Evaluating Imidazoline Inhibitors on Pre-Eroded X65 Steel Surfaces: Insights into Erosion-Corrosion Mitigation

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Abstract Solid particle erosion-corrosion is a major safety hazard in pipeline systems used for energy development and petrochemical processes. The synergistic effects of erosion wear and electrochemical corrosion often exacerbate the deterioration of metal materials. In this study, we investigated the impact of two different imidazoline corrosion inhibitors 2-(6-hexadecenyl)-3-imidazoline-1-ethanol (HEIE) and the tall oil diethylenetriamine imidazoline (TDEI) on pre-eroded X65 steel. Electrochemical tests and surface characterization techniques were employed to analyze the effects of HEIE and TDEI on the corrosion morphology of X65 pipeline steel and the adhesion of the inhibitors. The study spans various temperatures, concentrations, and surfaces with different pre-erosion structures. Additionally, density functional theory (DFT) calculations were used to elucidate the inhibition mechanisms of these compounds. The adsorption behavior of HEIE and TDEI on steel surfaces was also examined. Molecular dynamics simulations investigated the diffusion behavior of corrosive substances in both aqueous and inhibitor-adsorbed phases. Results indicate that the irregular structures on pre-eroded surfaces may hinder the uniform adsorption of corrosion inhibitors, thereby reducing their effectiveness. The inhibition efficiency was found to be lowest at a pre-erosion angle of 30°. Quantum chemical calculations further revealed that the side-chain amino groups of TDEI molecules provided more adsorption sites compared to HEIE molecules, favoring TDEI adsorption on the X65 surface. Additionally, molecular dynamics calculations shed light on the adsorption mechanisms of TDEI and HEIE on the X65 steel surface, elucidating the corrosion inhibitor action mechanism at a molecular level. Through comprehensive comparison, our study conclusively establishes the superiority of TDEI over HEIE in terms of corrosion inhibition. This study provides new insights and methods for improving protective measures on pre-eroded surfaces.

Keywords Imidazoline Corrosion Inhibitor; Pre-erosion Initial Structure; Electrochemistry; Adsorption; MD Simulation