

EXTENDED ESSAY

Chemistry

Topic: An investigation on the inhibitory effect of different concentrations of caffeine solutions on the corrosion of carbon steel (ST 37)

Research Question: “How do different concentrations of pure caffeine($C_8H_{10}N_4O_2$) as an inhibitor (absence of caffeine, 0.1 mol.dm^{-3} , 0.05 mol.dm^{-3} , 0.01 mol.dm^{-3} , $0.005 \text{ mol.dm}^{-3}$, $0.001 \text{ mol.dm}^{-3}$) present in 1 mol.dm^{-3} hydrochloric acid solution (HCl) affect the corrosion of carbon steel(ST 37) determined by the inhibition efficiency measured by mass loss of carbon steel(ST 37) specimens immersed to prepared solutions at 30.0°C and 50.0°C water baths for 24 hours?

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INTRODUCTION

Regarding the current conditions of systems and habitats on Earth and how they change through time under the circumstances of today; in order to preserve the ecological balance, the sanity of nature and to prevent the destruction of life, more environmentalist approaches against problems and obstacles are required. Embracing this statement, by carrying the most polluting and damaging effects, industries should adapt their conditions and come up with greener solutions against disruptive processes, such as corrosion.

Metals and alloys are the base structure of industrial framework, providing stability and resistance to force and heat. Despite of being widely functional and used in a great range of workspace; corrosion of steel has been a critical problem which has caused severe economic losses, led to serious environmental pollution, and carry high potential of risk for human health, in many different industries.

Corrosion is an electrochemical process in which a metal revolves to a more stable form by oxidizing and this damages the metal surface, and cause deterioration of the structure.¹ Many different methods have been tried to reduce and eliminate effects of corrosion. Use of corrosion resistance materials, protective coating with different materials such as paint, rubber, nylon, and polyester, metal plating which is coating with a metal material, environmental measures by simply reducing the oxygen and moist factors around the surrounding and design modifications that would likely to reduce the contact of metal surface and corroding surrounding are some of the examples.²

¹ *What is corrosion?* ECS. (2016, February 26). Retrieved July 4, 2022, from <https://www.electrochem.org/corrosion-science/>

² *How to Prevent Corrosion.* Materials UK. (n.d.). Retrieved July 4, 2022, from <https://www.thyssenkrupp-materials.co.uk/how-to-prevent-corrosion>

Inhibition is the preventive or retarding activity of a chemical process which is provided by another material, called the inhibitor or inhibitive. The effectiveness of an inhibitor is expressed with inhibitor efficiency, which is used to decide whether an inhibitor can provide the sufficient inhibiting property for a system.

Inhibitors differ from each other by their traits of being inorganic and organic. While inorganic inhibitors act in anodic and cathodic ways, organic inhibitors act by creating adsorption. Adsorption is the process of atoms, molecules or possibly other particles being attached and accumulated on a surface and creating a thin layer on that surface.³

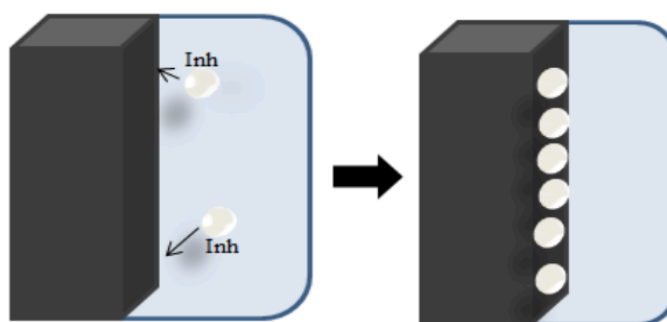


Figure 1⁴: Illustration of inhibitor molecules adsorbing onto a surface.

It is observed that organic products, such as caffeine (*1,3,7-trimethylxanthine*, $C_8H_{10}N_4O_2$), are capable of offering inhibitory trait against metals and alloys by causing adsorption on their surfaces.⁵ Additionally, compared to other alternative methods (by means of cost, external effects, and effectiveness), the most efficient of all the methods is corrosion inhibitory activity⁶.

³ Adsorption. Soft. (n.d.). Retrieved August 6, 2022, from <http://soft-matter.seas.harvard.edu/index.php/Adsorption>

⁴ G., C., & F., A. (2014). Corrosion inhibitors – principles, mechanisms and applications. *Developments in Corrosion Protection*. <https://doi.org/10.5772/57255>

⁵ de Souza, F. S., Giacomelli, C., Gonçalves, R. S., & Spinelli, A. (2012). Adsorption behavior of caffeine as a green corrosion inhibitor for copper. *Materials Science and Engineering: C*, 32(8), 2436–2444. <https://doi.org/10.1016/j.msec.2012.07.019>

⁶ Beda, R. H., Niamien, P. M., Avo Bilé, E. B., & Trokourey, A. (2017). Inhibition of aluminium corrosion in 1.0 M hcl by caffeine: Experimental and DFT Studies. *Advances in Chemistry*, 2017, 1–10. <https://doi.org/10.1155/2017/6975248>

Efficiency of an inhibitor depends on many factors such as the size of the molecule, number of bonding groups the molecule has, capability of the metal surface to form a complex with the atom. Inhibitor efficiency is measured with the given formula:

$$E_f = (R_i - R_0) / R_0 \times 100 \text{ } ^4$$

[E_f is inhibitor efficiency, R_f is rate of corrosion with inhibitor involved, R_0 is rate of corrosion without inhibitor involved.]

