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Palmitic acid based environmentally benign corrosion inhibiting formulation useful during acid cleansing process in MSF desalination plants

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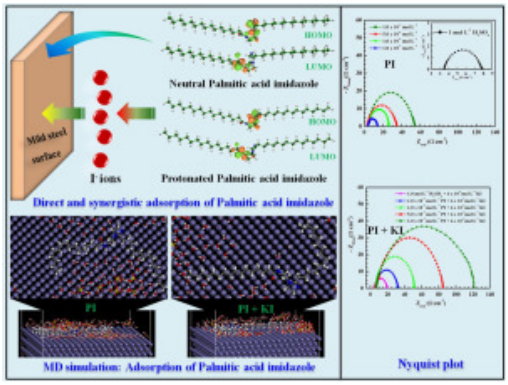
Abstract

Palmitic acid imidazole (PI) was synthesized in microwave reactor. The obtained product was explored to reveal the mild steel's corrosion inhibiting property in 1 mol L^{-1} H_2SO_4. It gave maximum inhibition efficiency of 90% at ambient condition. Addition of little amount of KI (6×10^{-3} mol L^{-1}) into 1×10^{-3} mol L^{-1} of PI further increased its efficiency up to 98%. High corrosion inhibiting property of PI was observed owing to its adsorption on mild steel surface. The synthesized inhibitor molecule adsorbs *via* physisorption and chemisorption phenomenon; and followed Langmuir adsorption isotherm. Synergistic effect of KI addition with inhibitors was investigated and the obtained synergism parameters revealed a co-operative mechanism. The surface topography analysis and water angle measurements exhibited surface protective and water repelling property of PI. Furthermore, DFT, FIs analysis, MD simulations and RDF analysis were performed for exploring intrinsic molecular property and insightful elucidation of corrosion inhibiting mechanism. It unveiled spontaneous and strong adsorption of both neutral and protonated PI on metals' surfaces in presence of iodide ions. The obtained outcomes suggested that the combination of KI and PI may be the preferable corrosion inhibitor during acid cleansing process in MSF desalination plants.

Graphical abstract



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Introduction

Carbon steel is widely employed in multi-stage flash (MSF) units owing to its suitable mechanical properties [[1], [2], [3], [4]]. It has been observed that the deposition of salts and scales on the MSF unit in desalination plants has caused a severe inconvenience and hampered its performances [5]. In order to get rid of such inconveniences and economic loss, sulphuric acid is used for removing salt deposits and scales from steel surfaces in several desalination plants [6]. No doubt, such acid cleansing procedures work well but it initiates the degradation of steel causing a huge economic loss as well as hygienic threats [[7], [8], [9]]. A remarkable measure to mitigate the metallic corrosion during de-scaling processes through acidic solutions is actually based on utilization of solution phase of organic compounds in certain concentration to inhibit the corrosion [[10], [11], [12], [13], [14]]. It is true that majority of organic molecules are environmentally pernicious, ultimately sets the challenges to find out environmentally benign organic inhibitors. Herein, major emphasis is given in finding out superior corrosion inhibiting compound having low toxicity [15].The use of ionic and non-ionic surfactants may be considered as suitable alternatives to replace pernicious, environmentally hazardous organic compounds specially focussing on hygienic issues [[16], [17], [18]].

Recently, it has been reported that the derivatives of imidazole molecules are environment friendly as well as non-toxic. Additionally, the imidazole derivatives are easily soluble in oil and water which facilitate its easy applicability for several purposes [[19], [20], [21], [22], [23]]. Furthermore, it is expected that the presence of nitrogen heteroatoms in the molecular skeleton act as sites for interacting with metal surface atoms. The nitrogen atoms are proficient in donating its lone pair electron to unfilled d-orbitals of metal, and it also possesses electron accommodating capacity in its anti-bonding orbital through back donation.

