

Experimental and Theoretical Studies of Black Cumin Seed (*Nigella sativa*) as Corrosion Inhibitor for ASTM A36 Steel

Black cumin seed extract (*Nigella sativa*) effectively controls corrosion of ASTM A36 steel in 1 M HCl solution. This study analysis black cumin seed extract as a corrosion inhibitor at 0, 100, 200, 300, 400, and 500 ppm by electrochemical methods including Potentiodynamic Polarization (PDP) and Electrochemical Impedance Spectroscopy (EIS). The results revealed that with the PDP method the highest inhibition efficiency (IE) was obtained 84.26% at a concentration of 500 ppm and with the EIS method an IE value of 77.77% was obtained at the same concentration. The black cumin seed extract functions as a mixed type inhibitor and adsorption of the inhibitor on the ASTM A36 steel surface through a physisorption mechanism at 298 K. The compounds of the extract were analyzed by GCMS an obtained major compounds namely linoleic acid (25.12%), methyl linoleate (22.70%), 4-cyclopentene-1,3-dione,4-3-methyl-2-butenyl (7.64%), methyl palmitate (6.66%), and palmitic acid (5.14%). A theoretical approach with computation was also carried out to investigate the interaction of major compounds in the extract that play a significant role as inhibitors. This was done using Density Functional Theory (DFT) method and Monte Carlo simulation. The results showed that methyl linoleate compound played the most significant role.

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