Corrosion inhibitory Potential, Thermodynamics, and Computational Studies of Poly(2-vinyl pyridine), Carboxymethylcellulose, and Poly(2-hydroethylmethacrylate) Blends on Mild Steel in 0.5M H_2SO_4

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Abstract Poly (2-vinyl pyridine) (PVP), carboxymethylcellulose (CMC), and poly (2-hydroxyethyl methacrylate) (PHEM) are three polymeric inhibitors whose anticorrosion properties were evaluated using both experimental and computational methods on mild steel in 0.5M H_2SO_4. The weight loss, corrosion inhibition, efficiency, degree of surface coverage, adsorption studies, electrochemical tests, kinetics and thermodynamic analysis, and computational studies were determined. The Gibbs free energy was determined using the Frumkin adsorption model. The Arrhenius plots were utilized to determine the activation energy, and the transition state equation was utilized to determine the enthalpy and entropy. Computational studies utilizing the molecular dynamics (MD) simulation were conducted using the Forcite module tool as contained in Material Studio software (7.0). The results demonstrated that the adsorption mechanism was temperature-dependent, as the polymer composite's protection effectiveness increased as temperature rose. Temperature and concentration increases were found to correlate with increases in surface angle, weight loss, and corrosion inhibition efficiency. PVP/CMC blend (1:3) at the concentration of 3.0g/l exhibited the highest inhibition efficiency at 24 hours, with 96.22 %, while PVP/PHEM (1:1) had the lowest, with 40.74 at 0.5g/l concentration at 168 hours. The results of the adsorption experiments were in agreement with the Freundlich, Langmuir, and Temkin isotherms, with nearly unit values and a linear graph obtained for each polymer blend. According to computational studies, all of the polymer blends showed a negative binding energy and a positive interaction energy, suggesting strong corrosion inhibition efficiency. With concentration, temperature, and exposure time having significant effects on their inhibition efficiency, these results validate the potential of the polymer blends as mild steel corrosion inhibitors.

Keywords Corrosion inhibitors, Thermodynamic, Langmuir, Chemical adsorption.