Materials Today Communications

Volume 21, Issue 1, 2019, Pages 100-720

Thermodynamic investigation on the adhesion and corrosion inhibitionproperties of a non-steroidal anti-inflammatory drug in HCl electrolyteapplied on mild steel material

Azeddine Addoun, Saida Bouyegh, Mohamed Dahmane, Ouassila Ferroukhi, Mohamed Trari

Abstract: In this paper, the inhibition mechanism of a pharmaceutical agent, piroxicam, on the corrosion behavior of carbon steel in HCl (1M) solution was investigated. The weight loss technique and quantum chemical calculations were carried out. The determined inhibition efficiency at 298 K was 86.90 % for a concentration of 600 ppm. The adsorption mode of the drug obeys to the Langmuir isotherm model. The free energy of adsorption (?Gads = ?32.84 kJ mol?¹) revealed a spontaneous process with a mixed interaction type, physical and chemical. The thermodynamic parameters (?Hads and ?Sads) governing the adsorption phenomenon and metal dissolution were investigated and discussed through thermodynamic and kinetic principles. The ?Hads and ?Sads were respectively ?17.86 kJ mol?¹ and 50.27 J mol?¹ K?¹ which indicates an exothermic process and an increased disorder at the interface. The DFT method was used to determine the adsorption centers of the chemical structure of the drug. EHOMO (?6.448 eV) reveals a high tendency of the drug to share its electrons with the metal. In addition, the SEM analysis was carried out for the surface characterization of the carbon steel after immersion into the aggressive medium in the absence and presence of the drug substance.

Keywords : Mild steel, Weight loss, adsorption, DFT