

Investigations Properties on the Corrosion Inhibition of *Kala Bansa* Leaf Extract on Mild Steel in an Acidic Environment

O. S. Yadav¹, S. Kumar¹, K. Yadav¹, R. Sharma¹ and R. Kumar²

¹Shyam Lal College Department of Chemistry Shahdara, Delhi, India

²Shyam Lal College Department of Physics Shahdara, Delhi, India

Corresponding author: opduchem@gmail.com

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Abstract

Different Ct of KBE from its leaves were used to study its effect on MS corrosion resistance. Electrochemical methods such as PDP, EIS and WL tests were herein used. Experimental results showed that, with higher Ct of KB, its IE(%) increased. The highest corrosion IE(%) of 98.41, at 1600 ppm KBE in a 0.5 M H₂SO₄ solution, was obtained. The inhibitor's adsorption onto the MS surface was excellent, since it created a monolayer. KBE's adsorption mechanism obeyed Langmuir's isotherm. SEM analysis established the development of a protective layer on the MS surface.

Keywords: CI; EIS; LPR; PDP; SEM; WL.

Introduction*

For a long time, steels and its alloys have been used in several industries for various purposes, such as pipelines. Every year, worldwide economic losses caused by corrosion amount to 75,000 billion dollars, which depletes world's GDP of 3-4% [1]. Metals corroding process may be prevented with the aid of CI [2, 3], which hinder metals dissolution by mineral acids attacks. Several types of un-eco friendly and toxic CI are used in industries, some of which are inorganic and organic synthesized substances. Nowadays, green and nontoxic CI are in high demand.

Various industries employ acids in the process of cleaning pipes and oil from surfaces [4-6]. CI usually behaves as adsorbents, which means they adsorb onto metals surfaces and form a chemical bond. However, there are some phenomena where they are attracted by metals, originating physical adsorption. Different plant parts are used to prepare green CI extracts, since they have good ability to cover metals surfaces, because their photochemical components possess aromatic structures with hetero atoms. Generally, CI added to AE has organic molecules that contain hetero atoms as prime chemical constituents. In several studies, the extracts of many plants have been used as efficient CI in various AE, such as: walnut green (*Juglans regia L.*) husk [7];

*The abbreviations and symbols definition lists are in pages 39-40.

Mish Gush [8], *Stachys byzantine* [9], *Thymus vulgaris* [10] and *Aloysia citrodora* [11] leaves; *Punica granatum* peel on SS-410 [12]; *Ammi visnaga* (which was also used as friendly antioxidant) [13]; *Allamanda cathartica* [14], and *Senggani* (*Melastoma candidum* D. don) [15] leaves; and iodide ions and *Xanthium strumarium* leaves [16].

KB is a deciduous flowering plant with diverse genera, of the *Acanthaceae* family. It is an Indian routine medicinal plant, which is used in various treatments of ailments. Its leaves contain various type of photochemical [17, 18], such as saponins, flavonoids and glycosides.

The novelty of the present work was to employ KBE as a green CI for MS in H₂SO₄. Employed electrochemical techniques were EIS, PDP and LPR, to test whether KBE behaved as a mixed-type CI. KB adsorption onto the MS surface in H₂SO₄ followed Langmuir's isotherm.

Materials and methods

KBE preparation

KBE was obtained via maceration process from 80% ethanol/water system. Then, it was filtered. The residues were removed by a solvent and eliminated via rotary evaporator. A concentrated blackish solid was obtained.

WL method

WL is an extensively used and predictable method for estimating CR. The prepared blank solution was made of geared 0.5 M H₂SO₄ (analytical reagent) and distilled water. CR values of MS were evaluated at different T (298, 308, 318 and 328 K), via WL method, with different Ct of KBE in the test solution, for 20 h. MS samples (1 x 1 x 1 cm) had the chemical composition by wt% of C-0.1, Si-0.033, Mn-0.335, Al-0.057, Cu-0.0476, Cr-0.02 and balance Fe. For 20 h, the MS samples were entirely immersed in a conical flask of 250 cm³ with a 0.5 M H₂SO₄ solution. Then, they were taken from the test solutions, and cleaned with acetone.

Instrumentation (electrochemical) measurements

Selected Ct ranges of KBE solutions for the current study were 400, 800, 1200 and 1600 ppm. They were diluted in 0.5 M H₂SO₄, which was also used as blank. All steps of this experimentation and measurement employed scientific programs have been delineated elsewhere [19-22]. The electrochemical potentiostat study was performed by CH Instruments, Inc. CHI760c. The SR adopted in PDP study was 1.0 mV/s⁻¹. EIS were recorded with an amplitude of 5 mV peak to peak, at OCP, with signals/disturbance in the frequency range from 10⁵ to 10⁻² Hz.

Study of surface characterization

MS coupons (1 × 1 cm × 2 mm) were used for the surface characterization study. Polished MS coupons were subjected to corrosion, in H₂SO₄, at the Ct range of KBE from 400 to 1600 ppm, to monitor IE(%), for 10 h. SEM studies were performed by Jeol Japan, Model No. JSM-6610 LV instrument.

GC-MS study

GC-MS study was performed with a Shimadzu GC-MS-QP 2010 Ultra fitted with an RTX-5 MS (30 m x 0.25 mm x 0.25 μm) capillary column. He gas was used as transporter, with the flow rate of 1.21 mL /min. The initial oven T was 60 $^{\circ}\text{C}$, for two min, and then it was increased to 260 $^{\circ}\text{C}$. The 2 mL sample was injected in split less mode, and total IT was 60 min. The ions source was heated at 220 $^{\circ}\text{C}$, and electron-impact ionization technique was used at a potential of 70 eV. Mass spectra of KBE with crude ethanol showed compounds identified from NIST and WILEY libraries, and their assessment agreed with those reported in literature [23].

