

Anticorrosion ability of pyrimidine derivative onto Q235 steel in oilfield acidizing fluid under hydrodynamic condition

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Abstract

The paper represents the green synthesis and inhibitive performance of pyrimidine derivative (PP) over Q235 steel in 15% HCl under dynamic conditions. The result of EIS suggests the rise in R_{ct} with the rising amount of PP amount. PDP result reveals the mixed nature of PP inhibitive action. The PP performance value is 93% at 200 mg/L. Surface study reveals the development of protective film of PP over the metal surface. Density functional theory (DFT) suggests that the protonated form of PP shows stronger adsorption ability than neutral one. Molecular dynamic simulation (MD) confirmed that the adsorption geometry of PDH⁺ on iron surfaces exhibits more parallel orientation than PP.

Keywords: Pyrimidine derivative; Acidization; Q235 steel; XPS; MD