SUMMARY AND CONCLUSION

The present study is aimed to synthesis some new nitrogen containing heterocycles, and study of their antioxidant activity and corrosion inhibition performance on mild steel. Optimization of variables such as temperature, concentration of the inhibitor and immersion time for the corrosion inhibition of mild steel in 0.5 M HCl solution has been made. Evaluation of corrosion current density as a function of concentration of inhibitors from Tafel slopes was also performed. The polarization resistance and double layer capacitance were taken for consideration. The obtained results were reproduced by electrochemical measurements. The surface adsorbed film was characterized by SEM, FTIR and EDAX studies.

The study includes characterization of newly synthesized compounds using spectroscopic methods such as elemental analysis, FT-IR, $^1$H-NMR, $^{13}$C-NMR and LC-MS. The synthesized compounds were subjected to antioxidant assay using DPPH, OH and NO radical scavenging assay procedures. The synthesized compounds were studied as corrosion inhibitors in 0.5 M hydrochloric acid at different temperature, concentrations and possible immersion time. Experimental set up for all the studied inhibitors followed from standard available literature.

First chapter deals with the general introduction. In section – I general introduction to corrosion, theories and mechanisms of corrosion reactions, classification of corrosion, rate of corrosion and factors affecting the corrosion rate were discussed. In section – II corrosion inhibitors, mechanisms of corrosion inhibitors, classification of corrosion inhibitors, adsorption and polarization were discussed. Section – III deals with antioxidant activity and corrosion inhibition. In Section – IV a review of literature on corrosion inhibition of MS by organic compounds in different media was made. Section – V describes the scope of the present work, and finally the references were listed.

Second chapter deals with the materials and methods used. It starts from techniques used, solution preparation, materials treatment, measurement of corrosion rate. The measurement of corrosion rate was made using weight loss, potentiodynamic polarization (Tafel slopes) and electrochemical impedance spectroscopy (EIS) technique. Characterization of the complex film of inhibitors formed on the metal surface as well as on the corroding surface was made using FT-IR spectroscopy and
SEM morphologies. Different parameters like corrosion current density, charge transfer resistance, double layer capacitance and inhibition efficiency were calculated. In this chapter the synthesized compounds were also screened for antioxidant assay using DPPH, hydroxyl radical scavenging and nitric oxide radical scavenging assay procedures.

In the third chapter, three derivatives of pyridine based 1,3,4-oxadiazoles were synthesized and characterized. The synthesized compounds were studied as anticorrosive agent using gravimetric and electrochemical methods. In mass loss method, temperature and concentrations were optimized and inhibition efficiencies were calculated. The $IE\ (%)$ increases with increase in concentrations of 6-MMOPP, 5-MPOP and 4-BPOMP at all temperatures, and when the concentration reaches to 300 ppm, $IE\ (%)$ of 6-MMOPP, 5-MPOP and 4-BPOMP reached to of 89.9 %, 85.9 % and 84.6 %, respectively. The adsorption of all the studied molecules obeyed the Langmuir isotherm model. The negative values of free energy of adsorption indicated that the adsorption of the oxadiazole molecules is spontaneous process. The calculated $\Delta G_{ads}$ and $\Delta H_{ads}$ values indicated that the adsorption mechanism of the synthesized oxadiazole derivatives on mild steel in 0.5 M HCl solution is physisorption. SEM analysis showed that the formed surface film has higher stability and low permeability in aggressive solution than uninhibited mild steel surface, and EDAX analysis indicated that the studied inhibitors protected the mild steel surface. Quantum chemical calculations are well correlated with the experimental findings. The inhibition ability of these compounds followed the order 6-MMOPP $>$ 5-MPOP $>$ 4-BPOMP, and the inhibition efficiencies as determined by polarization, EIS and weight loss methods are in good agreement with each other. Antioxidant activity was also studied and correlated with anticorrosion efficiency.

Fourth chapter deals with the study of pyrimidine derivatives as corrosion inhibitors. The derivatives show excellent inhibition property for the corrosion of mild steel in 0.5 M HCl solutions, and the inhibition efficiency increases with increasing concentration of the inhibitors and temperature of the medium. The studied inhibitors are effective at 50 and 60 °C, at 50 and 60 °C, it was found that there was a slight increase or constancy in inhibition efficiency with the increase of temperature. However beyond 60 °C, inhibition efficiency decreases. The optimum concentration for all the studied inhibitor was 0.25g/L. The inhibition ability of these compounds follows the
order, 6-MMMTTCH > 6-MMOTCH > 6-MMTTCE > 6-MMOTCE, and the inhibition efficiencies determined by polarization, EIS and weight loss methods are in good agreement with each other. The adsorption of all the studied molecules obeys the Langmuir isotherm model. The negative values of free energy of adsorption indicated that the adsorption of the pyrimidine derivatives is spontaneous process. The calculated $\Delta G_{\text{ads}}$ and $\Delta H_{\text{ads}}$ values indicated that the adsorption mechanism of the synthesized pyrimidine derivatives on mild steel in 0.5 M HCl solution is physisorption. SEM analysis shows that the formed surface film has higher stability and low permeability in aggressive solution than uninhibited mild steel surface. Hence, they show enhanced surface properties. The highest inhibition efficiency of 6-MMMTTCH is due to the presence of C=S group, which enhances the electron density on the molecule, and act as the active sites for adsorption. Antioxidant activity was also studied and correlated with anticorrosion efficiency.

