Experimental and theoretical analysis of an oxazinoquinoxaline derivative for corrosion inhibition of AISI 1018 steel

Joherbson Deivid dos S. Pereira[a], Jannyely M. Neri[a], Denise P. Emerenciano[a], Gutto Raffyson S. de Freitas[a], Maria Beatriz M. Cansanção Felipe[b], Miguel Ângelo F. de Souza[a], Fabrício G. Menezes[a] and Maria Aparecida M. Maciel[a,c*]

[a]Instituto de Química, Universidade Federal do Rio Grande do Norte, Natal, RN, 59072-970, Brasil.

[b]Núcleo de Pesquisa em Petróleo e Energias Renováveis, Universidade Federal do Rio Grande do Norte, Natal, RN, 59072-970, Brasil.

[c]Universidade Potiguar Laureate International Universities, Programa de Pós-graduação em Biotecnologia, Campus Salgado Filho, Natal, RN, 59075-000, Brazil.

*e-mail: mammaciel@quimica.ufrn.br

SUPPLEMENTARY MATERIAL

1 METALLOGRAPHIC ANALYSIS

In the metallographic analysis, a AISI 1018 mid steel specimen was cut (0.273 cm^2; 0.137 cm^3) and extensively abraded using several sandpaper sheets (grain size: 120, 400, 800 and 1200) until a like-mirror surface was obtained at 1200 gr. Then, the metallic surface was subjected to chemical treatment with 4% Nital (4% nitric acid and 96% ethanol). After this procedure, metallic surface images were acquired with an Olympus BX51 optical microscope using amplifications of 500x and 1000x (Figure S1). The number of phases in the material was determined from the below equation, according to previous reports.[1]

$V_V = \frac{V_f}{V}$ where V_V and V_f are the phase volume and V is the experimental volume.

The number of phases in the material was determined by measuring the volumetric fractions and counting the peaks at the surface. The number of peaks in the interest area was divided by the total number of peaks at the grade, giving the value of the equivalent to the volumetric fraction (Pp). For reliable results, this counting was repeated in different regions of the sample.[1] Then, the AISI 1018 mild steel surface was polished before and after each OAQX concentration test, with water sandpaper of different grain sizes (120, 400, 800 and 1200). After that procedure, the residual corrosion damage was removed affording a homogeneous steel surface, according to previous reports.[2]

Metallographic analysis is relevant to evaluate the properties of materials as well as the influence of the chemical components in many applications, such as corrosion, which in this work is studied in terms of the inhibition effect by the OAQX oxazinoquinoxaline derivative. Figure S1 shows the microstructure images acquired for the sample explored in this work. Two different phases were found, being clearer and darker, corresponding to ferrite (α-Fe) and perlite, respectively. It is possible to verify a body-centered crystalline system, which is in the ferrite phase. Percentages of 82.7% and 17.3% were found for ferrite and perlite, respectively, which is coherent to AISI 1018 mild steel.[3]

(a) (b)

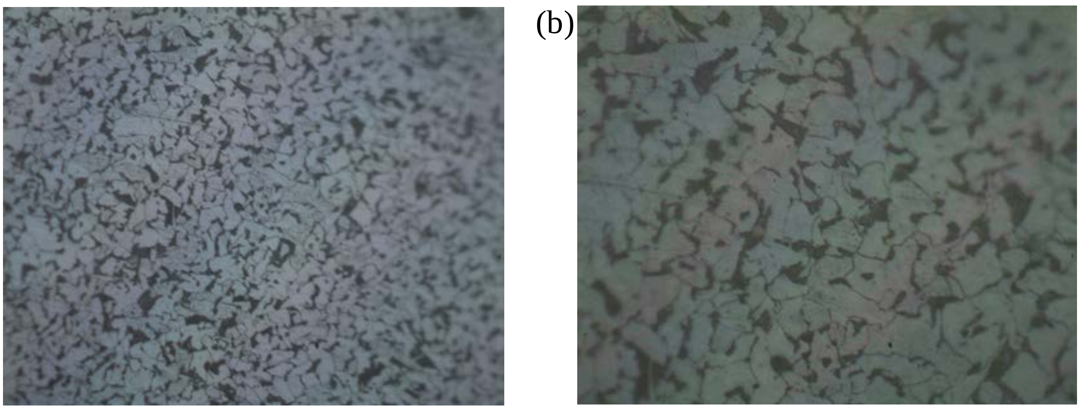

Figure S1*. Metallic surface images acquired for AISI 1018 sample with expansions of 500x (a) and 1000x (b)*

