염수 환경에서 탄소강의 피리디늄 이온 액체에 대한 부식 억제 평가 연구

Investigation of Pyridinium Ionic Liquids in Corrosion Inhibition of Carbon Steel in Saline Environments

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Abstract : This study investigates the anti-corrosion properties of two eco-friendly pyridinium ionic liquids; 4DMN and 4DMP, in a 3.5% NaCl solution. Utilizing weight loss tests, EIS, PDP, quantum chemical calculations, and molecular dynamics simulations, the study demonstrates concentration-dependent inhibition efficiencies of 94% and 92% for 4DMN and 4DMP, respectively. The compounds modulate both anodic and cathodic reactions without altering the corrosion mechanism. EIS data suggest that a protective layer forms, supported by FE-SEM and AFM surface analyses, which reveal improved morphology and reduced roughness. Computational validations corroborate these empirical findings, highlighting the feasibility of these ionic liquids for effective, sustainable corrosion mitigation.

키워드 : 부식 억제제, 탄소강, 이온성 액체, 양자 화학 계산, 분자 역학
Keywords : Corrosion Inhibitor; Carbon Steel; Ionic Liquids; Quantum Chemical Calculation; Molecular Dynamics.

1. Introduction

Carbon steel, ubiquitously utilized in diverse industrial applications, is intrinsically susceptible to corrosive deterioration, especially in environments containing 3.5 wt.% NaCl. This susceptibility has far-reaching economic, environmental, and safety implications, thereby necessitating the search for efficacious corrosion inhibitors that are also environmentally benign [1]. Ionic liquids, characterized by their low vapor pressures and exceptional thermal stabilities, have garnered academic and industrial attention as potential corrosion inhibitors. Pyridinium-based ionic liquids, a subclass of ionic liquids, are of particular interest due to their propensity to form stable adsorptive layers on metal surfaces, serving as effective barriers against corrosive agents [2].

Existing literature has documented the inhibitory capabilities of pyridinium-based ionic liquids, particularly in acidic mediums, yet indicates that comprehensive exploration remains an imperative. Moreover, advancements in computational methodologies, such as quantum chemical calculations and molecular dynamics simulations, provide nuanced insights into the mechanisms governing inhibitor efficacy.

The current research endeavors to offer an exhaustive analysis of the corrosion-inhibiting attributes of two specific pyridinium-based ionic liquids: 4-(dimethylamino)-1-nonylpyridin-1-ium Bromide (4DMN) and 4-(dimethylamino)-1-(prop-2-yn-1-yl)pyridin-1-ium Iodide (4DMP). Utilizing a multi-faceted approach encompassing weight loss tests, electrochemical assays, and advanced microscopic techniques, as well as computational simulations, the study aims to scrutinize both the effectiveness and mechanistic underpinnings of these ionic liquids in mitigating corrosion of carbon steel in saline solutions. Thus, the research aspires to contribute substantively to the extant literature on sustainable corrosion inhibition strategies. energy.

2. Materials and methods

In this study, carbon steel samples, composed of 0.061% C, 0.179% Mn, and minor alloying elements, were subjected to mechanical polishing and subsequent sonication in different solvents for surface preparation. A three-electrode electrochemical cell setup was utilized, with carbon steel serving as the working electrode. The study incorporated Electrochemical Impedance Spectroscopy (EIS) and Potentiodynamic Polarization (PDP) for electrochemical analyses. To supplement these findings, Field-Emission Scanning Electron Microscopy (FE-SEM) and Atomic Force Microscopy (AFM) were used for surface characterization, while quantum chemical calculations and molecular dynamics simulations elucidated the interaction mechanisms between the inhibitors and substrate.

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3. Results and discussion

Figure 1 provides a comprehensive overview of the mechanistic and morphological effects of 4DMN and 4DMP on carbon steel corrosion in a 3.5 wt.% NaCl medium. Panels 1(a) and 1(b) reveal remarkable differences in surface morphology between the untreated and inhibited metal surfaces through AFM imaging. It corroborates the EIS results in panel 1(c), which indicates an increased polarization at varying immersion times.

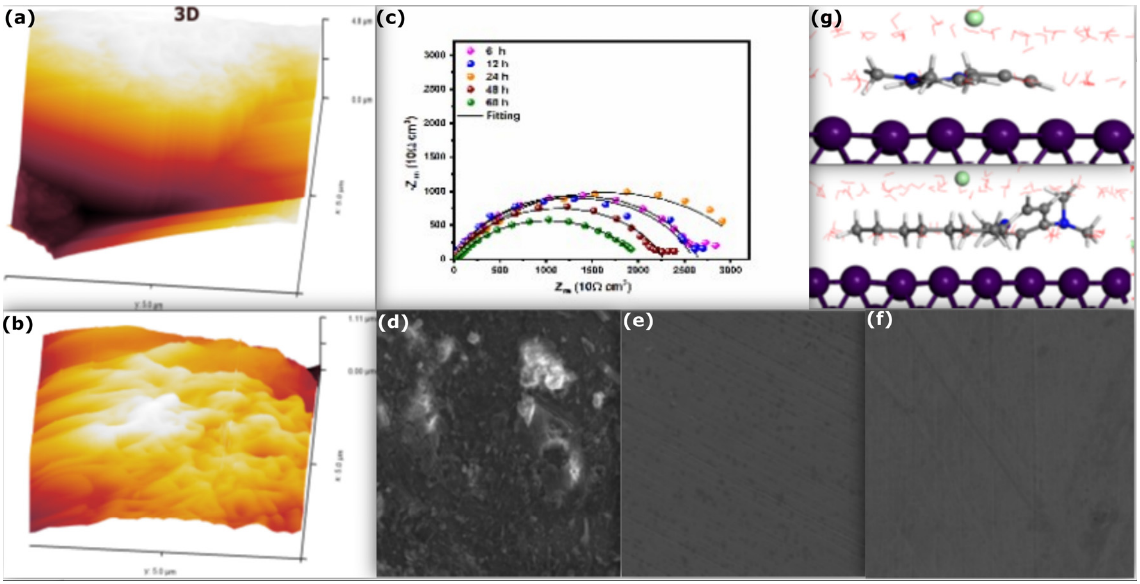

Figure 1. (a)–(b) AFM of blank and inhibited metal surface; (c) EIS results at different immersion periods; (d)–(f) SEM of blank and inhibited metal surface, and (g) Molecular dynamics simulation of ionic liquids on Fe(110) surface.

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The SEM images in panels 1(d) to 1(f) offer further validation, as they display an enhanced surface texture and minimized corrosive damage upon ionic liquid application. The findings are aligned with the conclusion that both ionic liquids act as mixed-type inhibitors and are highly stable at elevated temperatures and extended immersion durations.

Panel 1(g), elucidating molecular dynamics simulation results, serves to underscore the adsorptive strength and orientation of the ionic liquids on the Fe(110) surface. The near-parallel orientation demonstrated by MD simulation indicates optimal surface coverage, enhancing the inhibitory efficacy [3].

4. Conclusion

This study successfully synthesized and characterized 4DMN and 4DMP as eco-friendly, pyridinium-based ionic liquids for corrosion inhibition of carbon steel in saline media. Both compounds exhibited mixed-type inhibitory effects and high stability, especially 4DMN, which slightly outperformed 4DMP. Surface analyses through SEM and AFM confirmed improved morphological features, while quantum chemical calculations and molecular dynamics simulations provided computational validation. These results collectively demonstrate the promising utility of these ionic liquids as effective and sustainable corrosion inhibitors, setting a foundation for future research in broader industrial applications.

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