Results and discussion**WL calculation**

Data calculated via WL are listed in Table 1.

Table 1: WL parameters for MS, for 20 h IT in 0.5 M H_2SO_4 without and with KBE at various Ct and T (298-328 K).

| T | Ct (ppm) | WL (mg) | CR ($\text{mg}/\text{cm}^2/\text{h}^{-1}$) | IE% | SC (θ) |
|-------|----------|---------|--|-------|-----------------|
| 298 K | Blank | 0.4979 | 0.0277 | - | - |
| | 400 | 0.0471 | 0.0026 | 90.61 | 0.9061 |
| | 800 | 0.0362 | 0.0016 | 94.22 | 0.9422 |
| | 1200 | 0.0202 | 0.0011 | 96.02 | 0.9602 |
| | 1600 | 0.0092 | 0.0005 | 98.19 | 0.9819 |
| 308 K | Blank | 0.6187 | 0.0345 | - | - |
| | 400 | 0.0599 | 0.0034 | 90.14 | 0.9014 |
| | 800 | 0.0395 | 0.0022 | 93.62 | 0.9362 |
| | 1200 | 0.0260 | 0.0014 | 95.94 | 0.9594 |
| | 1600 | 0.0175 | 0.0009 | 97.39 | 0.9739 |
| 318 K | Blank | 0.8261 | 0.0460 | - | - |
| | 400 | 0.0872 | 0.0048 | 89.56 | 0.8956 |
| | 800 | 0.0710 | 0.0039 | 91.52 | 0.9152 |
| | 1200 | 0.0598 | 0.0033 | 92.82 | 0.9282 |
| | 1600 | 0.0361 | 0.0020 | 95.65 | 0.9565 |
| 328 K | Blank | 1.0471 | 0.0584 | - | - |
| | 400 | 0.2725 | 0.0152 | 73.97 | 0.7397 |
| | 800 | 0.1681 | 0.0093 | 84.07 | 0.8407 |
| | 1200 | 0.1051 | 0.0058 | 90.06 | 0.9006 |
| | 1600 | 0.0705 | 0.0039 | 93.32 | 0.9332 |

Due to MS corrosion in a 0.5 M H_2SO_4 solution, its WL was examined, with various Ct of KBE, at several T (298, 308, 318 and 328 K). CR (mm/yr^{-1}) was calculated using eq. (1).

$$C_R = \frac{K \times W}{A \times t \times \rho} \quad (1)$$

where W is WL, t is IT, ρ is density ($7.85 \text{ g}/\text{cm}^3$) and K denotes corrosion constant (8.76×10^4) [24]. C_R^A and C_R^I are CR of MS in H_2SO_4 without and with KBE, of which effect on CR is shown in Fig. 1.

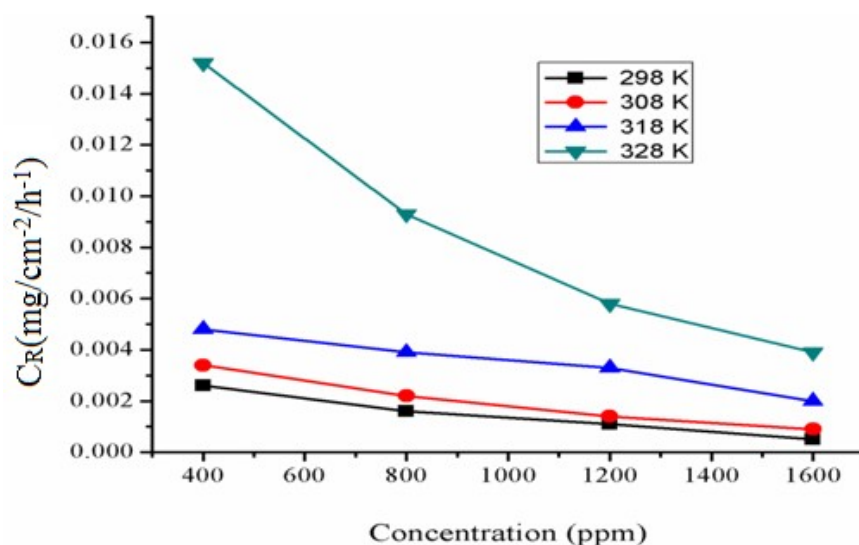


Figure 1: CR values with different Ct of KBE at T from 298 to 318 K.

With higher Ct of KBE, CR decreased, as shown in Fig. 2. The inhibitor’s molecules were adsorbed onto the MS surface, which hindered CR. The lower the Ct from KBE, the lower the IE(%).

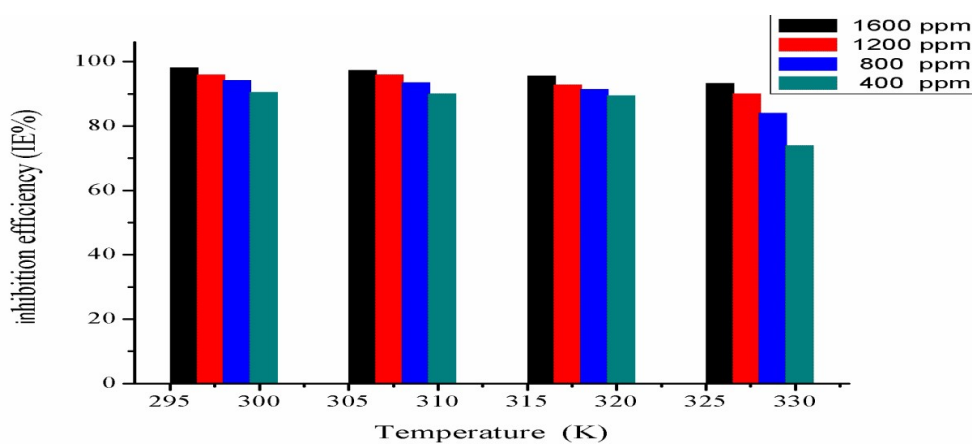


Figure 2: Variation in IE(%) with various Ct of KBE, at T from 298 to 328 K.