2 ELECTROCHEMICAL MEASUREMENTS

The anodic and cathodic polarization curves for AISI 1018 mild steel immersed in 0.6 mol L^{-1} NaCl solution and the organic solvent DMSO 0.627 x 10^{-4} mol L^{-1} were obtained in order to evaluate its corrosivity in saline medium, since it was applied to solubilize OAQX. The curves were performed using the same methodology described in the main text, section “Experimental”, subsection “Electrochemical assays”. It can be noticed from polarization curves (Figure S2) that the corrosion potential (E_{corr}) shifts 0.057 V towards more noble direction with a slight increase in polarization resistance (R_p) (Table S1) and consequently minor increase in corrosion inhibition. DMSO was able to positively influence the inhibition potential found for OAQX dissolved in DMSO system. DMSO polarity and strong hydration energy with surface cation favors its adorption on the metal surface and leads to decrease in anodic dissolution. Nevertheless, 0.627 x 10^{-4} mol L^{-1} DMSO solution had a minimal contribution reinforcing that the main corrosion inhibition effect was due to OQAX interaction with metal.

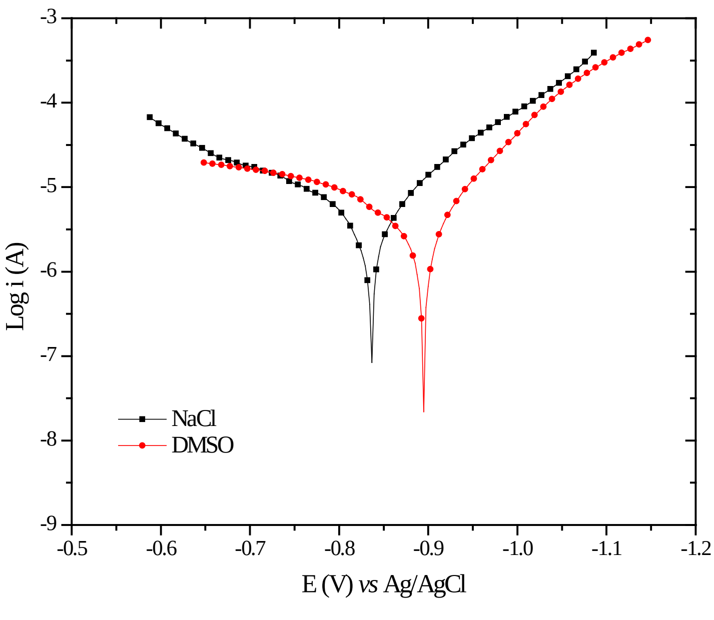

Figure S3. *Anodic and cathodic polarization curves for AISI 1018 mild steel in sodium chloride solution (0.6* mol L^{-1}*) in absence and presence of DMSO (0.627 x 10^{-4} mol L^{-1})*

Table S1. Parameters obtained from polarization curves for AISI 1018 mild steel, in 0.6 mol L^{-1} NaCl medium containing 0.627 x 10^{-4} mol L^{-1} DMSO

DMSO (mol L^{-1})	E_{corr} observed (V)	Rp (Ohm, x10^3)	η_P (%)
0	-0.837	6.120	0
0.627 x 10^{-4} mol L^{-1}	-0.894	7.020	12.86

3 REFERENCES

1. Padilha, A. F.; *Materiais de Engenharia: Microestrutura e Propriedades*, Hemus, São Paulo, **1997**.
2. Chauhan, L. R.; Gunasekaran, G.; Corros. Sci. **2007**, *49*, 1143.
3. Islam, M. A.; Alam, T.; Farhat, Z. N.; Mohamed, A.; Alfantazi, A.; *Wear* **2015**, *332-33*, 1080.