**ABSTRACT**

Corrosion inhibition of mild steel in 1 M H2SO4 was investigated in the absence and presence of different concentrations of quinoxaline derivatives namely (3E)-3-(phenylimino)-3,4-dihydroquinoxalin-2(1H)-one (PDQO), (3E)-3-[(2-methylphenyl) imino]-3,4-dihydroquinoxalin-2(1H)-one (MPDQO) and (3E)-3-[(2-methoxy-phenyl)imino]-3,4-dihydroquinoxalin-2(1H)one (MOPDQO). Weight loss, potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) measurements were employed. Impedance measurements showed that the charge transfer resistance increased and double layer capacitance decreased with increase in the inhibitor concentration. Potentiodynamic polarization study showed that the inhibitors acted as mixed-type inhibitors. The adsorption of these compounds on the mild steel surface obeys a Langmuir adsorption isotherm. Results obtained reveal that compound MOPDQO is the best inhibitor and the inhibition efficiency follows the sequence: MOPDQO > MPDQO > PDQO. Electronic properties such as highest occupied molecular orbital (EHOMO) and lowest unoccupied molecular orbital (ELUMO), the energy difference (ΔE) between EHOMO and ELUMO, dipole moment (μ), electronegativity (χ), electron affinity (A), hardness (η), softness (σ), ionization potential (I), the fraction of electrons transferred (ΔN), total energy (TE) were calculated and discussed. The results showed that the corrosion inhibition efficiency increased with an increase in the EHOMO values but decrease in the ELUMO values. Mulliken atomic charges, Fukui functions and softness indices were discussed in order to characterize the inhibition property of the inhibitors.