From Table 1, maximum IE(%) of KBE was 98.19, which was achieved at a Ct of 1600 ppm. The inhibitor’s IE(%) and SC (θ) values were calculated via eqs. (2) and (3), respectively.

$$IE(\%) = \frac{c_R^A - c_R^i}{c_R^A} \times 100 \quad (2)$$

$$SC(\theta) = \frac{c_R^A - c_R^i}{c_F^i} \quad (3)$$

Polarization investigations

Galvanostatic study and LRP

Polarization analyses were carried out thorough determination of KBE inhibition mechanism, at 298 K, using different Ct. From the experimental study, Tafel curve plot is shown in Fig. 3, and polarization is represented by Table 2. Improvement in corrosion IE(%) via i_{corr} was calculated by Eq. (4).

$$Tafel(IE\%) = \frac{I_{acid} - I_{inh}}{I_{acid}} \times 100 \quad (4)$$

where I_{inh} and I_{acid} are I_{inh} values without and with KBE in a 0.5 M H_2SO_4 solution, respectively.

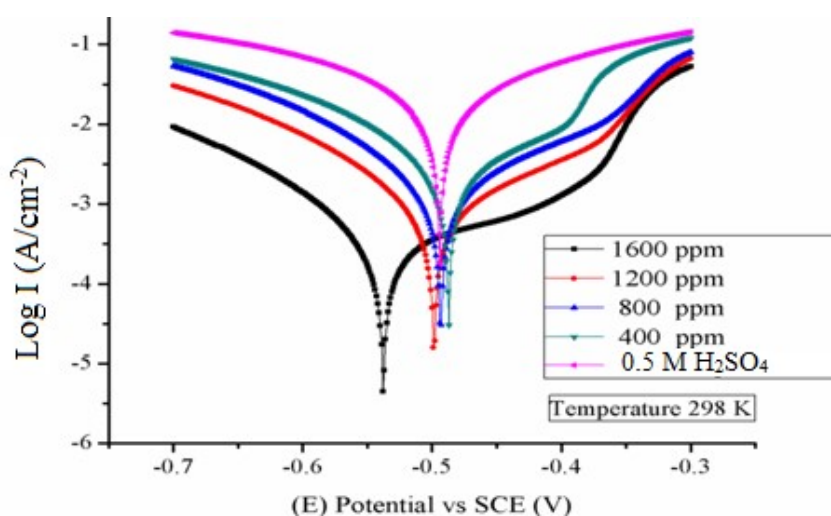


Figure 3: Galvanostatic polarization curves for MS in a 0.5 M H_2SO_4 solution with various Ct of KBE, at 298 K.

Table 2: Tafel and LPR parameters for MS in a 0.5 M H_2SO_4 solution with different Ct of KBE, at 298 K.

| Ct (ppm) | I_{corr} (A/cm^2) | E_{corr} (mV per SCE) | IE% | Tafel data | | LPR data | |
|----------|-------------------------|-------------------------|-------|--------------------|--------------------|-------------------------|-------|
| | | | | β_c (mV/dec) | β_a (mV/dec) | R_p (Ω/cm^2) | LPR% |
| Blank | 2.560 | 0.494 | - | 53.81 | 51.47 | 1.6 | - |
| 400 | 0.2165 | 0.487 | 91.54 | 73.45 | 98.54 | 15.4 | 89.57 |
| 800 | 0.1803 | 0.493 | 92.95 | 67.30 | 86.80 | 18.7 | 91.44 |
| 1200 | 0.09865 | 0.499 | 96.14 | 70.52 | 85.25 | 31.3 | 94.88 |
| 1600 | 0.04067 | 0.538 | 98.41 | 91.01 | 45.38 | 78.4 | 97.95 |

CI action in 0.5 M H_2SO_4 improved with higher Ct of KBE. E_{corr} experimental values' trend means that the inhibitor is an anti-corrosion catalyst of mixed type. With KBE, β_a and β_c noticeably changed in an irregular manner, due to the inhibition process that implied HER and MS dissolution. β_a was mainly slower than

β_c , phenomenon that may be temporary, as indicated by the suppressed anodic reaction of MS oxidation/dissolution via KBE action. Moreover, β_c differed, although slightly, and the inhibitor suppressed HER. Both reactions were limited by KBE-Fe complexes ($[\text{Fe-atoms-KBE}]_{\text{ads}}$) and $[\text{Fe-atoms-KBE-OH}]_{\text{ads}}$ on the substrate's surface, which led to complete active sites coverage [25]. LPR values specify KBE's adsorption onto the MS surface by the development of a physical barrier with a non-conducting nature.

EIS measurements

EIS experiments were performed to assess interfacial changes at the MS surface in 0.5 M H_2SO_4 with and without KBE, at 298 K. This study was used as a separate and additional method to properly measure IE(%), mechanistic and kinetic data of the electrochemical system under examination. Resulting Bode and Nyquist plots are shown in Figs. 4 and 5, and their parameters are specified in Table 3.

