

## Experimental and Theoretical Investigations Oil of Cymbopogon citratus as Corrosion Inhibitors on Copper in Sulfuric Acid Solution

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Abstract:

Lemongrass oil (*Cymbopogon citratus*) is effective in controlling corrosion of copper in sulfuric acid solution. This study analyzed lemongrass oil as a corrosion inhibitor at 0, 100, 200, 300, 400, and 500 ppm using electrochemical methods including potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS). These methods are used to determine the corrosion rate, inhibition efficiency, and adsorption isotherm value. The results revealed that with the PDP method the highest inhibition efficiency ( $\eta$ ) was obtained at 93.15% and with the EIS method the  $\eta$  value was obtained at 97.70% at the same concentration of 500 ppm. Lemongrass oil functions as a mixed type inhibitor and is included in the Langmuir isothermal adsorption type and inhibitor adsorption on the copper surface through a physisorption mechanism at a temperature of 298 K (room temperature). The extract compound components were analyzed by GCMS and the major compounds obtained were citrol/geraniol (32.48%), Z-citral (28.00%), and trans-Geraniol (14.69%). A theoretical approach with computational chemistry was also carried out to confirm the efficiency of lemongrass inhibitors against copper and to analyze the interaction of compounds in the extract that play a significant role as inhibitors. This was done using the Density Functional Theory (DFT) method and Monte Carlo simulation. The results showed that the citrol/geraniol compound played the most significant role.

Keywords: Corrosion Inhibitor, PDP, EIS, DFT, Monte Carlo, Isothermal Langmuir, Lemongrass Oil (*Cymbopogon citratus*).

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