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Experimental and computational studies of *Nicotiana tabacum* leaves extract as green corrosion inhibitor for mild steel in acidic medium

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Abstract In the present work corrosion inhibition of mild steel in 2 M H_2SO_4 solution by *Nicotiana tabacum* extract was studied by weight loss method. It has been found that the extract acts as an effective corrosion inhibitor for mild steel in Sulfuric acid medium. The inhibition process is attributed to the formation of an adsorbed film of inhibitor on the metal surface which protects the metal against corrosion. The inhibition efficiency (%IE) and surface coverage (θ) of *N. tabacum* extract increased with increase in inhibitor concentration but decreased with increasing the temperature. The adsorption of extract on the mild steel surface was found to obey Langmuir's adsorption isotherm. The free energy value (ΔG_{ads}) indicated that the adsorption of inhibitor molecules was typical of physisorption. The results obtained show that *N. tabacum* Extract could serve as an excellent eco-friendly green corrosion inhibitor. Quantum chemical parameters such as highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), energy gap (ΔE), dipole moment (μ) and Mulliken charges were calculated. Quantum chemical calculations also supported experimental data and the adsorption of inhibitor molecules onto the metal surface.

1. Introduction

Mild steel has been the most widely used alloy for structural and industrial applications such as, industries mining, construction and metal processing equipment [1]. The use of acid media in the study of corrosion of mild steel has become important because Sulfuric acids and Hydrochloric acid are the medium generally being used for pickling mild steel and industrial cleaning, and acid descaling [2,3]. The protection of metal against corrosion is a major industrial problem. The use of inhibitors is one of the best options of protecting metals against corrosion in acid solutions. Most organic compounds having heteroatoms and shows anti-corrosive activity [4]. Synthesis of these organic compounds is not only expensive but also toxic to both human beings and environments [2–5].

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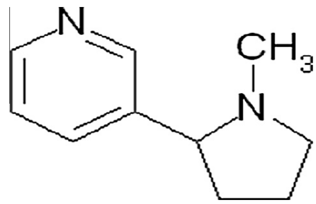

Figure 1 Basic structure of nicotine.

Thus, the researchers have been focused on the use of eco-friendly compounds and ecologically acceptable such as extract of common plants because these plant extracts are bio-degradable, cheap, easy available and renewable sources of materials [6]. Green corrosion inhibitors are biodegradable and do not contain heavy metals or other toxic compounds [7,8]. Extracts of plant materials contain a wide variety of organic compounds. Most of them contain heteroatoms such as P, N, S, and O. These atoms coordinate with the corroding metal atom (their ions), through their electrons and prevent corrosion by formation of protective layer on the metal surface [8]. A great number of scientific studies have been dedicated to the corrosion inhibition of mild steel in acidic media by natural products as corrosion inhibitors [1,3,4,6–8].

Nicotiana tabacum is perennial herbaceous plant and member of Solanaceae family. It has been reported to extract contain relatively high concentrations of alkaloids, fatty acids and nitrogen-, fluorine-, sulfur- and oxygen-containing compounds [9]. Recently GC/MS analysis performed by Njoku and co-researchers [9] and determined the major phytochemical constituent present in *N. tabacum* is nicotine, which can be acted as an active constituent and extract use as inhibitor (Fig. 1). To explore this possibility, an attempt has been made to ascertain its corrosion inhibition properties on mild steel in 2 M H_2SO_4 solution by weight loss method and computational method also.

2. Experimental work

2.1. Preparation of leaves extract

N. tabacum (Tobacco) leaves were used to make the aqueous extract. Tobacco purchased from local market, dried leaves powder weighed 25 g were thoroughly washed in distilled water and soked in 250 mL. distilled water for 24 hours then heated at 50–55 °C and extract was filtered through Whattman No. 1 filter paper. The extract of tobacco leaf obtained in this manner was used as an inhibitor.

2.2. Preparation of test solution

The aggressive solution (2 M H_2SO_4) was prepared by dilution of Analytical Grade 98% H_2SO_4 with double-distilled water. The solution volume was 100 mL with and without the addition of different concentrations of *N. tabacum* extract ranging from 2.5 g/L to 10 g/L.

2.3. Specimen preparation

Prior to all measurements, the mild steel samples were polished with different emery papers up to 300 grade, and rectangular specimen of mild steel was mechanically pressed cut to form different coupons, each of dimension exactly $4 \times 2 \times 0.1$ cm. Each coupon was degreased by washing with double distilled water then dried in acetone and preserved in a desiccator. All reagents for the present study were Analar grade and double distilled water was used for their preparation.

2.4. Weight Loss method

The Weight Loss technique is the conventional and simplest of all corrosion monitoring techniques. The method involves exposing a specimen of material (the coupon) to a process environment for a given period, then removing the specimen for measurement. The basic measurement which is determined from corrosion coupons is weight loss, the weight loss taking place over the period of exposure being expressed as corrosion rate [10,11].

In the Weight loss measurements, mild steel coupons in triplicate were completely immersed in 100 mL of the test solution of acidic environment (2 M H_2SO_4) in the presence and absence of the inhibitor at different temperatures. The metal specimens were withdrawn from the test solutions after 6 h at temperature 303 K $\pm$ 1 and 313 K $\pm$ 1. The polished samples were cleaned with acetone. The Weight loss was taken as the difference in weight of the specimens before and after immersion determined using DHONA 200 D analytical balance with sensitivity of ± 0.1 mg. The tests were performed in triplicate to guarantee the reliability of the results and the mean value of the weight loss is reported. Triplicate samples were used to check reproducibility of results. Weight loss allowed us to calculate the mean corrosion rate as expressed in mg cm^{-2} h^{-1}. Corrosion rate is calculated assuming uniform corrosion over the entire surface of the coupons. Corrosion rates, *CR* are calculated from weight loss methods. The formula used to calculate corrosion rate is as in Eq. (1). From the weight loss measurements, the corrosion rate will be calculated using the following relationship [10,11].

$$\text{Corrosion rate (mmpy)} = \frac{87.6 \times W}{DAT} \tag{1}$$

where mmpy = millimeter per year, W = weight loss (mg), D = density (gm/cm^3), A = area of specimen (cm^2), and T = time in hours.

The inhibition efficiency (%IE) and degree of surface coverage (θ) were calculated using Eqs. (2) and (3), respectively.

$$\%\text{IE} = \frac{(W1 - W2)}{W1} \times 100 \tag{2}$$

$$\theta = \frac{(W1 - W2)}{W1} \tag{3}$$

where $W1$ and $W2$ are the corrosion rates in the absence and presence of the inhibitor respectively.

2.5. Quantum chemical study

Quantum chemical calculations based on DFT/B3LYP level are performed to find the relation between the molecular structure of the inhibitor and the inhibition efficiency. All the calculations were performed with Gaussian 03 for windows [12]. The molecular structure of Nicotine was fully and geometrically optimized using the functional hybrid B3LYP (Becke,

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