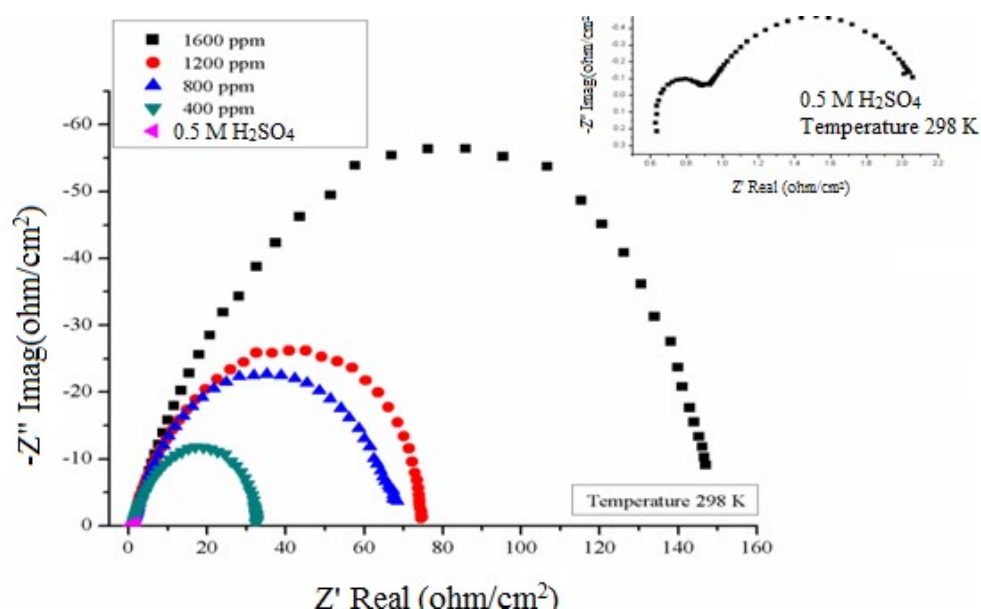


Figure 4: Nyquist's plots for MS in a 0.5 M H_2SO_4 solution without and with KBE at various R_{ct} , at 298 K.

The MS's surface irregularity and CI mechanism via single charge transfer was considered through the single semi-circle in the Nyquist plot, for all R_{ct} of KBE in H_2SO_4 [26]. The diameter in R_{ct} remarkable rose with increased R_{ct} of the inhibitor, which confirmed this mechanism. CR of MS decreased, after KBE created an insoluble protective layer. By using Eq. (5), IE(%) values were calculated [27].

$$(EIS)IE(\%) = \frac{R_{ct} - R_{ct}^0}{R_{ct}} \times 100 \quad (5)$$

where R_{ct} and R_{ct}^0 are R_{ct} values with and without KBE, respectively.

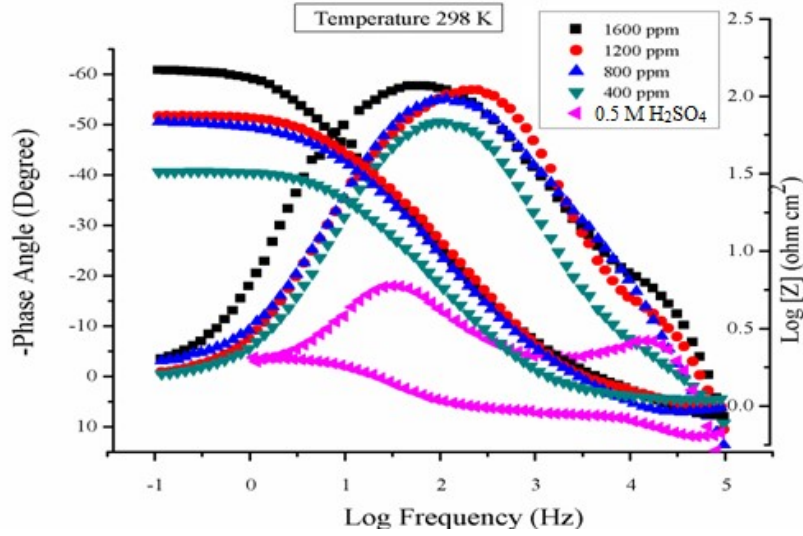


Figure 5: Bode's plot for MS in a 0.5 M H₂SO₄ solution without and with KBE in various Ct, at 298 K.

Table 3: Parameters of impedance for MS in 0.5 M H₂SO₄ without and with KBE, in various Ct, at 298 K.

| Ct (ppm) | R _s (Ω/cm ²) | n | Q (Ω ⁻¹ /cm ² S ⁿ) | R _{ct} (Ω/cm ²) | F _{max} (Hz) | C _{dl} (F/cm ²) | IE% |
|----------|-------------------------------------|--------|--|--------------------------------------|-----------------------|--------------------------------------|-------|
| Blank | 1.4 | 0.7105 | 0.876 | 1.720 | 6.50 | 0.14229 | |
| 400 | 1.2 | 0.8528 | 0.481 | 30.19 | 14.31 | 0.03682 | 94.38 |
| 800 | 1.3 | 0.8974 | 0.116 | 70.31 | 17.28 | 0.001312 | 97.55 |
| 1200 | 1.4 | 0.9296 | 0.0424 | 75.37 | 23.39 | 0.0007996 | 97.71 |
| 1600 | 1.1 | 0.9510 | 0.016 | 155.77 | 69.75 | 0.0001464 | 98.89 |

C_{dl} was measured by using Eq. (6), of which values increased with higher Ct of KBE.

$$Cdl = \frac{1}{2\pi R_{ct} f_{max}} \quad (6)$$

where f_{max} is maxima frequency via Nyquist curve.

