A Mechanistic Study of the Inhibition of Mild Steel Corrosion in Acidic Medium

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Abstract

The corrosion inhibition efficiency of mild steel in 1.0 M HCl was investigated using five imidazole based compounds theoretically using DFT and electrochemically using EIS and PDP. DFT calculations indicated that the iodo-substituted imidazole adsorbs better towards steel surface forming a linked network than other molecules studied. Theoretical conclusions were subsequently correlated experimentally using potentiodynamic polarization, linear polarization resistance, electrochemical impedance spectroscopy and surface analytical techniques (SEM and AFM). The results will be used to construct a model for predicting the corrosion inhibition performance of simple organic inhibitors.

Introduction

Amongst the major problems facing the oil and gas industry today are those related to corrosion. This phenomenon affects every aspect of exploration, production, transportation and storage, as well as refinery operations. Corrosion of metal and alloys represent a large portion of the total costs for oil and gas producing companies every year worldwide, hence the need to device strategies for its prevention and control. Moreover, appropriate corrosion control help avoid many potential disasters which often times lead to loss of life, negative social impacts, and water resource and environmental pollution [1]. One of the efficient and cost-effective approaches to mitigate this problem is thus the application of corrosion inhibitors.

A corrosion inhibitor is a chemical substance which, when added in small concentrations to an aggressive environment, minimizes or prevents corrosion [2]. Several classes of inhibitors have been developed, and these include pyridine derivatives [3], surfactants [4], rare earth metal compounds [5], and imidazole based compounds [6].

In the current study, we examine a series of closely related functional imidazole based compounds for corrosion inhibition efficiency. First principles simulations based on quantum mechanical density functional theory (DFT) which serve as powerful predictive tool in the design and development of effective corrosion inhibitors will be employed. Results from computational work will be correlated with electrochemical corrosion measurements to achieve sound conclusions from the study.

Significance of Study

In the United States alone the cost of corrosion to the economy has been estimated at between 10 and 15 billion dollars annually.

Material and Methods

- Theoretical calculations were performed with VASP 5.4.1 using the PBE functional. Iron (Fe) surface was modelled with 3x3x7 and 4x4x4 slabs and fully optimized. Adsorption energies of the compounds under study were further obtained.
- Electrochemical studies were carried out on mild steel (AISI 1018) in 1 M HCl at room temperature using a Gamry potentiostat/galvanostat/ZRA (Reference 600) with a Gamry framework system.
- Surface characterizations which include SEM and AFM were carried out on the mild steel sample before and after subjecting to the medium with and without the inhibitors.

Results

Theoretical Studies

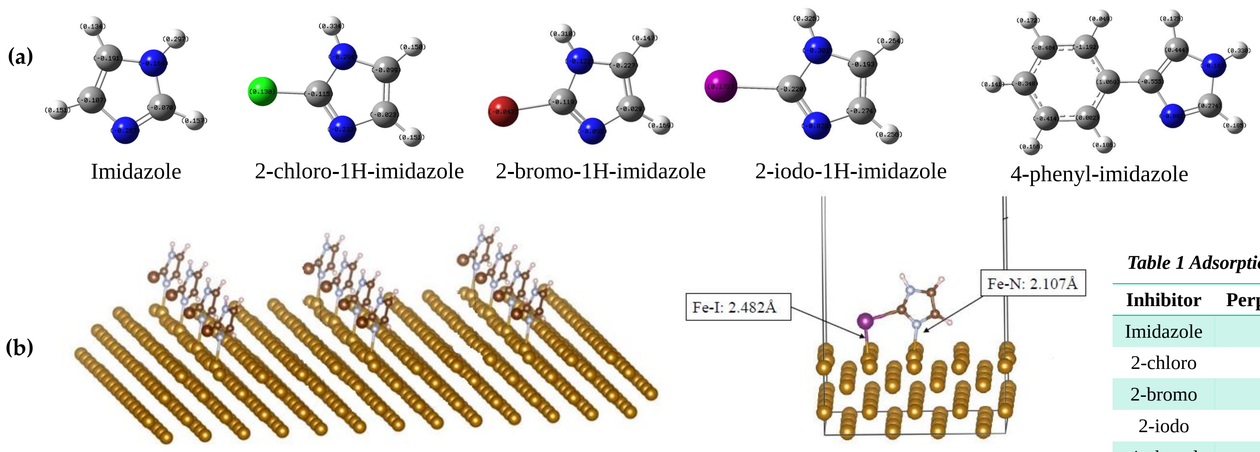

Fig. 1 (a) Optimized structures of the studied compounds, (b) Interaction of the inhibitors with Fe(100) surface

Table 1 Adsorption energies (Kcal/mol)

Inhibitor	Perpendicular	Tilted
Imidazole	-16.9	-23.6
2-chloro	-14.2	-83.7
2-bromo	-17.2	-87.6
2-iodo	-24.1	-89.6
4-phenyl	-16.5	NA

