Chapter 9

CHAPTER-9

SUMMARY AND CONCLUSION

In the present investigation, the acid corrosion of mild steel which finds enormous industrial applications has been studied in the presence and absence of the synthesized benzoheteroazepine derivatives as inhibitors. The inhibition efficiency was studied by weight loss method and electrochemical measurements. Three class of benzoheteroazepines namely, benzodiazepines, benzothiazepines and benzoxazepines have been synthesized and subjected to corrosion inhibition studies.1M H_2SO_4 was used as corrosive solution. Mass loss measurements have been carried out at various concentrations and temperatures. Potentiodynamic polarization measurements were carried in the potential range of -200 mV to +200 mV with respect to OCP, with a scan rate of 1mV/s. The associated polarization parameters such as E_{corr}, I_{corr}, Tafel slopes were obtained and recorded.EIS measurements of benzoheteroazepines were done at open circuit potential with peak to peak amplitude of 10 mV. Nyquist plots in the form of semicircle were obtained in presence and absence of optimum concentration of inhibitor. Curve fitting was performed using Randle's equivalent circuit model. The impedance parameters were obtained with the help of IVIUM SOFT software. The adsorption of the inhibitors on the metallic surface was confirmed by SEM/EDX, AFM studies. The micrograph of the corroded and inhibited mild steel was recorded on scanning electron microscope, CARL ZEISS UK. The surface morphology of the inhibited metal surface was further confirmed by AFM studies, VEECO CP II. The effect of surfactant (CTAB and SDS) on the inhibition performance was studied in 1M H_2SO_4.

The experimentally calculated inhibition efficiency was correlated with molecular parameters obtained using theoretical calculations. Density functional theory with Becke's three parameter exchange functional along with Lee-Yang-Parr non-local correlation functional (B3LYP) with 6-31+G(d,p) basis set for neutral and protonated molecules were adopted using Gaussian 09 software.

The following conclusions were arrived from the investigations.

- The compounds were found to be good inhibitor showing 41-93% inhibition efficiency.
- IE depends on concentration of the inhibitor and temperature.
- The order of inhibition efficiency of the synthesized benzodiazepines (series I and series II) at 1M H_2SO_4 concentration is

  Series I

  MDPBD > DPBD > MPBD > TEBD ~ TMBD

  Series II

  TMPBD > EPBD > MEPBD > PBD > MBD
- Benzothiazepines showed greater inhibition efficiency than benzodiazepines and benzoxazepines due to the presence of less electronegative sulphur atom.
- All the synthesized benzoheteroazepines obeyed Langmuir adsorption isotherm.
- Benzodiazepines were found to display better corrosion inhibition for mild steel and copper compared to aluminium.
- Electrochemical impedance spectroscopy measurements have shown that an increase in inhibitor concentration causes an increase in charge transfer resistance and a decrease in C_{dl}, owing to the increased thickness of the adsorbed layer.
- Potentiodynamic polarization studies indicate that benzoheteroazepines behave as mixed type inhibitors.
- Addition of CTAB and SDS to the inhibitors DPBD and TMBD shows an increase in inhibition efficiency.
- Molecular parameters derived from quantum chemical studies correlated well with experimental order of inhibition efficiency.