Eq. (7) represents an inverse relation between C_{dl} and thickness (d) of the shielding layer. Experimental parameters are listed in Table 3, which shows a decrease in C_{dl} value with higher Ct of KBE. This means that the protecting layer thickness increased.

$$Cdl = \frac{A\epsilon\epsilon_0}{d} \quad (7)$$

where A is the surface area of the MS substrate, ε and ε₀ are constants dielectric for the vacuum permittivity with the medium and d is the shielding layer thickness.

The significance of single time constant is illustrated by Bode graphs of Fig. 5, for each Ct of KBE. The phase angle approached to 90⁰, which was further confirmed by stronger homogeneous MS surface substrate [28]. Other parameters include (n)

values phase shift from Eq. (8), which are nearer to unity with KBE addition, and associated with less heterogeneity on the MS surface without inhibitor [29-31].

$$Cdl = Q(\omega)^{n-1} = Q(2\pi f_{Zim-max})^{n-1} \quad (8)$$

where Q is CPE, ω is angular frequency, which is an imaginary part with the maximum value of electrochemical impedance plot and $f_{Zim-max}$ is maxima frequencies.

Study of T's kinetics

Adsorption isotherm

The relation between KBE's molecules and the MS's surface was studied via the adsorption mechanism characteristics, employing various isotherms. Experimental data established that the relation with best fit was for Langmuir's adsorption isotherm, with linear R^2 values (0.999 - 1) obtained by the plotting graph C/θ vs. Ct, at different T, which generated straight lines [32-37] (Fig. 6).

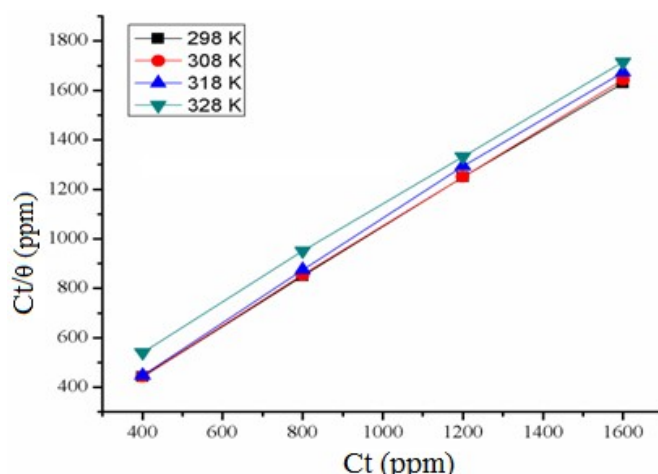


Figure 6: Langmuir's isotherm for KBE (at different Ct) adsorption onto MS in a 0.5 M H₂SO₄ solution, at various T.

From Eq. (9), Langmuir's isotherm was calculated. It depends on the Ct of KBE's molecules in the H₂SO₄ solution, which have performed SC (θ) of MS.

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \quad (9)$$

where C_{inh} is Ct of KBE (Fig. 7). R^2 value had a recognized major role on the relations between KBE's molecules adsorbed on to the MS surface substrate, which were linked on to cathodic and anodic reactive sites. In the investigated system, the additive molecules blankets on cathodic and anodic sites were formed by the adsorption mechanism and the development of a multi-molecular layer that obeyed Langmuir's isotherm.

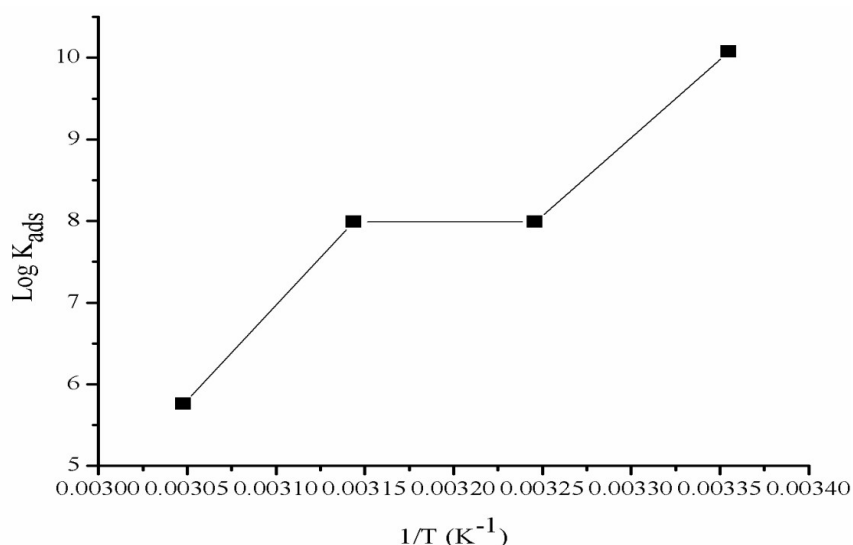


Figure 7: Graph ($\log K_{ads}$ versus $1/T$) of ΔG_{ads}° KBE on the MS surface.

K_{ads} values were employed to determine ΔG_{ads}° via Eq. (10), indicating KBE strong adsorption onto the MS surface. The adsorption was strong, since more hetero atoms with lone pair and aromatic rings were delocalized from pi electrons in KBE's molecules. According to [38], ΔG_{ads}° values closer to -40 kJ/mol^{-1} indicate chemisorption, and those nearer to -20 kJ/mol^{-1} show physisorption. For this study, calculated values and parameters are listed in Table 4, which were near to -40 kJ/mol^{-1} , at different T, revealing a chemisorption process, which indicates its spontaneous nature.

