4-HYDROXY-3-METHOXYBENZALDEHYDE AS A VOLATILE INHIBITOR ON THE ATMOSPHERIC CORROSION OF CARBON STEEL

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ABSTRACT

The 4-hydroxy-3-methoxybenzaldehyde was studied as a nontoxic efficient volatile corrosion inhibitor for the temporary protection of mild steel. The corrosion inhibition property was evaluated under simulated operational conditions. Electrochemical measurements were applied to study the inhibition effect of compounds on the corrosion of carbon steel with a thin stimulated atmospheric corrosion water layer. Polarization data indicated that the studied inhibitor is a mixed-type inhibitor. Adsorption of components on the carbon steel surfaces was investigated by scanning electron microscope (SEM). The electronic parameters calculated include: \( E_{\text{HOMO}} \), \( E_{\text{LUMO}} \), energy gap, etc. The calculated results show that all the molecules have high propensity as electron donors, low energy gap and hardness (high reactivity), and they are good nucleophiles characterized by low values of global electrophilicity index, and the energy change associated with the charge transfer to the mild steel surface \( \Delta E \), are all favourable (negative). Depending on the results, the inhibitive mechanism is proposed from the viewpoint of adsorption theory.

Keywords: atmospheric corrosion, 4-hydroxy-3-methoxybenzaldehyde, volatile inhibitors, films, DFT calculation.

INTRODUCTION

Atmospheric corrosion of metals in closed spaces, such as in parcels, and during storage and shipment, can be temporarily prevented by the use of certain substances called vapour phase corrosion inhibitors [1 - 5]. Most of the volatile corrosion inhibitors are synthetic chemicals, expensive, and hazardous to environments. Natural products are known to be incredibly rich sources of naturally synthesized chemicals for most applications. Plant extracts are bio-degradable, non-toxic and of potentially low cost.

Thus, an alternative of environmental-friendly VPIs is under consideration promising raw materials for the development of VPIs, we can mention organic substances of vegetable origin because the natural raw materials contain a large number of biologically active substances and the process of extraction is, more cost-efficient than chemical synthesis [6 - 10]. In the literature, one can also find no information about possible applications of the plants extract and its extracted compounds for the development of volatile corrosion inhibitors. Only several works devoted to the study of natural compounds like wood bark oil [11] and thyme [12, 13] as VCl. In continuation of our work, some plant extracts have been studied as effective volatile corrosion inhibitors of steel namely Rapeseed cake, Hope Cones, Brushes and skins of grapes and Lavanda, Artemisia extracts [14, 15]. The inhibition of mild steel corrosion by the studied species of plant raw materials [16] is probably attributed to the presence of most important compounds such as aldehydes - 4-hydroxy-3-methoxybenzaldehyde. It has many advantages such as low cost, non-toxicity and easy production.
Noticeably, the plant extract is a mixture of various components, which result in the complex inhibitive mechanism. It is rather difficult to determine what components present in plant extract create their relatively high ability to inhibit corrosion. A better way is to isolate the components and to investigate the inhibition of each single component, but it is still difficult to isolate all the components. In addition, it takes long time to isolate the components. Thus, testing the inhibition potential of major components using available pure compounds could be an alternative choice to study the corrosion inhibition of plant extract. Furthermore, the potential usages of 4-hydroxy-3-methoxybenzaldehyde discussed in this research are in line with the recent trend of the environment-friendly concept. El-Etre investigated the effect of 4-hydroxy-3-methoxybenzaldehyde on the corrosion of aluminum in 5.0 M HCl. Afterwards, Emergül and Hayvalı studied the corrosion inhibition of 4-hydroxy-3-methoxybenzaldehyde on steel in 2.0 M HCl, and the inhibition efficiency is about 85 % [17 - 19]. However 4-hydroxy-3-methoxybenzaldehyde has not been studied as volatile atmospheric corrosion inhibitor of steel. 4-hydroxy-3-methoxybenzaldehyde is examined and proved to possess tremendous potential for industrial usage. Unlike the pure synthetic product that requires enormous investment scale, 4-hydroxy-3-methoxybenzaldehyde can be produced at any type of industrial scale, which is potentially capable of eradicating the disparity among the communities, especially in the third world.