Surface Characterization

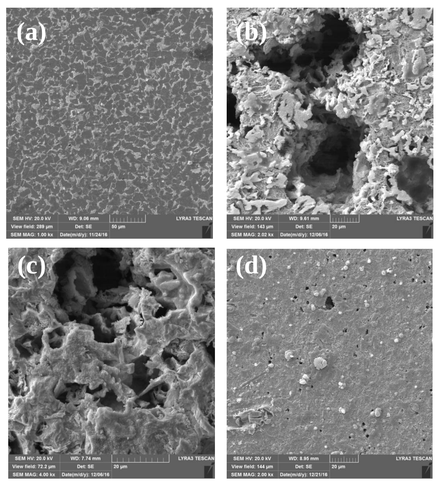

Fig. 2. SEM images of steel sample (a) as received, and after immersion in (b) 1 M HCl, (c) 2-chloro-1H-imidazole, (d) 2-iodo-1H-imidazole, for 24 h

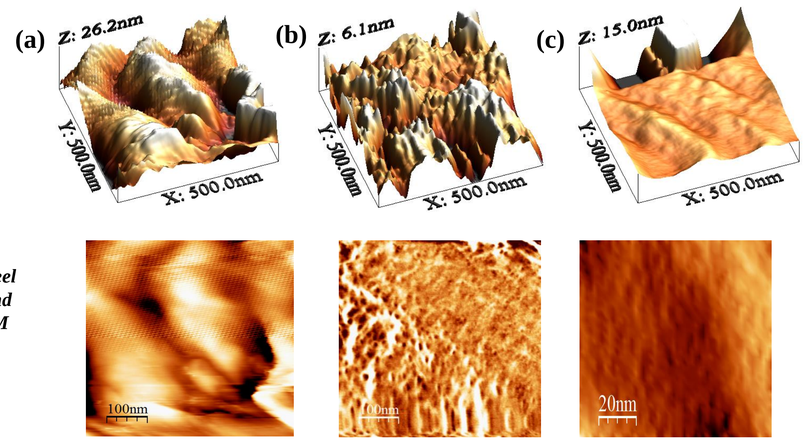

Fig. 3. AFM images of (a) bare steel sample, (b) 2-chloro-1H-imidazole, (c) 2-iodo-1H-imidazole immersed sample

Electrochemical Studies

Table 2. Tafel summary of preliminary studies

Inhibitor	$C_{inhibitor}$ (mM)	E_{corr} (mV vs SCE)	βa (mV/dec)	-βc (mV/dec)	Current density (x 10^{-4} A/cm^2)	Corrosion rate (mpy)	% Inhibition (%)
Blank (1 M HCl)	0	-520.0	79.70	109.1	2.29	104.5	-
2-Chloro	5	-532.0	88.10	96.20	2.21	100.8	3.5
Imidazole	5	-528.0	82.40	103.3	2.12	96.66	7.5
2-Bromo	5	-517.0	65.80	97.80	1.52	69.33	33.7
4-Phenyl	5	-544.0	284.9	309.0	1.38	63.26	39.5
2-Iodo	5	-476.0	126.4	136.7	1.10	50.48	51.7

Preliminary studies carried out using 5 mM concentration of the five compounds in the inhibition of mild steel corrosion in 1 M HCl showed that the iodo substituted compound provided a better inhibition efficiency

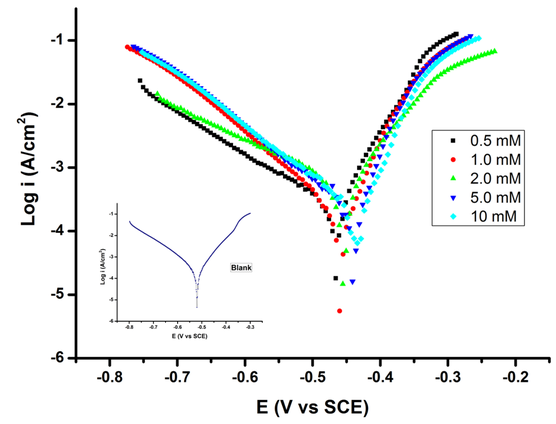

Fig. 4. Tafel plots of 2-iodo-1H-imidazole in 1 M HCl at various concentrations; Inset: blank 1 M HCl.

Conclusion

In conclusion, a preliminary study on the inhibition efficiency of a series of substituted imidazole compounds have been successfully carried out. The results showed that the iodo-substituted compound adsorb better on steel surface preventing the intrusion of the corrosive medium. Subsequent studies will hence be carried out to see the effect of having larger functional groups on the imidazole molecule.

References

1. Garcia, L.A.C.J., et al., Electrochimica Acta, 2001. **46**(24–25): 3879-3886.
2. Tiu, B.D.B., Advincula, R. C., Reactive and Functional Polymers, 2015. **95**: 25-45.
3. Ansari, K.R., Quraishi, M. A., Singh, A., Measurement, 2015. **76**: p. 136-147.
4. Shaban, S.M., et al., *J.* Industrial and Engineering Chem, 2015. **21**: 1029-1038.
5. Behrsing, T., Deacon, G. B., Junk, P. C., *Rare Earth-Based Corrosion Inhibitors*. 2014, Woodhead Publishing: 1-37.
6. Zhang, H.-h., et al., Applied Surface Science, 2015. **356**: p. 63-72.