Table 4: Thermodynamic parameters for KBE's adsorption onto the MS surface in 0.5 M H_2SO_4 , at different T.

| T | Log K | R ² | ΔH_{ads} (kJ/mol) | ΔS_{ads} (j/mol/K) | ΔG_{ads} (kJ/mol) |
|-----|-------|----------------|------------------------------|-------------------------------|------------------------------|
| 298 | 6.29 | 0.9997 | -51.65 | -49.22 | -45.83 |
| 308 | 5.31 | 0.9999 | | | -41.59 |
| 318 | 5.30 | 0.9993 | | | -42.88 |
| 328 | 4.79 | 0.9997 | | | -41.02 |

$$\Delta G_{ads}^{\circ} = -2.303RT [\log(55.5) + \log K_{ads}] \quad (10)$$

where R is universal gas constant. The water's molecule Ct was 55.5 mol/L. In the present study, obtained ΔS_{ads}° value was -49.22 kJ/mol , which suggested that the arrangement of KBE's molecules on the MS surface followed the process of exothermic adsorption [39].

E_a parameter and T effect

The study of T effect, via WL calculations, on MS (coupon) in 0.5 M H_2SO_4 with different Ct of KBE, is listed in Table 1, which shows CR, SC (θ) and IE(%) values.

In the solution without KBE, CR of MS exponentially rose from 298 to 328 K, whereas with the inhibitor, it slightly decreased. IE(%) declined with T rise from 298 to 328 K. By using Arrhenius equation (11), E_a was determined [40].

$$\log \partial = \log A - \frac{E_a}{2.303 RT} \quad (11)$$

where A is pre-exponential factor of Arrhenius. The plot derived by Arrhenius and Eyring equations is shown in Fig. 8.

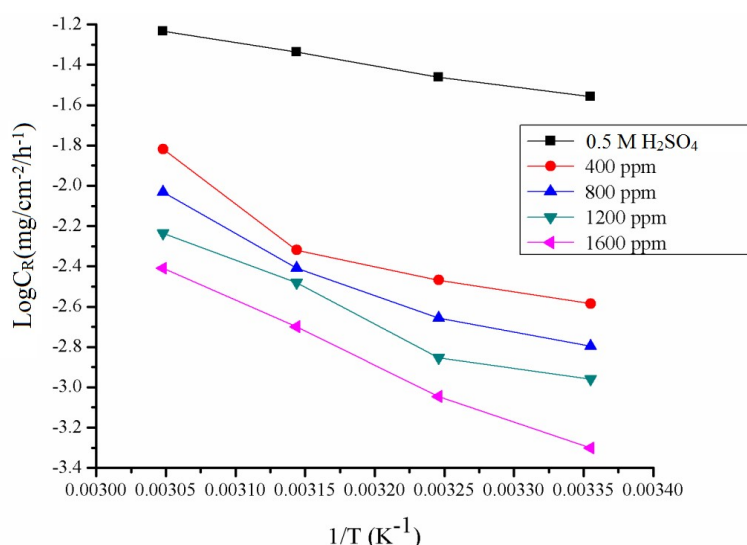


Figure 8: Arrhenius plots of Log CR against T^{-1} for MS in a 0.5 M H_2SO_4 solution containing different Ct of KBE.

Calculated values for ΔH°_{ads} and ΔS°_{ads} are listed in Table 5. E_a values were calculated via a straight line of the slope ($E_a = \text{slope} \times 2.303 R^2$), resulting from Arrhenius plot $\log \partial$ vs. $1/T$ curve. E_a observed value for the systems with KBE were larger than those without it, which suggests that the adsorption process was chemical. ΔH°_{ads} and ΔS°_{ads} values were calculated by using Eq. (12).

$$\partial = \frac{RT}{Nh} \exp\left(\frac{\Delta S^{\circ}_{ads}}{R}\right) \exp\left(-\frac{\Delta H^{\circ}_{ads}}{RT}\right) \quad (12)$$

where N is Avogadro number and h is Plank constant [41].

Table 5: E_a parameters for MS in 0.5 M H_2SO_4 with and without KBE in different Ct.

| Ct (ppm) | E_a (kJ/mol) | ΔH°_{ads} (kJ/mol) | ΔS°_{ads} (j/mol/K) |
|-------------|-------------------|--------------------------------------|---------------------------------------|
| 1600 | 56.49 | 54.24 | -110.21 |
| 1200 | 47.30 | 44.98 | -74.11 |
| 800 | 47.25 | 44.25 | -73.98 |
| 400 | 45.37 | 42.81 | -61.29 |
| Blank | 20.44 | 19.11 | -120.87 |

Through the adsorption route, reactants molecules were improved to activate the complex, in which the phyto chemicals disordering took place. $\Delta S^{\circ}_{\text{ads}}$ negative values reveal the associative mechanism that marks the progress of an activated complex, of which step was rate determining [42]. $\Delta S^{\circ}_{\text{ads}}$ positive values correspond to the endothermicity of MS's dissolution reaction. They were higher with KBE, which means that the energy barrier for MS dissolution reaction was drastically improved by the CI in H_2SO_4 [23].

Morphological investigation

SEM

The micrographs (Figs. 9a-9d) obtained via SEM in a 0.5 M H_2SO_4 solution with out and with KBE (1600 and 400 ppm) show the changes caused by the corrosion process.

