ABSTRACT

Corrosion manifests itself in multifarious forms in our daily lives. It affects the economy of the country and causes severe material science problem. The seriousness of the problem has made the corrosion scientist aware and conscious. Corrosion prevention technology has many options at its disposal for the successful corrosion mitigation of materials. An important method of minimizing corrosion today is the use of inhibitors. Corrosion inhibitors are extensively used in various applications and many plant operations are dependent on their successful operation.

The present work deals with the studies on the inhibitive action of heterocyclic compounds containing nitrogen, oxygen or sulphur atoms for corrosion of mild steel in acid medium.

The objectives of the present study are:

(1) To synthesize some heterocyclic compounds namely isoxazolines, hydroxy pyrazolines, pyrimidines and some bis-derivtives starting from chalcones.

(2) To test the inhibition effect of the synthesized compounds for mild steel corrosion in 1M H_2SO_4 by various techniques.

(3) To identify the optimal experimental condition for their maximum inhibition efficiency.

(4) To derive the adsorption kinetics from the weight loss data.

(5) To study the nature of the inhibition process and to determine the type of inhibition, whether anodic or cathodic or mixed.

(6) To investigate the nature of the surface film formed during the inhibition process.

(7) To study the mechanism of corrosion inhibition by the synthesized compounds.

(8) To compare the inhibitive effect of some selected compounds in 1M H_2SO_4 and 2M HCl.

(9) To study the synergistic influence of added anions and surfactants on the inhibition efficiency of isoxazolines and hydroxy pyrazolines.

The corrosion inhibitive properties of the synthesized inhibtitors have been studied using weight loss, potentiodynamic polarization and impedance spectroscopic analysis methods. From the experimental data various corrosion kinetic parameters such as inhibitor efficiency (IE %), corrosion rate, surface coverage, R_{ct}, C_{dl}, E_{corr}, I_{corr} *etc.*, have

been calculated. Analysis of the corrodent solutions for Fe^{2+} ions was done by Atomic absorption spectroscopy (AAS). Surface morphology of the mild steel plates FTIR, scanning electron microscopy – energy dispersive X-ray analysis (SEM - EDS), X-ray diffraction (XRD) and atomic force microscopy (AFM) techniques. Quantum chemical calculations have been performed using DFT in aqueous phase in both non-protonated and protonated form. Various quantum chemical parameters were calculated and correlated with the inhibitive effect of the selected inhibitors.