In the fifth chapter, three benzimidazole derivatives were synthesized and characterized. All the synthesized benzimidazole derivatives showed excellent inhibition property for the corrosion of mild steel in 0.5 M HCl solutions, and the inhibition efficiency increases with increasing concentration of the inhibitors. The studied inhibitors are effective at 30 °C, beyond 30 °C, it was found that inhibition efficiency decreases with the increase of temperature. The optimum concentration for all the studied inhibitor was 1.5 mM. The inhibition ability of these compounds follow the order, BDB > BPMP > BFB, and the inhibition efficiencies determined by polarization, EIS and weight loss methods are in good agreement with each other. The adsorption of all the studied molecules obeys the Langmuir isotherm model. The negative values of free energy of adsorption indicated that the adsorption of the benzimidazole molecule is spontaneous process. The results obtained from potentiodynamic polarization indicated that the synthesized inhibitors represent a mixed-type of inhibitors. The calculated $\Delta G_{\text{ads}}$ and $\Delta H_{\text{ads}}$ values indicated that the adsorption mechanism of the synthesized benzimidazole derivatives on mild steel in 0.5 M HCl solution is physisorption. SEM analysis shows that the formed surface film has higher stability and low permeability in aggressive solution than uninhibited mild steel surface. Antioxidant activity was also studied and correlated with anticorrosion efficiency.
Sixth chapter deals with the study of new 1,2,4-triazoles as corrosion inhibitors and antioxidant agents. The synthesised compounds showed excellent inhibition property for the corrosion of mild steel in 0.5 M HCl solutions, and the inhibition efficiency increases with increasing concentration of the inhibitors. The studied inhibitors are effective at 30 °C, beyond 30 °C, it was found that inhibition efficiency decreases with the increase of temperature. The optimum concentration for all the studied inhibitors was 0.5 mM. The inhibition ability of these compounds follows the order, 8-BMPTP > 8-BFMMTP > 8-BFDMTP, and the inhibition efficiencies determined by polarization, EIS and weight loss methods are in good agreement with each other. The adsorption of all the studied molecules obeys the Langmuir isotherm model. The negative values of free energy of adsorption indicated that the adsorption of the triazole molecule is spontaneous process. The results obtained from potentiodynamic polarization indicated that the synthesized inhibitors represent a mixed-type of inhibitors. The calculated ΔG_{ads} and ΔH_{ads} values indicated that the adsorption mechanism of the synthesized triazole derivatives on mild steel in 0.5 M HCl solution is physisorption. SEM analysis showed that the formed surface film has higher stability and low permeability in aggressive solution than uninhibited mild steel surface. The antioxidant activity and anticorrosion property of the synthesized triazole derivatives were correlated with each other.

In the seventh chapter, three new organic compounds containing nitrogen were synthesized and characterized. All the synthesized compounds showed excellent inhibition property for the corrosion of mild steel in 0.5 M HCl solutions, and the inhibition efficiency increases with increasing concentration of the inhibitors. The studied inhibitors are effective at 30 °C, beyond 30 °C, it was found that inhibition efficiency decreases with the increase of temperature. The optimum concentration for all the studied inhibitors is 1.309 mM. The inhibition ability of these compounds follow the order, 3-MPTT > 4-AMTT > 3-MHA, and the inhibition efficiencies determined by polarization, EIS and weight loss methods are in good agreement with each other. The adsorption of all the studied molecules obeys the Langmuir isotherm model. The negative values of free energy of adsorption indicated that the adsorption of the synthesized molecules is spontaneous process. The calculated ΔG_{ads} and ΔH_{ads} values indicated that the adsorption mechanism of the synthesized compounds on mild steel in 0.5 M HCl solution is physisorption. The greater inhibition efficiency of these inhibitors
is due to unshared electron pairs on hetero atoms and π- electrons of carbonyl group, >C-SH group and aromatic rings. SEM analysis shows that the formed surface film has higher stability and low permeability in aggressive solution than uninhibited mild steel surface. The antioxidant activity and anticorrosion property of the synthesized compounds were correlated with each other.

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