The present study is designed to report the effects of 4-hydroxy-3-methoxybenzaldehyde as volatile corrosion inhibitor of steel.

**EXPERIMENTAL**

**Materials and Apparatus**

The corrosion test and electrochemical measurements were carried out using mild steel strips. The composition of the mild steel is given in %: C - 60.15; Mn - 0.20-0.45; P - 0.03; S - 0.035 and Al, P - 0.02.

Steel specimens (50×20×1.5 mm) were used for volatile inhibiting sieve test (VIS). The strips were polished by emery paper of 1/0, 2/0 and 3/0, rinsed with double distilled water, degreased and dried at room temperature.

The inhibitor used was 4-hydroxy-3-methoxybenzaldehyde with the concentration range from 200 to 1,000 ppm, obtained from Merck and used without further purification. The purity is 99.0 % on dries basis. Fig. 1 shows the molecular structure of 4-hydroxy-3-methoxybenzaldehyde. As an inhibitor, an 2-propanol 4-hydroxy-3-methoxybenzaldehyde solution with a concentration of 25 mg/L is used.

**Gravimetric measurements**

Volatile inhibiting sieve test was applied to evaluate the inhibition effect of the VCIs. To obtain reproducible results three samples were used in each test simultaneously. There was a hole in each plate drilled to suspend the sample by a nylon thread. The samples were grinded with SiC paper to 1000 mesh and were then cleaned in alcohol and rinsed before drying at room temperature. The final geometrical area was 25 cm$^2$. The gravimetric measurement was conducted by suspending the samples in a 250 cm$^3$ conical flask with a tight-fitting rubber cork containing a small dish. The VCIs were dispersed in the dish. The samples with freshly prepared surface were mounted on the flask with and without 1.0 g inhibitor, respectively. After inhibitor film-forming period of 3 days, 15 cm$^3$ deionized water was added. The test process included cyclic warming and cooling of the samples in a corrosion testing chamber of varying humidity. One cycle included an 8 h exposure in the thermostat (50 ± 1°C), and 16 h exposure at room temperature.

Corrosion rates and inhibitor effectiveness are calculated by means of the following equations:

$$CR = \frac{W_0 - W_1}{A \times T},$$

$$IE = \frac{CR_1 - CR_2}{CR_1} \times 100,$$

where CRs is in g m$^{-2}$ h$^{-1}$; A is the sample area, m$^2$; $W_0$ is initial weight of the sample, and $W_1$ is sample weight, g, after the immersion period, T is the immersion period, h, and CR$1$ and CR$2$ are the corrosion rates without and with inhibitor, respectively.
Electrochemical measurements
To determine the influence of protective surface films on the cathodic and anodic electrode AC processes for mild steel, we plotted the potentiodynamic polarization curves for a three-electrode electrochemical cell in air by separating the anolyte from the catholyte (the volume of working solution was 60 cm$^3$). We used a cylindrical copper electrode pressed into a Teflon holder and a platinum plate as an auxiliary electrode. The disk end face of the mild steel electrode 0.385 cm$^2$ in area served as the working surface. We plotted the polarization curves in a $0.5 \text{ M Na}_2\text{SO}_4$ solution used as a model of aggressive medium of the AC of metals. As a specific feature of our electrochemical investigations, we can mention the following fact: the disk-shaped surface of the end face of the working electrode was immersed in surface layers of the working solution by at most 1 - 2 mm [20]. This enabled us to perform more exact modeling of the AC running on the metal surface in thin layers of condensed moisture. A capillary from the reference electrode was placed near the surface of the working electrode from below. Prior to processing in the VIAC vapor, the working electrode was polished and degreased with acetone. The VIAC film on the surface was preliminarily formed in vapors of the isopropanol extract and distilled water for 24 h. Polarization curves studies were carried out using EG&G Instruments potentiostat-galvanostat (Model 263A). The potential of mild steel was measured relative to the silver-chloride reference electrode. The induced electrode potentials were recalculated relative to the normal hydrogen electrode.