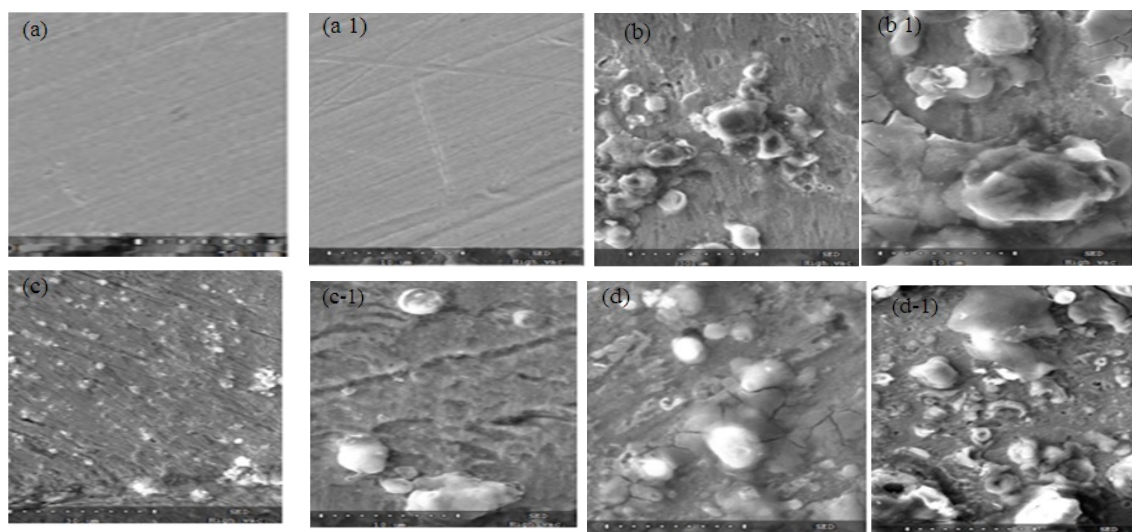


Figure 9: SEM micrographs with magnification 1000 (1) 3000 of MS surfaces - (a) bare; with 0.5 M H_2SO_4 -(b) blank, (c)with 1600 ppm KBE, and (d) with 1200 ppm KBE.

The MS surface in 0.5 M H_2SO_4 was damaged, as shown in Fig 9 (b). Its morphology appreciably improved (Fig. 9c) with the addition of 1600 ppm KBE, and less damages occurred compared to the sample with blank 0.5 M H_2SO_4 . The MS surface roughness level was reduced when the Ct of KBE was increased from 400 to 1600 ppm. This enhancement in MS morphology was due to the excellent protective layer [43, 44] formed by KBE on its surface, which was responsible for CI.

GC-MS analysis

In the current investigation, GC-MS identified 15 compounds among the 45 constituents recognized in MS immersed in KBE with ethanol, as shown in Fig.10.

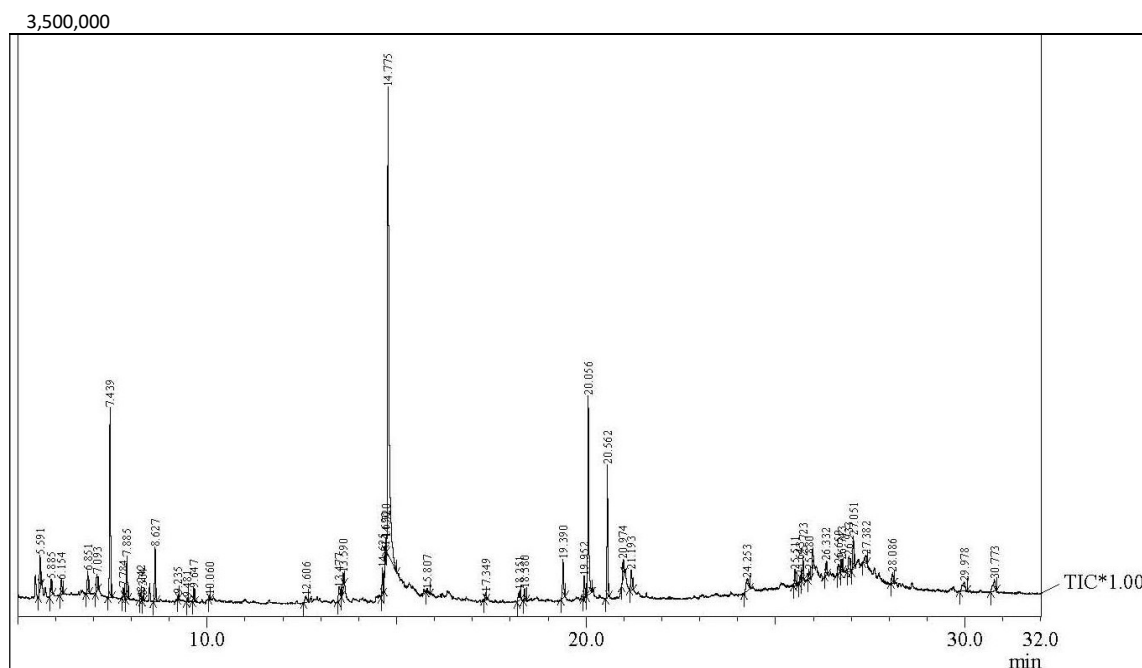


Figure 10: GC-MS of MS and KBE.

Table 6 characterizes the identified compounds, such as their MF, MW, IT, PA and SI. The phytochemical examination of KBE exposed the presence of heterocyclic organic compounds that can be largely classified as sterols, long chain alkenes (cyclic), long chain fatty acids and purine nucleosides. The majority of detected phytocomponents have been reported as effective green CI [45-52]. The existence of multiple bonds with electrons, hetero atoms and some other substances in these organic compounds provides for excellent CI properties [53], due to the synergy among all of them.