Caffeine is a xanthine alkaloid compound (also known as purine alkaloids, alkaloids containing xanthine as their nitrogenous base)⁷ found in different plants' beans, leaves and fruits, extracted by use of different methods such as water extraction, direct & indirect organic solvent extraction and supercritical carbon dioxide extraction.⁸ It is a cathodic inhibitor which reduces the rate of corrosion due to cathodic reactions by causing an insoluble compound to be formed as a barrier layer.⁹ This is called a cathodic protection, in which electrons from an external source, caffeine in this case, flows to the surface of the material and oxidation is prevented by adsorption.¹⁰

⁷ Ashihara, H., Mizuno, K., Yokota, T., & Crozier, A. (2017). Xanthine alkaloids: Occurrence, biosynthesis, and function in plants. *Progress in the Chemistry of Organic Natural Products* 105, 1–88. https://doi.org/10.1007/978-3-319-49712-9_1, 2017, accessed June 1, 2022

⁸ Lawandi, J. (2019, May 1). *How caffeine is removed from coffee*. Kitchn. Retrieved August 6, 2022, from <https://www.thekitchn.com/how-caffeine-is-removed-from-coffee-221230>

⁹ *Materials engineering*. Corrosion inhibitors [SubsTech]. (2012, May 31). Retrieved March 14, 2023, from https://www.substech.com/dokuwiki/doku.php?id=corrosion_inhibitors

¹⁰ *Materials engineering*. Cathodic protection [SubsTech]. (2015, July 21). Retrieved March 14, 2023, from https://www.substech.com/dokuwiki/doku.php?id=cathodic_protection



Figure 2: 2D Structure of Caffeine Molecule¹¹

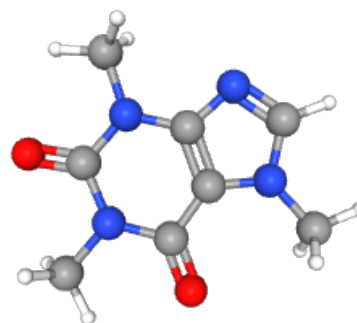


Figure 3: 3D Structure of Caffeine Molecule¹⁰

ST 37 is a carbon metal, low in carbon content. It is an alloy composed of iron, carbon, manganese, sulphur, and phosphorus. Due to its high melting point, low hardness, and high ductility, ST 37 is broadly used in industrial area: construction, machines, bolts...¹²

For this investigation, carbon steel (ST 37) is used as the metal product that will be exposed to acidic environment and observe the inhibitory effect of caffeine on the resultant corrosion.

BACKGROUND INFORMATION

Rate of reaction determines how independent variable affects reactions' occurrence speed. To measure this rate, different aspects could be referenced: change in mass, concentration and volume are some examples. It is also known that rate of reaction depends on several factors. Temperature, surface area and presence of catalyser are directly proportional with rate of reaction while concentration of solution, and ... are inversely proportional. Rate of reaction is calculated with the following formula:

$$\frac{\text{change in (concentration - volume - mass)}}{\text{unit time}}$$

¹¹ U.S. National Library of Medicine. (n.d.). *Caffeine*. National Center for Biotechnology Information. PubChem Compound Database. Retrieved January 9, 2023, from <https://pubchem.ncbi.nlm.nih.gov/compound/Caffeine#section=3D-Conformer>

¹² Sebayang, M. D. (2021). ST37 steel carburization with coconut charcoal. *Journal of Technomaterials Physics*, 3(1), 29–35. <https://doi.org/10.32734/jotp.v3i1.5713>

The inhibiting activity of caffeine on metals have been experimented and proven on different articles, as presented in Table.1:

| Materials | Methodology | Summary | Reference |
|---|--|---|--|
| 1 moldm ⁻³ HCl, mild steel, caffeine | Potentiodynamic polarization and electrochemical impedance spectroscopy techniques were applied, and weight loss was measured. | According to potentiodynamic polarization study, caffeine is a cathodic type inhibitor. Since caffeine has a capability of adsorption by forming a barrier film on the mild steel surface, researchers proved that caffeine has high corrosion inhibition efficiency. | H. Elmsellem, A. Aouniti, M.H. Youssoufi, H. Bendaha, T. Ben hadda, A. Chetouani, I. Warad, B. Hammouti |
| 1 moldm ⁻³ HCl, aluminium, caffeine | Mass loss technique, in addition to quantum chemical calculations based on DFT. | In this study, corrosion inhibition of caffeine on aluminium in 1.0 M hydrochloric acid solution was studied. The inhibition efficiency was observed to increase with increasing concentration of caffeine but decreases with a rise in temperature. The molecule shows the highest inhibition efficiency of 74% at 10 ⁻² M for T = 303K. | R. H. B. Beda, P. M. Niamien, E. B. Avo Bilé, and A. Trokourey ¹³ |
| NaCl, mild carbon steel, caffeine | Weight-loss measurement method was used and data were collected by observing the microstructures of corroded mild steel specimens by using an optical microscope. | It was observed that increasing caffeine amount in environment medium, results in a decrease in the mild steel specimen's weight loss. More caffeine was introduced to the atmosphere, which reduced the rate of specimen deterioration. From optical microscopic analysis, it appears that caffeine's inhibitory effect occurred through creating a barrier to stop further corrosion of mild steel in NaCl solution. | L.P. Xuan, M.A. Anwar, T. Kurniawan, H. M. AyuI, R. Daud. & Y. P. Asmara ¹⁴ |
| 0.1 moldm ⁻³ sulfuric acid (H ₂ SO ₄), copper, caffeine | Potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), contact angle measurements, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and fluorescence experiments. | Corrosion behaviour of copper in aerated 0.1 mol L ⁻¹ H ₂ SO ₄ solutions in the presence of three xanthine derivatives with similar chemical structures is evaluated. By creating adsorption onto the copper surface and creating hydrophobic protective film, caffeine acts as cathodic type inhibitor. This film covers up to 72% of the total active surface, acts as a protective barrier and prevents interaction between the metal, water, and oxygen molecules. | Fernando Sílvia de Souza, Cristiano Giacomelli, Reinaldo Simões Gonçalves & Almir Spinelli ¹⁵ |

Table 1: Previous experiments on the inhibitory effect of caffeine on metals in literature

¹³ Beda, R. H., Niamien, P. M., Avo Bilé, E. B., & Trokourey, A. (2017). Inhibition of aluminium corrosion in 1.0 M hcl by caffeine: Experimental and DFT Studies. *Advances in Chemistry*, 2017, 1–10. <https://doi.org/10.1155/2017/6975248>

¹⁴ Xuan, L. P., Anwar, M. A., Kurniawan, T., Ayu, H. M., Daud, R., & Asmara, Y. P. (2019). Caffeine as a natural corrosion inhibitor for mild steel in Nacl solution. *JOURNAL OF SCIENCE AND APPLIED ENGINEERING*, 2(2), 63. <https://doi.org/10.31328/jsae.v2i2.1186>

¹⁵ de Souza, F. S., Giacomelli, C., Gonçalves, R. S., & Spinelli, A. (2012). Adsorption behavior of caffeine as a green corrosion inhibitor for copper. *Materials Science and Engineering: C*, 32(8), 2436–2444. <https://doi.org/10.1016/j.msec.2012.07.019>

PRELIMINARY EXPERIMENTS

There have been many preliminary trials due to obstructive factors affecting the expected flow of the experiment and cause occurrence of unwanted reactions before successful results were reached.