Scanning electron microscope (SEM)
The surface morphology and coating were examined by FEI E-SEM XL 30. For SEM images, 1 cm$^2$ specimen samples were taken.

Fourier Transformation Infrared Spectroscopic Studies (FT-IR)
The extract of plant material was tested on IR - Fourier - spectrometer Jasco FT/IR – 4000. To characterize adsorbed film on the metal, 1 cm$^2$ surface area of mild steel was exposed to both gas mediums for certain hours and used for surface analysis by FT/IR spectrum. The registration of IR-reflectance spectra of the sample surface pretreated volatile corrosion inhibitors was performed by IR Fourier-transformed spectroscopy (Perkin Elmer) in the range of 4000 - 630 cm$^{-1}$.

Quantum chemical calculations
Quantum chemical calculations have been performed by the HyperChem 7 [21] package. The geometry optimization was obtained by application of the restricted Hartree-Fock method (RHF) using MNDO approach with PM3 parameterization [22]. Quantum chemical calculations have been found to be successful in providing insight into chemical reactivity and selectivity in terms of global molecular properties, such as electronegativity ($\chi$) and chemical potential ($\mu$) [23]. Thus, for an N-electron system with total electronic energy ($E$) and an external potential $v(r)$; the chemical potential ($\mu$), which is also the negative of the electronegativity ($\chi$), has been defined as the first derivative of the E with respect to N at constant $v(r)$ [24]. According to Koopman’s theorem, the frontier orbital energies $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ are related to the ionization potential, $I$, and the electron affinity, $A$, of iron and the inhibitor molecule by the following relations: $A = -E_{\text{LUMO}}$, $I = -E_{\text{HOMO}}$ [25 - 27]

\[ \chi = -\mu = \frac{1}{2}(I + A) \]  

The hardness $\eta$ of an electronic system is defined as [28]:

\[ \eta = \frac{1}{2}(I - A) \]

where $I$ and $A$ are the ionization potential and electron affinity [27].

The global softness ($S$), is the inverse of global hardness and is given as [28]:

\[ S = \frac{1}{2\eta} \]

It has been reported that the more stable molecular structure has the largest HOMO-LUMO energy gap [29]. Therefore, an electronic system with a larger HOMO-LUMO gap should be less reactive than one having a smaller gap. This relationship is based on the Maximum Hardness Principle [30], which states that ‘there seems to be a rule of nature that molecules arrange themselves so as to be as hard as possible’. This principle is among the most widely accepted electronic principles of chemical reactivity and a formal proof of this principle was given by Parr and Chattaraj [31]. If bulk iron metal and the inhibitor molecule are brought together, the flow of
electrons will occur from the molecule of lower electronegativity to the iron that has higher electronegativity until the value of the chemical potential becomes equal. The fraction of electrons transferred from the inhibitor molecule to the iron atom will then be given by \[15\].

The global electrophilicity index (\(\omega\)) was introduced by Parr et al. \[32\]. Using the parabolic model, it was shown that global electrophilicity index, can also be written as:

\[
\omega = \frac{(I + A)^2}{8(I + A)}
\]

The electron charge transfer, \(\Delta N\), from base B to acid A, and the associated energy change \(\Delta E\) is given as \[27\]:

\[
\Delta N = \frac{\mu_B - \mu_A}{2(\eta_A + \eta_B)} = \frac{\Phi - \chi_{mol}}{2\eta_{mol}}
\]

\[
\Delta A = \frac{(\mu_B - \mu_A)^2}{2(\eta_A - \eta_B)} = \frac{(\Phi - \chi_{mol})^2}{4\eta_{mol}}
\]

The electronegativity of metal surface is replaced by the work function for Fe (110) surface, \(\Phi\), theoretically equals 4.82 eV and the hardness, \(m_{metal}\) which equals 0 eV for bulk metals \[33\].

