Experimental and Theoretical Approach for the Corrosion Deceleration of Mild Steel in Hydrochloric Acid Medium by Two Sulfonamide Derivatives

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In the pursuit to find corrosion inhibitors of superior efficacy, N-(pyrimidin-2-yl)-4-[(quinazoline-4-yl)amino]benzene-1-sulfonamide (PQS) and N-(4-methylpyrimidin-2-yl)-4-[(quinazoline-4-yl)amino]benzene-1-sulfonamide (MQS) are the two new sulfonamides employed, which have decelerating effect on mild steel (MS) corrosion in a medium 0.5 M HCl and were found to have an efficiency of 98.7% and 96.8% respectively (303 K for 40 ppm concentration) deliberated through the electrochemical techniques (PDP and EIS). The inhibitory efficacy relies on the temperature of the solution and inhibitor concentration. PQS had greater stability than MQS at higher temperatures which is indicative in the obtained experimental data. The relative adsorption process was in consonance with the Langmuir adsorption isotherm. The SEM, EDS, FT-IR, and AFM analysis validated PQS and MQS to form a barrier on MS, opposing corrosion. The potential energy surfaces (PES) scan and a theoretical study for PQS and MQS were probed employing density functional theory (DFT) at B3LYP/6-311+G(d, p) basis set level that explicated the formation of a complex between the sulfonamides and MS. The corrosion inhibition efficiency of PQS and MQS inferred from experimental and theoretical data comply, making them credible corrosion inhibitors.

Introduction

Mild steel (MS) executes a prominent role in the construction and marine industry due to its exemplary properties and economic feasibility, although the metal is prone to wasteful oxidation on its exposure to a corrosive environment. Corrosion of a metal is an electrochemical process that evinces cathodic and anodic reactions that constitute in eventual loss of metal. The role of a corrosion inhibitor is pivotal in corrosion control and organic inhibitors have proved to be efficient inhibitors.[1] The organic inhibitors in aqueous solutions tend to form a barrier/protective layer on the metal exterior, preventing the interaction of the corrosive environment which otherwise proceeds into the wasteful oxidation of the metal. The efficacy of the organic inhibitors is credited to the high polarizability value and electronegativity of the elements/functional groups on the molecule. There are several organic inhibitors like amines, polyamines, aldehydes, ketones, triazoles, phosphonates, sulfonates, sulfonamides, tannins, surfactants, organic acids and their salts exhibiting good efficacy in mitigation of corrosion. Inhibitors made of Schiff base and heterocyclic compounds with nitrogen, oxygen, phosphorus and sulphur elements have been reported to have superior corrosion inhibition efficacy in acidic solutions with O > N > S > P order which is ascribed to the π-electrons on them and their electronegativities.[2–6]

The organic inhibitors PQS and MQS investigated in this paper are the derivatives of sulfonamides which comprise quinazoline, sulfonamide and pyrimidine moieties. Quinazoline sulfonamides are the potential organic inhibitors that are eco-friendly and are extensively used for therapeutic use.[7] The presence of heteroatoms in their structure gives them a unique edge to armour the metal against wasteful oxidation. Sulfonamides under investigation comprise sulfur, oxygen and nitrogen in their moiety, which are the chief adsorption centers to the metallic surface. Preceding literature has indicated that sulfonamides have a staggering corrosion inhibitor propensity. The existence of the SO_2 group in sulfonamides has been the preferred site of interaction and their electron donating ability makes them effectual inhibitors.[8] Sulfamethazine, sulfabenzamide, sulfachloropyridiazine, sulfaquinaoxazoline are the notable sulfonamides in therapeutic use, that are categorized as green inhibitors due to their applicability in pharmaceuticals and delving findings in corrosion studies.[9] Pyrimidine derivatives are versatile in their corrosion inhibition, reviewed as environmentally viable through their electron donor-acceptor mechanism with the metal surface.[10,11]

The two sulfonamides PQS and MQS depicted in Figure 1 were synthesised, characterised and their molecular structure was confirmed in our previous research work.[12] They are

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