Preliminary Experiment 1: Determination of Material Properties

In one of the made trials, carbon steel obtained from steel wool, is used as the metal product. Pieces of steel with same weights are placed in 1 moldm⁻³ HCl solutions with different concentrations (0,1 moldm⁻³, 0.05 moldm⁻³, 0.01 moldm⁻³, 0.005 moldm⁻³, 0.001 moldm⁻³) of impure caffeine supplement. The metals were waited inside the solutions for 30 minutes. Any useful and predict result could not be obtained. Impurity of both materials prevented the expected result to be reached to, therefore it is determined that used materials should be pure.

Preliminary Experiment 2: Determination of Materials

In this trial, copper (Cu) was used as the metal material and placed into 1 moldm⁻³ H₂SO₄ solutions with no caffeine and 0.01 moldm⁻³ caffeine concentrations and made waited for a period of time. Unfortunately, the experiment again did not respond as expected.

Preliminary Experiment 3: Determination of Materials & Method

In another trial, Aluminium (Al) was used as the metal and 1 moldm⁻³ HCl was used as acid. Aluminium pieces were sanded sufficiently, later immersed into acetone and washed with distilled water and made dry by using an oven for 1.5 hours. Mass of caffeine for different caffeine solutions were calculated taking the impurity rate into consideration. The solutions were prepared by calculating the exact mass of pure caffeine present in caffeine tablets taking the fraction of present material inside one tablet into consideration and later added into the solutions. Later, without any loss of caffeine or acid throughout the process, solutions were

placed into water baths at 40°C, in order to achieve maximum efficiency of the reaction and enable caffeine to be dissolved inside acids. After Aluminium specimens were placed inside the beakers, they were kept in for 1 hour, but results were again not proportional with expected.

Preliminary Experiment 4: Determination of Materials & Method

In the last failed trial, different metals were chosen (Zinc (Zn), Iron (Fe) and Aluminium (Al)) and placed inside solutions concentrated at 0 mol dm^{-3} , 0,1 mol dm^{-3} , 0,05 mol dm^{-3} , 0,01 mol dm^{-3} , 0,005 mol dm^{-3} , proportions, prepared with 1M HCl and pure caffeine. All metals were sanded until the visible oxidized layer is removed and were kept inside 0.5M HCl of 300 ml, for 5 minutes, so that the oxidized layers were resolved as sufficiently as possible. Metals were taken out of the acid and sequentially washed under tap water, immersed into acetone, and washed with distilled water in order to clean as much as possible under laboratory circumstances. Specimens were placed into oven for full dryness, for 30 minutes. Specimens were made waited inside acid solutions for 24 hours and after being taken out, they were again washed with tap water and placed inside oven for full dryness before mass measurement was repeated. Yet, no expected results were obtained.

In the last experiment, in order to eliminate the effect that the difference in metal specimens may have created, even though they are preserved under same conditions; steel specimens were directly ordered from a factory, made cut in exact same sizes and in order to prevent a possible corrosion before they were used in the experiment, they were covered in oil. Caffeine that was used was again pure.

HYPOTHESIS: Metals within the acid solutions including higher concentrations of caffeine will be corroding less and relatively lower mass loss will be observed. As the concentration of caffeine is decreased, there will be more corrosion observed and higher mass loss will be measured.

VARIABLES

| | | REASON |
|----------------|---|---|
| INDEPENDENT V. | Caffeine concentration (absence, 0.1 moldm ⁻³ , 0.05 moldm ⁻³ , 0.01 moldm ⁻³ , 0.005 moldm ⁻³ , 0.001 moldm ⁻³) | Amount of corrosion in the presence of different caffeine concentrations will be measured. |
| | Temperature (30°C & 50°C) | Rate of reaction is directly proportional with temperature and an increase in temperature will increase the effectiveness of caffeine's inhibitory activity. Given temperatures were chosen considering the solubility of caffeine in the solution: the chosen temperature levels would provide dissolution of caffeine without interfering with the structure of materials or causing other effects during experiment. |
| DEPENDENT | Mass Loss of ST37 specimens due to corrosion | Amount of corrosion of aluminium specimens will be measured via mass loss and increased concentration of caffeine in solutions will impact the mass loss. |

Table 2: Independent and Dependent Variables

| | | REASON & METHOD of CONTROL |
|----------------------|--|---|
| CONTROLLED VARIABLES | Duration of exposure to acid | Amount of corrosion of metal surfaces may vary as the duration of metals remaining in acid solutions differ. Therefore, duration of exposure to acid was kept constant for each trial. |
| | Properties of metal specimens | Caffeine shows inhibitory impact by adsorbing onto the surface. As a consequence, difference of the surface sizes may cause a change of the amount of adsorbed material. Additionally, as adsorption is made onto the surface, surface properties (e.g. impurities, surface oxidation) are effective on the activity. Therefore, specimens were standardized by being ordered from factory. |
| | Measurement methods & apparatus | Measurements were made with same apparatus and with same methodology applied in order to prevent any systematic error that possibly could occur during the measurements which were done on millimetric level, and the smallest change may have caused a differentiation of values. |
| | Physical conditions of environment (Stability of temperature, location of measurement) | The smallest differentiation that could occur was prevented by keeping the physical conditions same: the specific temperature of the environment was kept stable by use of water baths, and measurements were made at the exact same location in order to eliminate the smallest changing factor, for example the small breeze. |
| | Concentration of acid | Effect of the concentration of caffeine is trying to be observed. If the concentration of acid is changed, the impact it would create would prevent the object to be reached. |

Table 3: Independent, Dependent and Controlled Variables and Reasoning

METHOD

Material List

| Chemicals | Apparatus | Safety |
|---|---|---|
| <ul style="list-style-type: none">Merck: 36% Hydrochloric acid (HCl) | <ul style="list-style-type: none">40×50 cm³ beaker100 cm³ Graduated Cylinder (±0.5)1 dm³ Volumetric Flask (±0.3) | <ul style="list-style-type: none">GlovesGogglesLaboratory Apron |
| <ul style="list-style-type: none">Sigma Aldrich: 99% Anhydrous Caffeine (C₈H₁₀N₄O₂) | <ul style="list-style-type: none">Precision scale (±0.001)SpatulaForcepsStirring rod | <ul style="list-style-type: none">Acid waste container |
| <ul style="list-style-type: none">39× 2x2 cm² ST37 Steel | <ul style="list-style-type: none">Water bath (±0.1) | |
| <ul style="list-style-type: none">46% (v/v) Ethanol (C₂H₅OH) | <ul style="list-style-type: none">OvenChronometer (±0.1) | |

Procedure

1. Gloves, goggles, and laboratory apron were worn for precaution.

Preparation of Metal Specimens

2. In order to provide maximum standardization, metal specimens were ordered from a factory; all 40 of them were made cut from the same carbon steel (ST37) piece in 2x2 cm² dimensions. (Metal specimens were covered in grease in order to prevent any possible corrosion during import.)
3. Metal specimens that were covered in grease were immersed in 46% v/v ethanol solution in order to solve the grease on them and remove the impurities.
4. Metal specimens were gotten out of ethanol solution and washed under tap water.