**RESULTS AND DISCUSSION**

Visual inspection was carried out following the criterion for the volatile corrosion inhibition test. Corrosion rate and inhibition effectiveness for the test samples are shown in Table 1. The analysis of the results of accelerated corrosion tests shows that the 4-hydroxy-3-methoxybenzaldehyde protects steel from corrosion under the conditions of periodic moisture condensation. Inhibition effectiveness for the compounds varies between 96 – 99 %. The degree of protection varies within the range 64.4 - 99.8 % depending on the test conditions. The results indicate that compounds can form a protective film on the metal surface, which protects the metal against further corrosion.

It was investigated the influence of the pre-treatment immersion time of steel in the volatile phase of 4-hydroxy-3-methoxybenzaldehyde on corrosion effect under the conditions of periodic moisture condensation. It should be noted that the corrosion rate decreases with increasing the time film formation. The inhibition efficiency (IE) increases in the range 86.71 - 91.9 % (Table 2). The protective film on the steel surface is formed nonuniformly for 40 - 48 h of its treatment with volatile compounds of the extract.

**Table 1. Calculated corrosion rates (g m\(^{-2}\) h\(^{-1}\)) and inhibition efficiency (%) for volatile corrosion inhibition test VCIs. (Period of film-forming, 48 h).**

<table>
<thead>
<tr>
<th>Distilled water</th>
<th>Corrosion rates</th>
<th>Inhibition efficiency (IE), %</th>
</tr>
</thead>
<tbody>
<tr>
<td>30 mg/dm(^3) NaCl; 50 mg/dm(^3) Na(_2)SO(_4)</td>
<td>0,002</td>
<td>98,9</td>
</tr>
<tr>
<td>100 mg/dm(^3) NaCl, 100 mg/dm(^3) NaHCO(_3), 100 mg/dm(^3) Na(_2)SO(_4)</td>
<td>0,0681</td>
<td>64,6</td>
</tr>
</tbody>
</table>

**Fig. 2.** Polarization curves of St3 steel in 1N Na\(_2\)SO\(_4\) without protective film (curve 1) and with a film formed after holding for 24, 48, 72 h in the vapor phase of the 2-propanol solution of 4-hydroxy-3-methoxy-benzaldehyde.
The effects of 4-hydroxy-3-methoxybenzaldehyde on the corrosion reactions were determined by polarisation measurements. Potentiodynamic polarization curves for mild steel in 1 N Na₂SO₄ are shown in Fig. 2.

The corresponding corrosion potentials (E_{corr}), corrosion current density (i_{corr}), anodic Tafel slopes (b_a), cathodic Tafel slopes (b_c), and corrosion rate (CR) are listed in Table 3.

Fig. 2 shows the potentiodynamic polarization curves for steel in 1N Na₂SO₄ solutions without and with pre-treatment with 4-hydroxy-3-methoxybenzaldehyde (immersion time is 24, 48, 72 h). It is observed that the pretreatments with 4-hydroxy-3-methoxybenzaldehyde larger reduces the rates of both the cathodic hydrogen evolution and the anodic Fe dissolution. The corrosion potential (E_{corr}) obviously changes. As a result of treatment of the metal by the 4-hydroxy-3-methoxybenzaldehyde, the current less potential shifts to the positive side (E = – 0.43 V) even after holding for 24 h. The inhibitor has a significant effect on the rate of oxygen evolution reaction. On the other hand, the presence of these inhibitor shifts both anodic and cathodic curves to lower values of current densities to more extent. Both the cathodic slopes and the anodic slopes do not change, which indicates that the mechanism of the corrosion reaction does not change and the corrosion reaction is inhibited by a simple adsorption mode.

