

## Investigation of Acidizing Corrosion Inhibitors for Mild Steel in Hydrochloric Acid: Theoretical and Experimental Approaches

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**Abstract :** The corrosion inhibition performance of pyran derivatives (AP) on mild steel in 15% HCl was investigated by electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, weight loss, contact angle, and scanning electron microscopy (SEM) measurements, DFT and molecular dynamic simulation. The adsorption of APs on the surface of mild steel obeyed Langmuir isotherm. The potentiodynamic polarization study confirmed that inhibitors are mixed type with cathodic predominance. Molecular dynamic simulation was applied to search for the most stable configuration and adsorption energies for the interaction of the inhibitors with Fe (110) surface. The theoretical data obtained are, in most cases, in agreement with experimental results.

**Keywords :** acidizing inhibitor, pyran derivatives, DFT, molecular simulation, mild steel, EIS

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