5. Specimens were placed into the oven at the highest temperature possible, for full dryness and made waited 90 minutes.

Preparation of Caffeine-Hydrochloric Acid Solutions

6. 12 moldm⁻³ hydrochloric acid (HCl) stock solution is obtained from Merck.
7. Necessary calculations were made in order to dilute HCl to 1 moldm⁻³. By addition of $83.3 \pm 0.5 \text{ cm}^3$ 12 moldm⁻³ HCl to water in 1000 cm³ volumetric flask.
8. Put empty 100 cm³ beaker on precision scale and push tare for calibration before mass of caffeine is measured.
9. By using spatula, add 1.942 ± 0.0001 grams of caffeine into the beaker and wait until the value on precision scale is constant.
10. Add $100 \pm 0.5 \text{ cm}^3$ diluted 1 moldm⁻³ HCl acid into the beaker by measuring it with the graduated cylinder and stir it with glassing stirring rod.

(Repeat steps 4 & 5 for other solutions of different concentrations. Required amount of caffeine that will be measured can be seen from Table.10)

(At this point, one should have 100 cm³ HCl-caffeine solutions of 0.1 moldm⁻³, 0.05 moldm⁻³, 0.01 moldm⁻³, 0.005 moldm⁻³, 0.001 moldm⁻³ concentrations and 100 cm³ of only HCl with no caffeine in it, two of each for two different temperatures (30°C and 50°C).)

11. Metal specimens were taken out of the oven by use of heat resistant gloves and mass measurements were made for each piece.

Corrosion of ST37 Steel Specimens in Acidic Medium

12. Each specimen was replaced inside one caffeine – HCl solution, with a specific concentration.
13. Set water baths to 30°C and 50°C.

14. Caffeine – HCl solutions of different concentrations with ST37 steel specimens in them are replaced inside water baths that were previously heated to 30°C and 50°C and left waited for 24 hours being checked by chronometer.
15. Metal specimens were taken out of acid solutions by use of forceps and washed under tap water.
16. Specimens were replaced inside oven for dryness, at highest temperature and made waited for 2 hours.
17. Weights of steels were measured on precision scale, and mass loss was calculated.
18. All used materials (metal specimens and acid solutions) were disposed properly.

ETHICAL CONSIDERATIONS & RISK ASSESSMENT

Fundamental precautions such as laboratory clothes (gloves, apron, glasses, heat resistant gloves while working with oven) were worn in order to prevent any touch with chemicals, specifically acids and irritating material.

In order to reduce any touch with chemicals, metal specimens were immersed, carried, and taken out from acidic environment only with forceps.

Solutions were prepared in a way that would reduce the reaction reactivity to minimum. For example, acid was added on top of water during dilution and acid was added on top of caffeine.

Lastly, all used materials were collected separately in special bins, and made sure that they are disposed carefully without any leakage or interference to other materials and mediums, which may cause serious environmental issues.

There is no ethical concern for this experiment.

DATA COLLECTION

Raw Data

Tables below display the mass values of ST37 specimens before and after they were replaced in caffeine-HCl solutions.

| | Trial.1 (g) (±0.001) | Trial.2 (g) (±0.001) | Trial.3 (g) (±0.001) | Trial.4 (g) (±0.001) | Trial.5 (g) (±0.001) |
|-----------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| no caffeine | 25.888 | 26.045 | 25.968 | 25.997 | 25.687 |
| 0.1 (±0.6%) moldm ⁻³ | 26.044 | 26.020 | 26.003 | 25.986 | 26.029 |
| 0.05 (±0.6%) moldm ⁻³ | 26.075 | 26.036 | 25.932 | 26.054 | 25.989 |
| 0.01 (±0.6%) moldm ⁻³ | 26.086 | 26.428 | 26.406 | 26.065 | 26.031 |
| 0.005 (±0.6%) moldm ⁻³ | 26.047 | 26.498 | 26.357 | 26.043 | 26.071 |
| 0.001 (±0.6%) moldm ⁻³ | 26.014 | 26.228 | 26.341 | 25.997 | 26.012 |

Table 4: Initial masses of steel (ST 37) specimens replaced in 30°C.

| | Trial.1 (g) (±0.001) | Trial.2 (g) (±0.001) | Trial.3 (g) (±0.001) | Trial.4 (g) (±0.001) | Trial.5 (g) (±0.001) |
|-----------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| no caffeine | 25.273 | 25.438 | 25.358 | 25.380 | 25.085 |
| 0.1 (±0.6%) moldm ⁻³ | 25.896 | 25.870 | 25.857 | 25.845 | 25.880 |
| 0.05 (±0.6%) moldm ⁻³ | 25.885 | 25.868 | 25.754 | 25.882 | 25.804 |
| 0.01 (±0.6%) moldm ⁻³ | 25.883 | 26.156 | 26.183 | 25.809 | 25.794 |
| 0.005 (±0.6%) moldm ⁻³ | 25.787 | 26.211 | 26.078 | 25.760 | 25.792 |
| 0.001 (±0.6%) moldm ⁻³ | 25.608 | 25.794 | 25.908 | 25.556 | 25.589 |

Table 5: Final masses of steel (ST 37) specimens replaced in 30°C.