Table 6: Phytocomponents detected in KBE.

| S. no | Compounds | MF | MW | IT | PA% | SI |
|-------|--|--|-----|--------|-------|----|
| 1 | 1,2,4-trimethylbenzene | C ₉ H ₁₂ | 120 | 5.885 | 0.98 | 93 |
| 2 | Cyclopropylbenzene | C ₉ H ₁₀ | 118 | 6.851 | 1.28 | 93 |
| 3 | 3a,4,5,6,7,7a-hexahydro-4,7-methanoindene | C ₁₀ H ₁₄ | 134 | 7.439 | 9.22 | 96 |
| 4 | 4,7-Methano-1H-indene, octahydro- | C ₁₀ H ₁₆ | 136 | 7.885 | 2.03 | 95 |
| 5 | Tricyclo[5.2.1.0(2,6)]dec-4-ene, 4-methyl | C ₁₁ H ₁₆ | 148 | 8.627 | 2.49 | 89 |
| 6 | 3H-1,2,4-triazol-3-one, 4-amino-2,4-dihydro-2-methyl-5-phenyl | C ₉ H ₁₀ N ₄ O | 190 | 14.690 | 0.74 | 75 |
| 7 | Decanoic acid, methyl ester | C ₁₁ H ₂₂ O ₂ | 186 | 18.251 | 0.88 | 87 |
| 8 | 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R] | C ₂₀ H ₄₀ O | 296 | 20.056 | 10.61 | 97 |
| 9 | Bis(trimethylsilyl) ether of 1,4-anhydro-3-deoxypentitol | C ₁₁ H ₂₆ O ₃ Si ₂ | 262 | 25.511 | 0.84 | 59 |
| 10 | D-erythro-pentopyranose, 2-deoxy-1,3,4-tris-o-(trimethylsilyl) | C ₁₄ H ₃₄ O ₄ Si ₃ | 350 | 26.933 | 1.23 | 57 |
| 11 | 5-Hydroxymethyl-2,2,5-trimethyl-1,3-dioxane, | C ₁₁ H ₂₄ O ₃ Si | 232 | 26.332 | 0.76 | 56 |
| 12 | Cis-4-Trimethylsilyloxy-cyclohexyl(trimethylsilyl)carboxy | C ₁₃ H ₂₈ O ₃ Si ₂ | 288 | 28.086 | 0.75 | 50 |
| 13 | (1-butoxybutoxy)trimethylsilane | C ₁₁ H ₂₆ O ₂ Si | 218 | 13.590 | 0.90 | 74 |
| 14 | Phytol, acetate | C ₂₂ H ₄₂ O ₂ | 338 | 20.562 | 5.95 | 76 |
| 15 | D-Erythro-Pentofuranose, 2-deoxy-1,3,5-tris-O-(trimethylsilyl) | C ₁₄ H ₃₄ O ₄ Si ₃ | 350 | 27.051 | 2.02 | 55 |

Proposed mechanism of CI

KBE protected MS against corrosion in a 0.5 M H₂SO₄ solution by the adsorption process. CI mechanism is based on molecules interactions of acceptor and donor electrons between KBE and unoccupied d- orbital's on the MS surface. In other words, KBE's hetero atoms interacted with the vacant d-orbital of the MS surface. At higher Ct, Its CI potential in AE, namely H₂SO₄, was stronger [54].

Conclusions

KBE showed excellent CI results against MS corrosion in a 0.5 M H₂SO₄ solution. Its IE(%) increased with higher Ct. The highest IE(%) of 98.41% was observed for the Ct of 1600 ppm. All electrochemical measurements showed an analogous trend of IE(%). KBE adsorption onto the MS surface obeyed Langmuir's isotherm. It was a monolayer adsorption, and its nature was spontaneous and comprehensive. Surface morphology study via SEM confirmed the MS surface improvement, due to KBE adsorption onto it. KBE corrosion protection of MS, at particularly low Ct, makes it an ideal material for creating self-healing coatings.

Authors' contributions

O. S. Yadav: planned the original research works; performed experiments and analysis; interpreted the results; wrote the manuscript. **S. Kumar and K. Yadav:** treated experimental data; validated results; prepared the draft. **R. Sharma and R. Kumar:** validated results; prepared the draft.

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Abbreviations

AE: acidic environment
AFM: atomic force microscopy
C_{dl}: double layer capacitance
CI: corrosion inhibitor
C_{inh}: inhibitor concentration
CPE: constant phase element
CR: corrosion rate
Ct: concentration
E_{corr}: corrosion potential
EIS: electrochemical impedance spectroscopy
GC-MS: gas chromatography/mass spectrometry
H₂SO₄: sulfuric acid

HER: hydrogen evolution reaction
 i_{corr} : corrosion current density
IT: immersion time
KB: *Kala Bansa (Barleria Prionitis)*
KBE: *Kala Bansa* extract
LPR: linear polarization resistance
MF: molecular formula
MS: mild steel
MW: molecular weight
OCP: open circuit potential
PA: peak area
PDP: potentiodynamic polarization
ppm: parts per million
 R^2 : regression coefficient
 R_{ct} : charge transfer resistance
SC: surface coverage
SEM: scanning electron microscopy
SI: similarity index
SR: scan rate
T: temperature
WL: weight loss

Symbols definition

β_a : anodic Tafel slope
 β_c : cathodic Tafel slope
 $\Delta G^{\circ}_{\text{ads}}$: standard free energy for Gibbs
 $\Delta H^{\circ}_{\text{ads}}$: standard enthalpy
 $\Delta S^{\circ}_{\text{ads}}$: standard entropy
 E_a : activation energy for Arrhenius equation

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