.0152*T^3 - 5.0071*T^2 + 821.29*T - 53829\ ;R^2 = 99.5\%}$$

This equation has an important application in corrosion rate prediction of this type of metal just two variables functionwhich are temperature and concentration of selective medium. The proposed equation can be programmed using assembly language for sensor corrosion measure application.

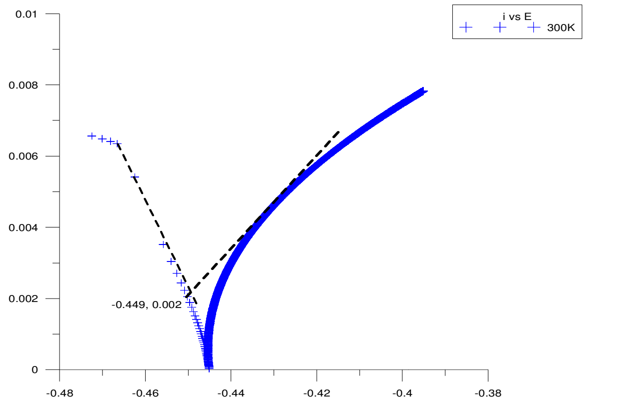

Figure 11 Tafel polarization curves for 1M NaCl at 300 k

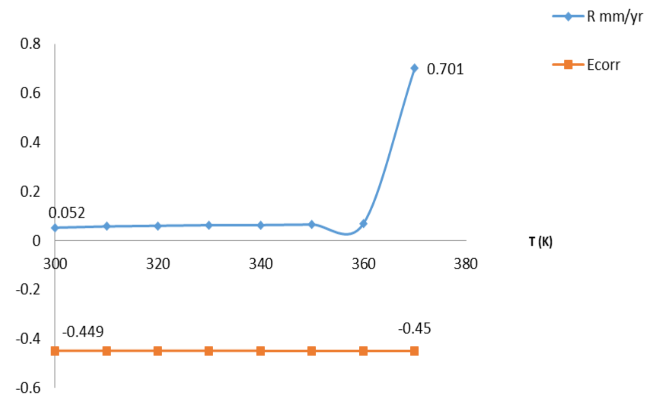

Figure 12 Corrosion rate vs temperature

Table 1 shows results obtained from mechanical molecular and semi-empirical method used to determine some proprieties for monomer and polymer, the molecule that have low electronegativity than base metal can protect the studied material from corrosion.

Table 1: Theoretical estimation of Efficient Inhibitors

Molecule	Efficient of inhibitor%
C_7H_7N	6.781
C_7H_7N-C	8.489
C_7H_7N-C-C	6.540
(C_7H_7N)-Br-$(BaSO_4)$	3.203
Na_2HPO_4	18.767
(Na_2HPO_4)-C_7NH_7	2.616
(Na_2HPO_4)-$(C_7NH_7)_2$	3.470
(Na_2HPO_4)-H-$(C_7NH_7)_2$	8.089
$(H_2N$-CS-$NH_2)$-C_7H_7N	7.635

Theoretical estimation

Quantum chemical calculations have been carried out by estimation inhibition effect for some polymers. In addition to that, geometric structure optimization has been established using molecular mechanic force field, and MM+ option based on electrostatic interactions used to find the coordinates of a molecular structure with potential minimum energy figures (13, 15). The Mullikan atomic charge is used to indicate chemical reactivity figure 14.

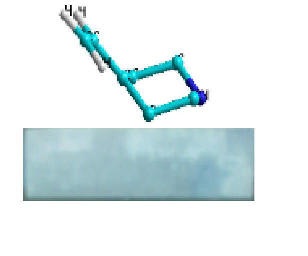

Figure 13 C7H7N Pattern on MB

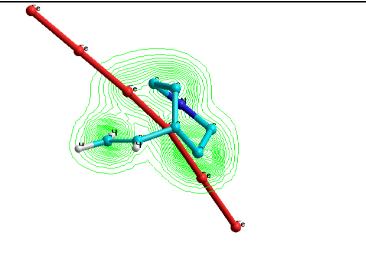

Figure 14 Charge density distribution

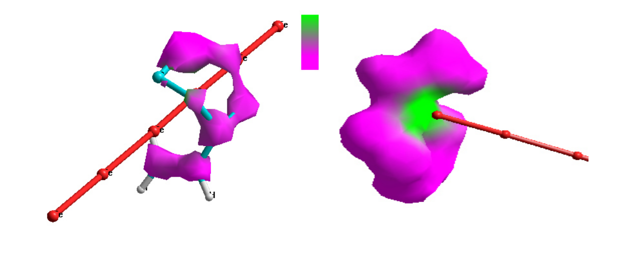

Figure 15. Electrostatic potential distributions (by using method MM+)