| | Trial.1 (g) (±0.001) | Trial.2 (g) (±0.001) | Trial.3 (g) (±0.001) | Trial.4 (g) (±0.001) | Trial.5 (g) (±0.001) |
|-----------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| no caffeine | 25.972 | 26.243 | 26.219 | 25.378 | 26.092 |
| 0.1 (±0.6%) moldm ⁻³ | 26.035 | 26.000 | 26.010 | 25.877 | 25.963 |
| 0.05 (±0.6%) moldm ⁻³ | 26.427 | 26.350 | 26.212 | 26.021 | 25.997 |
| 0.01 (±0.6%) moldm ⁻³ | 25.977 | 25.872 | 26.011 | 25.978 | 26.008 |
| 0.005 (±0.6%) moldm ⁻³ | 26.730 | 25.590 | 25.879 | 25.931 | 26.021 |
| 0.001 (±0.6%) moldm ⁻³ | 25.868 | 26.484 | 25.995 | 25.867 | 26.002 |

Table 6: Initial masses of steel (ST 37) specimens replaced in 50°C.

| | Trial.1 (g) (±0.001) | Trial.2 (g) (±0.001) | Trial.3 (g) (±0.001) | Trial.4 (g) (±0.001) | Trial.5 (g) (±0.001) |
|-----------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| no caffeine | 23.389 | 23.574 | 23.766 | 22.833 | 23.594 |
| 0.1 (±0.6%) moldm ⁻³ | 25.242 | 25.215 | 25.248 | 25.089 | 25.198 |
| 0.05 (±0.6%) moldm ⁻³ | 25.689 | 25.800 | 25.314 | 25.358 | 25.225 |
| 0.01 (±0.6%) moldm ⁻³ | 25.035 | 24.919 | 25.088 | 25.044 | 25.066 |
| 0.005 (±0.6%) moldm ⁻³ | 25.641 | 24.585 | 24.877 | 24.913 | 24.998 |
| 0.001 (±0.6%) moldm ⁻³ | 24.187 | 24.845 | 24.338 | 24.204 | 24.328 |

Table 7.: Final masses of steel (ST 37) specimens replaced in 50°C.

Processed Data

Tables below display the mass loss of ST37 specimens occurred due to corrosion in caffeine-HCl solutions. Values in the table were calculated as: $(\text{Change of Mass} = \text{Final mass}(\text{given in Table 5 and 7}) - \text{Initial mass}(\text{given in Table 4 and 6}))$.

Although mass loss values calculated by this formula are negative, they are given as positive since it is corrosion.

Sample Calculation: for 0.1 mol.dm^{-3} at $30.0 \text{ }^\circ\text{C}$ (Trial 1) $\Delta m = 25.896 - 26.044 = -0.148 \text{ g}$

| | Trial.1 (g) (± 0.002) | Trial.2 (g) (± 0.002) | Trial.3 (g) (± 0.002) | Trial.4 (g) (± 0.002) | Trial.5 (g) (± 0.002) |
|---|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| no caffeine | 0.615 | 0.607 | 0.610 | 0.617 | 0.602 |
| $0.1 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.148 | 0.150 | 0.146 | 0.141 | 0.149 |
| $0.05 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.190 | 0.168 | 0.178 | 0.172 | 0.185 |
| $0.01 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.203 | 0.272 | 0.223 | 0.256 | 0.237 |
| $0.005 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.260 | 0.287 | 0.279 | 0.283 | 0.279 |
| $0.001 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.406 | 0.434 | 0.433 | 0.441 | 0.423 |

Table 8: Change in mass of steel (ST 37) specimens replaced in 30°C .

| | Trial.1 (g) (± 0.002) | Trial.2 (g) (± 0.002) | Trial.3 (g) (± 0.002) | Trial.4 (g) (± 0.002) | Trial.5 (g) (± 0.002) |
|---|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| no caffeine | 2.583 | 2.669 | 2.453 | 2.545 | 2.498 |
| $0.1 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.793 | 0.785 | 0.762 | 0.788 | 0.765 |
| $0.05 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.738 | 0.550 | 0.898 | 0.663 | 0.772 |
| $0.01 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 0.942 | 0.953 | 0.923 | 0.934 | 0.942 |
| $0.005 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 1.089 | 1.005 | 1.002 | 1.018 | 1.023 |
| $0.001 (\pm 0.6\%) \text{ mol dm}^{-3}$ | 1.681 | 1.639 | 1.657 | 1.663 | 1.674 |

Table 9: Change in mass of steel (ST 37) specimens replaced in 50°C .

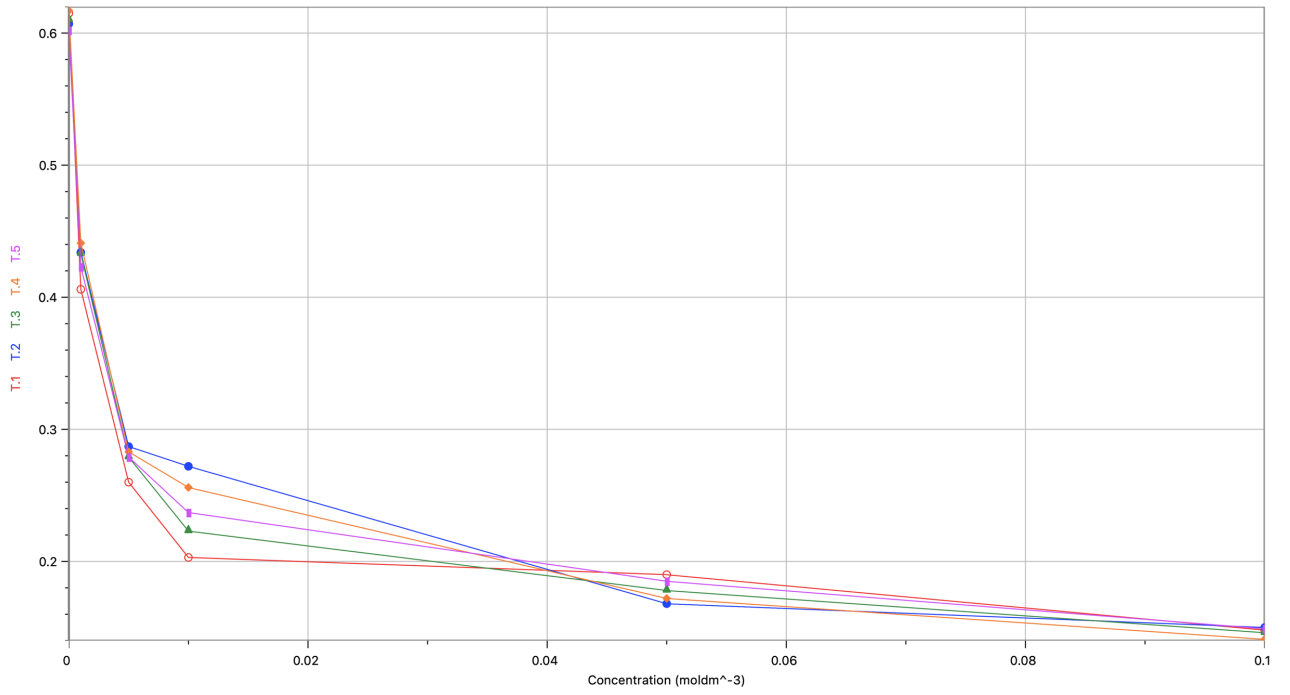


Figure 4: Graph of change of mass due to corrosion at different concentrations of caffeine-HCl solutions, on each trial (labelled as T.1-T.2-T.3-T.4-T.5) at 30°C.