As the time of treatment of the metal by the volatile compounds of 4-hydroxy-3-methoxybenzaldehyde increases to 48 h, the increase in the inhibiting efficiency becomes especially pronounced, which corresponds to the saturation of the surface with the inhibitor and the

### Table 2. Calculated corrosion rates (g m⁻² h⁻¹) and inhibition efficiency (%) for volatile corrosion inhibition test (Test conditions distilled water).

<table>
<thead>
<tr>
<th>Samples</th>
<th>Period of film-forming</th>
<th>IE, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Treated by vapour phase of Vanillin</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>86,7</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>96,8</td>
</tr>
<tr>
<td></td>
<td>48</td>
<td>98,9</td>
</tr>
<tr>
<td></td>
<td>72</td>
<td>99,0</td>
</tr>
</tbody>
</table>

### Table 3. Characteristics of the Polarization Curves of St3 Steel in 1N Na₂SO₄ after the formation of protective film from the vapor phase of the 2-propanol solution of 4-hydroxy-3-methoxy-benzaldehyde.

<table>
<thead>
<tr>
<th>Holding time</th>
<th>Currentless potential, V</th>
<th>Electrode polarization (ΔE), V</th>
<th>Tafel coefficients, V</th>
<th>I_{corr}, A/cm²10⁻⁵</th>
<th>IE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Anodic process in i=1,9*10⁻⁵ A/cm²</td>
<td>Cathodic process in i=1,9*10⁻⁵ A/cm²</td>
<td>b_a</td>
<td>b_c</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>-0,46</td>
<td>-</td>
<td>0,10</td>
<td>0,15</td>
<td>13,6</td>
</tr>
<tr>
<td>24</td>
<td>-0,46</td>
<td>0,040</td>
<td>-0,02</td>
<td>0,10</td>
<td>0,15</td>
</tr>
<tr>
<td>48</td>
<td>-0,45</td>
<td>0,035</td>
<td>-0,05</td>
<td>0,10</td>
<td>0,15</td>
</tr>
<tr>
<td>72</td>
<td>-0,45</td>
<td>0,036</td>
<td>-0,07</td>
<td>0,10</td>
<td>0,16</td>
</tr>
</tbody>
</table>
formation of the strongest bonds between the inhibitor and the metal. It is also seen that at all samples the corrosion potential shifts significantly to noble direction therefore it is predominantly anodic-cathodic inhibitor. The inhibition efficiency increases as the immersion time is increased. Both anodic and cathodic reactions are drastically inhibited after 72 h of exposure of the film-forming. In the presence of 4-hydroxy-3-methoxybenzaldehyde, the slight change of both $b_c$ and $b_a$ indicates that the corrosion mechanism of steel does not change. These results infer that the inhibitor acts by simple blocking of the available surface area. These components can be arranged as mixed-type inhibitors.

Furthermore, the inhibition efficiencies obtained from weight loss and polarization curves are in reasonably good agreement.

SEM analyses were conducted in order to characterize the protective layer that formed on the low carbon steel surface. SEM images of the initial surface and after 72 h for VCI film-forming are shown in Fig. 3. The surface morphology of the sample before exposure to volatiles of 4-hydroxy-3-methoxybenzaldehyde indicates that there were a few scratches from the mechanical polishing treatment. This image displays a freshly polished steel surface. The image on Fig. 3b is of the steel surface after 72 h of exposure for the film-forming of 4-hydroxy-3-methoxybenzaldehyde. It shows a thin and covering surface film. The steel surface after 72 h of 4-hydroxy-3-methoxybenzaldehyde film-forming was slightly rougher than that before film-forming. It shows a thin and covering surface film composed of many particles. Investigation by Stratmann [4] suggested that adsorption of VCI may form a few protective monolayers.