Presently, a few researchers have explored and reported the corrosion inhibition properties of a couple of imidazole derivatives for examples methylimidazole, vinylimidazole, phenylimidazole, benzimidazole, *etc* on aluminum, copper, carbon steel and mild steel [[24], [25], [26], [27], [28], [29], [30], [31], [32], [33]]. In these studies, the effect of aliphatic chain on the imidazole molecule has not been well explored. Additionally, a keen literature survey reveals that only a few imidazole molecules with small aliphatic chain have been explored for its corrosion inhibition property as shown in Table 1. It suggests that such derivatives of imidazole molecules are less explored both experimentally and theoretically. The detailed theoretical explanation on the adsorption and corrosion inhibition efficiency for such derivatives is also limited in literatures [[34], [35], [36], [37], [38], [39]].

In the present investigation, a palmitic acid imidazole (PI) has been synthesized *via* environmentally friendly microwave technique. PI may serve as efficient corrosion inhibiting molecule due to the presence of

long aliphatic chain, heteroatoms and π-bonds. Since, PI exhibit innocuous property, it motivated us to study its corrosion inhibition activities. The exhaustive literature survey reveals that no previous reports on PI as corrosion inhibiting molecule on mild steel against sulphuric acid are available. The palmitic imidazole is a derivative of imidazole containing one aliphatic chain *namely* pentadecane unit directly attached with the imidazole moiety and one palmitic unit attached with the imidazole moiety through ethanamine unit. This molecule is expected to be a better contender in the realm of corrosion inhibitor against the corrosive 1 mol L^{-1} H_2SO_4 medium. This is to be noted that in desalination plant, H_2SO_4 is preferred over HCl due to its low cost and it does not cause pitting corrosion *like* HCl. In this work, the corrosion inhibition efficiency of PI has been analysed by easy to handle and non-destructive electrochemical technique such as potentiodynamic polarization and electrochemical impedance spectroscopy, respectively. Apart from it, synergistic effect of KI with the synthesized PI has been precisely explored.

Herein, the investigation of the molecular property of PI molecule was executed using density functional theory (DFT) which is a proficient technical procedure to perform theoretical calculations with accuracy and small time interval. The energy of highest occupied molecular orbital (E_{HOMO}), the energy of lowest unoccupied molecular orbital (E_{LUMO}), E_{LUMO} - E_{LUMO} gap, fraction of electron transfer (ΔN) and global softness of the PI molecule have been calculated and explained. Following it, the local reactivity of different sites present in the inhibitor molecule has been analysed through Fukui indices (FIs) analysis. In addition to it, molecular dynamics (MD) simulation was also carried out to explore adsorption capability of synthesized PI on Fe (110) plane. Interaction and binding energy for adsorption of PI molecule have been calculated and explained. The MD simulation results also revealed the actual form of synthesized molecule adsorbed on mild steel surface accompanying other species such as H_2O, H_3O^+, SO_4^{2-} and with or without I^- anions. Furthermore, radial distribution function (RDF) for the inhibitor molecule has been analysed in order to explore the inhibitor-metal interactions.

Section snippets

Materials

The chemicals such as diethylenetriamine, palmitic acid, calcium oxide and ethyl acetate were procured from Sigma Aldrich. These chemicals were of analytical grade and used as received. GR grade 95–98% H_2SO_4 and the solvents *e.g.,* acetonitrile, methanol and diethylether of analytical grade were procured from Merck, India; and used as received.…

Instrumentations

The electrochemical measurements were carried out in CH Instrument make electrochemical workstation (model CHI660B) at room temperature (~25 °C). The…

Potentiodynamic polarization study

Generally, it is well known that when mild steels are exposed to corrosive electrolyte, the iron atoms loses its electron into electrolyte solution which is known as anodic reaction. On the other hand, H^+ ions consume those released electrons and produce H_2 gas at cathode. Now, when the inhibitor molecule is added in such medium then the adsorption of molecule hinders impending degradation of mild steel surface (anodic reaction) and H_2 evolution is retarded (cathodic reaction). The…

Conclusions

Corrosion inhibiting efficacy of palmitic imidazole (PI) for mild steels in 1 mol L^{-1} H_2SO_4 medium was evaluated and discussed using experimental measurements, quantum chemical calculations and MD simulation. Based on outcomes obtained from these experimentations, it can be concluded that PI can be used as an efficient molecule to inhibit corrosion of mild steels exposed in corrosive solution of 1 mol L^{-1} H_2SO_4. The adding of KI with PI molecule exhibits synergistic effect increasing the…

Acknowledgements

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