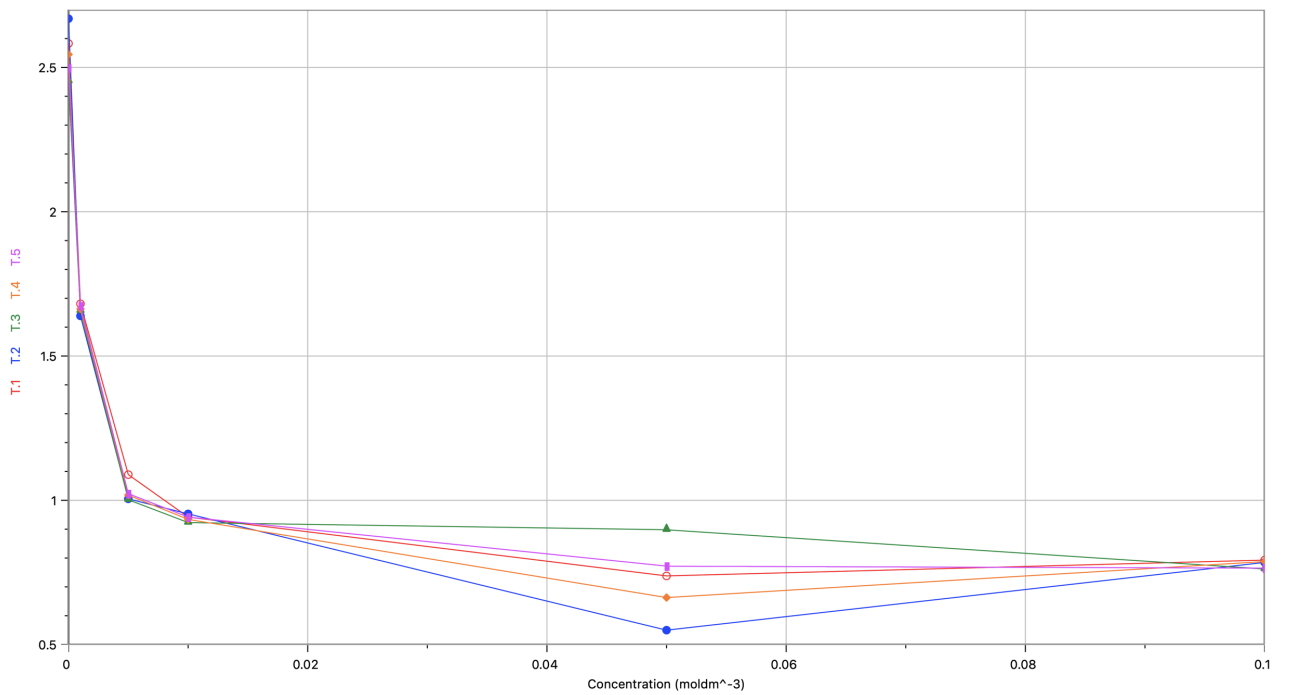


Figure 5: Graph of change of mass due to corrosion at different concentrations of caffeine-HCl solutions, on each trial (labelled as T.1-T.2-T.3-T.4-T.5) at 50°C.

CALCULATIONS & DATA PROCESSING

1. Molarity Calculations for Caffeine

Solutions of 0.1 moldm⁻³, 0.05 moldm⁻³, 0.01 moldm⁻³, 0.005 moldm⁻³, 0.001 moldm⁻³ concentration were prepared with 250 ml 1.0 moldm⁻³ hydrochloric acid. In order to prepare, 1 moldm⁻³ solution of 0.1 litre, 19.419 grams of caffeine (C₈H₁₀N₄O₂) is required.

| 1 moldm ⁻³ | 0.1 moldm ⁻³ | 0.05 moldm ⁻³ | 0.01 moldm ⁻³ | 0.005 moldm ⁻³ | 0.001 moldm ⁻³ |
|--------------------------|-----------------------------|------------------------------|------------------------------|----------------------------|-------------------------------|
| 19.419 (±0.001) grams | 1.9419 (±0.001) grams | 0.97095 (±0.001) grams | 0.19419 (±0.001) grams | 0.097095 (±0.001) grams | 0.019419 (±0.001) grams |

Table 10: Calculations for molarity in caffeine - HCl solution. Molarity, amount of HCl, required mass of caffeine.

2. Rate of Reaction

Rate of reaction was calculated, by taking mass loss as reference, by using the following equation: *change of mass (initial mass – final mass) / change of time (hours)*.

Change of mass values are given in Table.6 and Table.7, and the change of time remains 24 hours for all reactions. Uncertainty values for each rate were calculated to be different. Thus, were given in Table.19 & Table.20.