The values of softness η and hardness θ figure 16 were estimated by using the relationship between ionization potential I and electron affinity A obtained from theoreticalcalculation .These quantities are related in turn energy of the highest occupied orbital EHOMO and energy of the lower occupied orbital ELUMO:

$$A = -E_{LUMO} \quad (1)$$

$$I = -E_{HOMO} \quad (2)$$

$$\eta = (I-A)/2 \quad (3)$$

$$\theta = 1/\eta \quad (4)$$

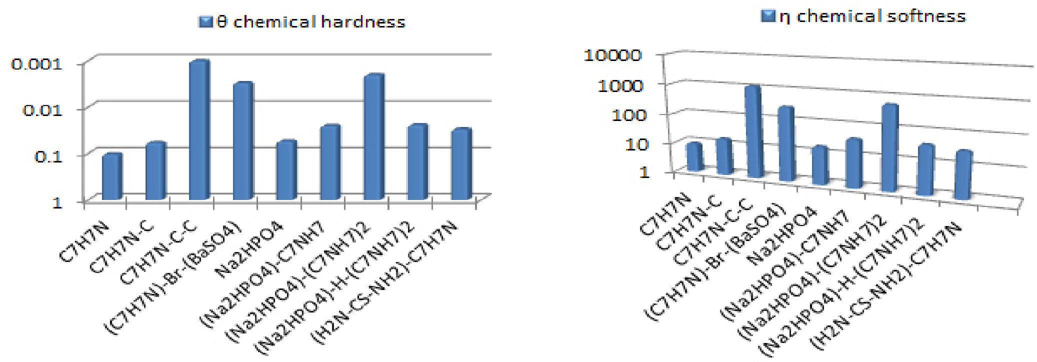

Figure 16 Chemical softness η and hardness θ

Conclusions

1. The thermal choc and nature of cooling fluid were found to have direct influence on corrosion behavior of $C_{0.12\%}Mn_{1.02\%}Si_{0.29\%}$ steel in Selected Physicochemical medium as like NaCl.
2. The corrosion rate has relationship with shape, size of samples and concentration of aggressive medium.
3. The current density and acidity of medium increase by increasing of temperature which has a direct effecton corrosion behavior of metal.
4. The molecule has low electronegativity than base metal can be protected it from aggressive medium.
5. The polymer $(C_7H_7N)_n$ has good cover area on base metal proved by charge density distribution and electrostatic potential.

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References

1. Benmoussat A., Traisnel M., *Springer Science. B.V. Proceedings of the NATO Advanced Research Workshop. (*2011).
2. Fatah M.C., *ASM International.JMEPEG. (*2013) 236–244.
3. Larabi L., Harek Y., *P.Electrochim.Acta*. 22 (2004) 227–247.
4. Abed Y., Arrar Z., Hammouti B., Aouniti A., Kertit S., Mansri A., *J. Chim. Phys.* 96 (1999) 1347-1355.
5. Hagiwara R., Ito Y., *J. Fluorine Chem.* 105 (2000) 221–227.
6. Chetouani A., Medjahed K., Al-Deyab S.S., Hammouti B., Warad I, Mansri A., Aouniti A., *Int. J. Electrochem. Sci.* 7 (2012) 6025 – 6043.
7. Bhandari H., Choudhary V., *Synth. Met.* 161 (2011) 753.
8. Kertit S., ChaouketF., *J. App. Electrochem.* 24 (1994) 1139.
9. Skothaim T.A., *Dekker M.NY.2. Handbook of Conducting Polymers.* (1986).
10. Matsushima I., Revie R.W., *John Wiley Sons. Inc. Uhlig's Corrosion Handbook.* (2000) p.515.
11. Matsushima I., *Journal of the Society of Materials Science, Japan*, 19 (1980) 19.
12. Sastri V.S., Ghali E., Elboujdaini M., *John Wiley. Sons Ltd.* ISBN: 9780470024546 (2007).
13. Larabi L., Harek Y., Traisnel M., Mansri A., *J. App. Electrochem.* 34 (2004) 833–839.
14. Belahcene B., Mansri A., Benmoussat A., *ETASR*. 4 N° 6 (2014) 711-713.