The results obtained from weight loss and potentiodynamic polarization are in good agreement, and the inhibition action could also be evidenced by surface SEM images. FT-IR analysis of the carbon steel specimens in the absence and after the formation of a film for 72 h in the gas-vapor atmosphere in the presence of 4-hydroxy-3-methoxybenzaldehyde was carried out between 500 and 3000 cm$^{-1}$.
and 4000 cm$^{-1}$. The FT-IR spectrum of 4-hydroxy-3-methoxybenzaldehyde (Fig. 4) indicates the presence of peaks at 3540 cm$^{-1}$ corresponded to the characteristic stretching O-H group. The band at 1696 cm$^{-1}$ was attributed to C = O group. The peaks at 1268 and 1035 cm$^{-1}$ indicate the presence of stretching bands C-O. Fig. 5 shows the spectra for specimens in the absence of volatile components, no characteristic peak was observed except that of water (Fig. 5, curve 1). The infrared spectrum of mild steel treated in vapor phase of 4-hydroxy-3-methoxybenzaldehyde (for 72 h) indicates the presence of hydroxyl group (3670 - 3580 cm$^{-1}$), carbonyl group (1630 - 1610 cm$^{-1}$), aromatic hydrogen group (3000 - 2920 cm$^{-1}$) and aromatic ring (1550, 1094 cm$^{-1}$) (Fig. 5, curve 2).

The results show that the film forming after exposure steel in the gas-vapor atmosphere in the presence of 4-hydroxy-3-methoxybenzaldehyde infrared spectra observed shifts oscillations in the range the C-O-H and stretching O-H group. These shifts with respect to the individual compounds indicate that there is interaction between Fe in the mild steel and some of the inhibitor molecules. It is also evident from the analyzed FT-IR spectra that after the initial mechanism of physical adsorption, chemical adsorption of the inhibitor molecules on Fe (in mild steel) also occurred.

It was investigated the effect of films formed on the metal surface after preliminary holding of the specimens in the vapor of the isopropanol solution of 4-hydroxy-3-methoxybenzaldehyde. It was shown (Table 4) that these films give the required aftereffect under the conditions of periodic condensation of moisture over 1N Na$_2$SO$_4$ aqueous solutions.

These results infer that the inhibition of corrosion steel is due to blocking of steel surfaces of chemically adsorbed molecules compounds.

To confirm the mechanism of adsorption of 4-hydroxy-3-methoxybenzaldehyde it was investigated adsorption power of the molecules. 4-hydroxy-3-methoxybenzaldehyde used, quantum chemical concepts and the density functional theory (DFT) was applied to study the geometrical and electronic structures of the compounds. The inhibitor molecules structure obtained after a geometric optimization procedure using Hyper Chem 7.0 computer package (RHF calculation, singlet state, PM3 parameterization) are given in Fig. 6.

In Table 5 are listed the values of selected quantum chemical parameters calculated for these inhibitor molecule by using DFT method.

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Table 4. Aftereffect of the films formed on St3 steel from the vapor phase of the isopropanol solution of 4-hydroxy-3-methoxy-benzaldehyde (time of formation 120 h; time of experiment 504 h).

<table>
<thead>
<tr>
<th>Volatile Corrosion Inhibitor</th>
<th>Corrosion rate K$_m$ g/(m$^2$h)</th>
<th>Inhibition efficiency, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-hydroxy-3-methoxy-benzaldehyde</td>
<td>0,0730</td>
<td>60,85</td>
</tr>
</tbody>
</table>
These parameters will provide insights into the mechanism of interaction of the 4-hydroxy-3-methoxybenzaldehyde with mild steel surface. Fig. 4 shows the electric/orbital density distribution of HOMO and LUMO for 4-hydroxy-3-methoxybenzaldehyde. It is found that the electron density of the frontier orbital is well proportioned. Such results indicate 4-hydroxy-3-methoxybenzaldehyde could be both the acceptor of the electrons and the donor of the electrons. That is, there is electron transferring in the interaction between the inhibitor molecule and metal surface.