Sample Calculation for 0.1 moldm⁻³ concentration at 30°C: $\frac{0.148}{24} = 0.0062$

| | Trial.1 (gh ⁻¹) | Trial.2 (gh ⁻¹) | Trial.3 (gh ⁻¹) | Trial.4 (gh ⁻¹) | Trial.5 (gh ⁻¹) |
|---------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| no caffeine | 0.0256 | 0.0253 | 0.0254 | 0.0257 | 0.0251 |
| 0.1 moldm ⁻³ | 0.00617 | 0.00625 | 0.00608 | 0.00588 | 0.00621 |
| 0.05 moldm ⁻³ | 0.00792 | 0.00700 | 0.00742 | 0.00717 | 0.00771 |
| 0.01 moldm ⁻³ | 0.00846 | 0.0113 | 0.00929 | 0.0108 | 0.00988 |
| 0.005 moldm ⁻³ | 0.0108 | 0.0120 | 0.0116 | 0.0118 | 0.0116 |
| 0.001 moldm ⁻³ | 0.0169 | 0.0181 | 0.0180 | 0.0183 | 0.0176 |

Table 11: Rate of change of mass loss due to corrosion (moldm⁻³h⁻¹) at 30°C.

| | Trial.1 (gh ⁻¹) | Trial.2 (gh ⁻¹) | Trial.3 (gh ⁻¹) | Trial.4 (gh ⁻¹) | Trial.5 (gh ⁻¹) |
|---------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| no caffeine | 0.108 | 0.111 | 0.102 | 0.106 | 0.104 |
| 0.1 moldm ⁻³ | 0.033 | 0.033 | 0.032 | 0.033 | 0.032 |
| 0.05 moldm ⁻³ | 0.031 | 0.023 | 0.037 | 0.028 | 0.032 |
| 0.01 moldm ⁻³ | 0.039 | 0.040 | 0.038 | 0.039 | 0.039 |
| 0.005 moldm ⁻³ | 0.045 | 0.042 | 0.042 | 0.042 | 0.043 |
| 0.001 moldm ⁻³ | 0.070 | 0.068 | 0.069 | 0.069 | 0.070 |

Table 12: Rate of change of mass loss due to corrosion (moldm⁻³h⁻¹) at 50°C.

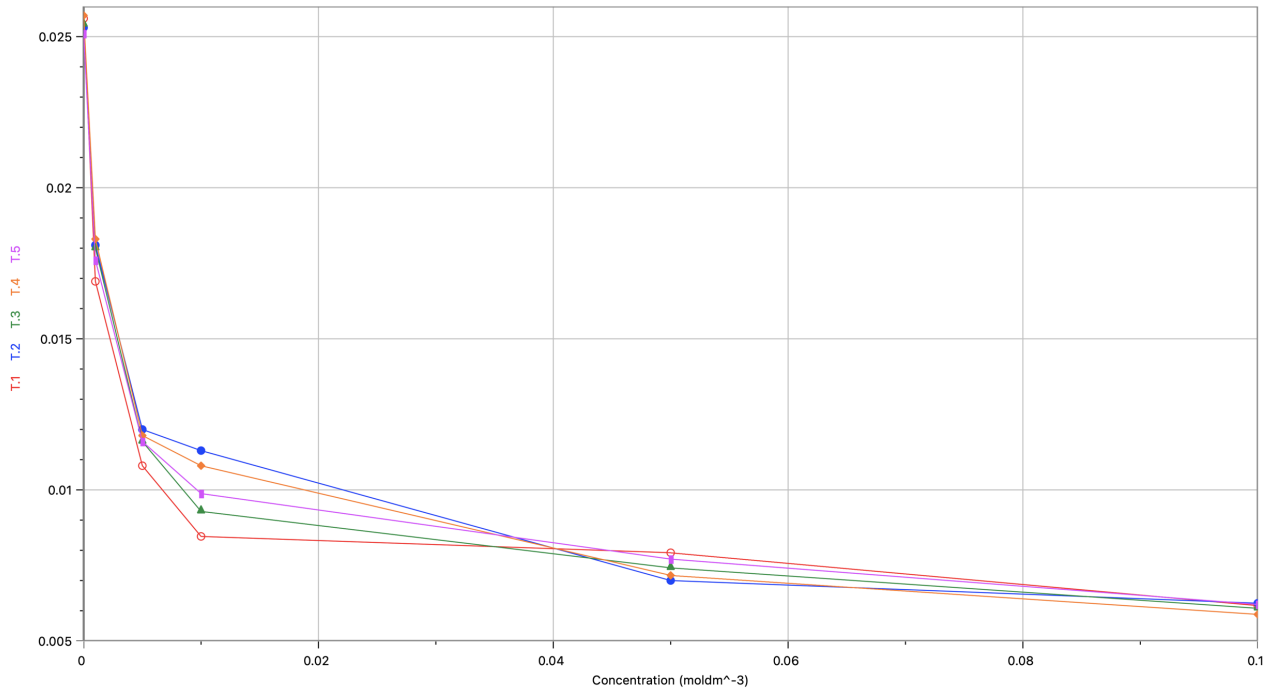


Figure 6: Graph of rate of change of mass loss at different concentrations of caffeine-HCl solutions due to corrosion on each trial (labelled as T.1-T.2-T.3-T.4-T.5) at 30°C.