The smaller HOMO–LUMO energy gap implies soft–soft interaction will be expected. The data in Table 6 show that the ∆E value of 4-hydroxy-3-methoxybenzaldehyde is lower, which can facilitate its adsorption on the metal surface so it has higher inhibition efficiency. To obtain a clear picture of the interaction between the molecules studied and mild steel surface, intermolecular parameters such as charge transfer descriptors and the associated energy change should be taken into account. Electrophilicity is an index which measures the propensity of chemical specie to accept electrons. The higher the value of ω is, the higher is the capacity of the molecule to accept electrons. Thus, a good nucleophile is characterized by low values of μ and ω; whereas a good electrophile is characterized by high values of μ and ω. It is clear (Table 6) that the molecules have low electrophilicity index values and are good nucleophiles.

The amount of charge transfer, ΔN, between the molecules and the mild steel Fe surface as calculated is given in Table 6. A positive value of ΔN indicates that the molecules act as an electron acceptor, while a negative value of ΔN indicates that the molecules act as electron donors [32]. Thus all the molecules studied act as electron acceptors except ∆E which acts as electron donor. According to Lukovits, if ΔN < 3.6, the molecules can be assumed to possess charge transfer ability towards the metal surface [32, 33].

The molecules studied possess charge transfer abilities towards mild steel. The energy change (∆E) associated with the charge transfer process were all negative and exothermic indicating a favourable transfer of charge process from the organic molecules onto steel surface.

**CONCLUSIONS**

In this study, it was shown that 4-hydroxy-3-methoxybenzaldehyde is an effective inhibitor of corrosion of mild steel.

Under conditions of modeling of the atmospheric corrosion of mild steel, the VIAC films from the developed components decrease the rate of cathodic process more intensely than the rate of anodic process. It is shown that the inhibition of the atmospheric corrosion of steels after treatment in the vapor of volatile compound 4-hydroxy-3-methoxybenzaldehyde, occurs due to the
blocking of the metal surface by chemically adsorbed molecules.

The quantum-chemical calculations were carried out to predict the adsorption activity of the developed components. The calculated results show that all the molecules have high propensity for donating electrons, low $\Delta \varepsilon$ and $\eta$ (high reactivity), they are good nucleophiles which is characterized by low values of $\omega$, and the energy change associated with the charge transfer to the mild steel surface $\Delta E$, and are all favourable (negative).

REFERENCES

1. Ch. Thee, Long Hao, Junhua Dong, Xin Mu, Xin Wei, Xiaofang Li, Wei Ke, Atmospheric corrosion monitoring of a weathering steel under an electrolyte film in cyclic wet dry condition, Corrosion Science, 78, 2014, 130-137.
2. Da-quan Zhang, Zhong-xun Ana, Qing-yi Panb, Li-xin Gaoa, Guo-ding Zhou, Comparative study of bis-piperidiniummethyl-urea and mono-piperidiniummethyl-urea as volatile corrosion inhibitors for mild steel, Corrosion Science, 48, 6, 2006, 1437-1448.
5. F. Andreatta L. Fedrizzi, Corrosion Inhibitors, Active Protective Coatings, 233, 2016, 59-84.
10. N. Poongothai, P. Rajendran, M. Natesan, N. Palaniswamy, Wood Bark Oils as Vapor Phase Corrosion Inhibitors for Metals in NaCl and S$_2$O$_2$ Environments, Indian Journal of Chemical Technology, 12, 2005, 641.
20. Gökhan Gece, The use of quantum chemical
29. Marco Franco-Pérez, José L. Gázquez, Paul W. Ayers, Alberto Vela, Revisiting the definition of the electronic chemical potential, chemical hardness, and softness at finite temperatures, The Journal of Chemical Physics, 143, 2015, 154103.