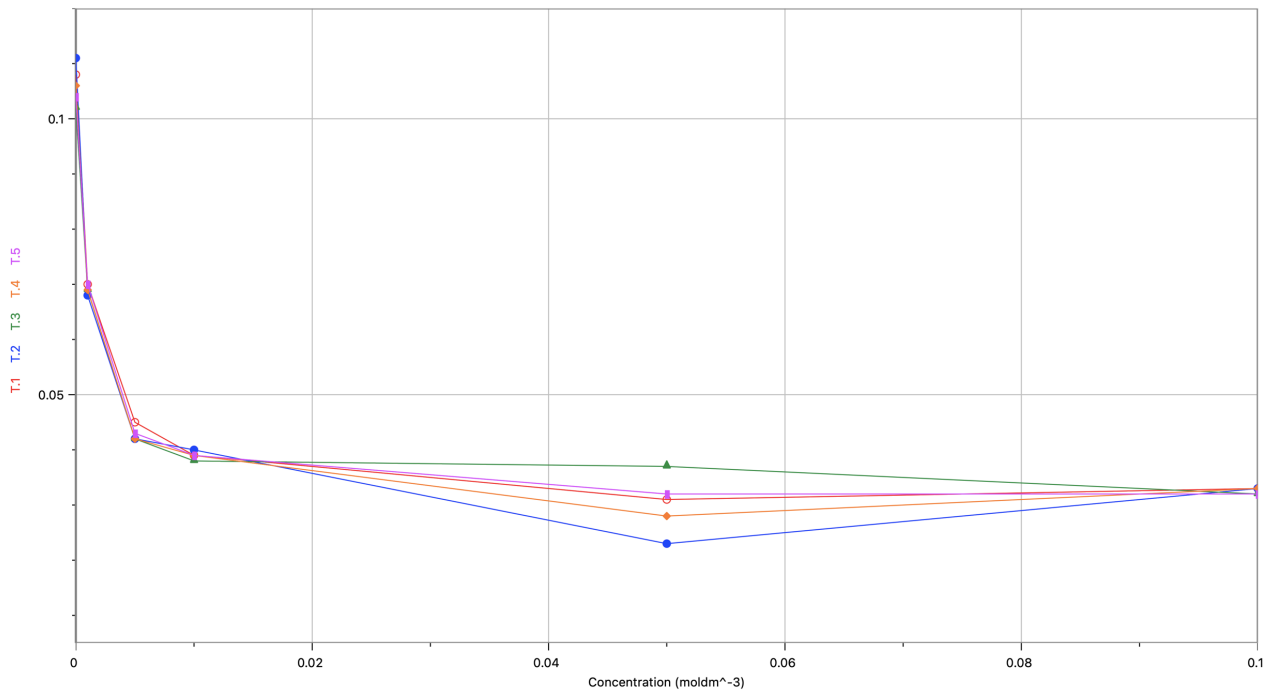


Figure 7: Graph of rate of change of mass loss at different concentrations of caffeine-HCl solutions due to corrosion on each trial (labelled as T.1-T.2-T.3-T.4-T.5) at 50°C.

3. Inhibition Efficiency

Efficiency percentage of the inhibitor (caffeine) is observed by taking rate of reaction at different concentrations as reference. Used equation is following: $E_f = (R_i - R_0) / R_0 \times 100$

(R_i : Rate of corrosion with inhibitor, present at a certain concentration, R_0 is corrosion rate in absence of inhibitor.)

Sample Calculation 0.1 moldm⁻³ concentration at 30°C: $\left| \frac{0.00617 - 0.0256}{0.0256} * 100 \right| = 75.93$

| | Trial.1 (gh ⁻¹) | Trial.2 (gh ⁻¹) | Trial.3 (gh ⁻¹) | Trial.4 (gh ⁻¹) | Trial.5 (gh ⁻¹) |
|---------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| 0.1 moldm ⁻³ | 75.93 | 75.29 | 76.07 | 77.15 | 75.25 |
| 0.05 moldm ⁻³ | 69.11 | 72.32 | 70.82 | 72.12 | 69.27 |
| 0.01 moldm ⁻³ | 66.99 | 55.19 | 63.44 | 58.51 | 60.63 |
| 0.005 moldm ⁻³ | 57.72 | 52.72 | 54.26 | 54.13 | 53.65 |
| 0.001 moldm ⁻³ | 33.98 | 28.50 | 29.02 | 28.53 | 29.73 |

Table 13: Inhibition efficiency percentage of caffeine at differently concentrated HCl-caffeine solutions at 30°C.

| | Trial.1 (gh ⁻¹) | Trial.2 (gh ⁻¹) | Trial.3 (gh ⁻¹) | Trial.4 (gh ⁻¹) | Trial.5 (gh ⁻¹) |
|---------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| 0.1 moldm ⁻³ | 69.30 | 70.59 | 68.94 | 69.04 | 69.38 |
| 0.05 moldm ⁻³ | 71.43 | 79.39 | 63.39 | 73.95 | 69.10 |
| 0.01 moldm ⁻³ | 63.53 | 64.29 | 62.37 | 63.30 | 62.29 |
| 0.005 moldm ⁻³ | 57.84 | 62.35 | 59.15 | 60.00 | 59.05 |
| 0.001 moldm ⁻³ | 34.92 | 38.59 | 32.45 | 34.66 | 32.99 |

Table 14: Inhibition efficiency percentage of caffeine at differently concentrated HCl-caffeine solutions at 50°C.

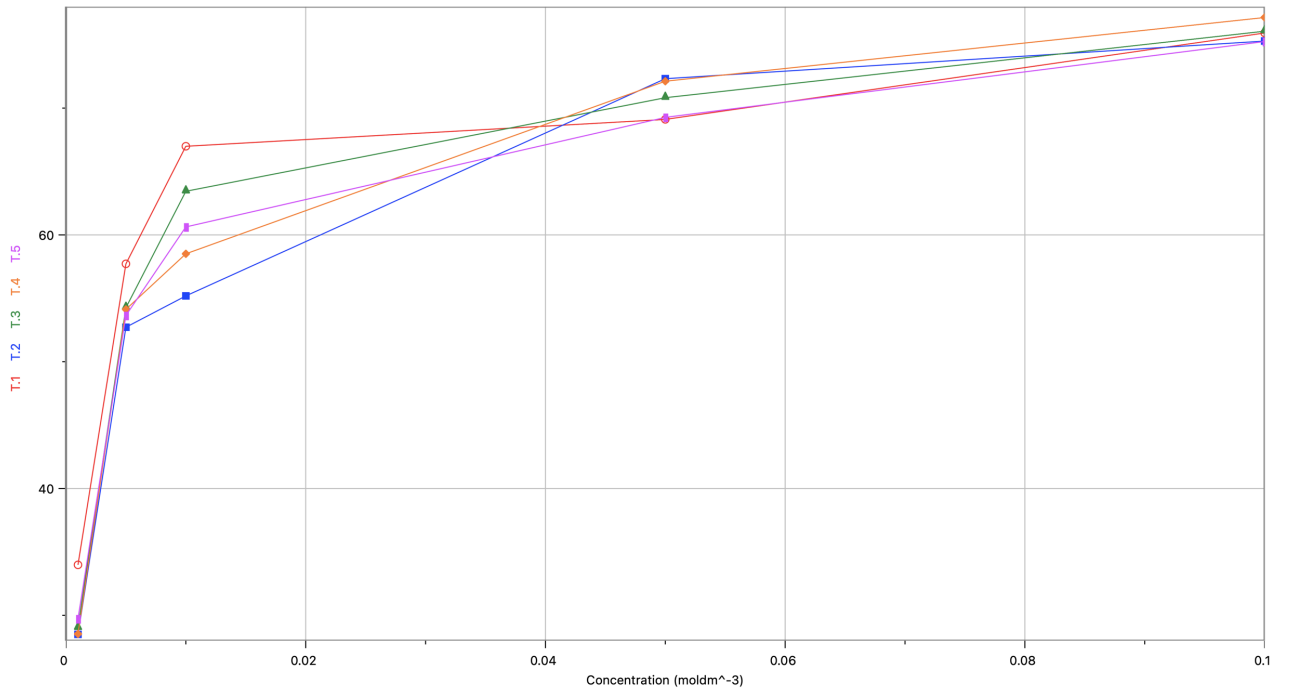


Figure 8: Inhibition Efficiency of Caffeine at 30°C.

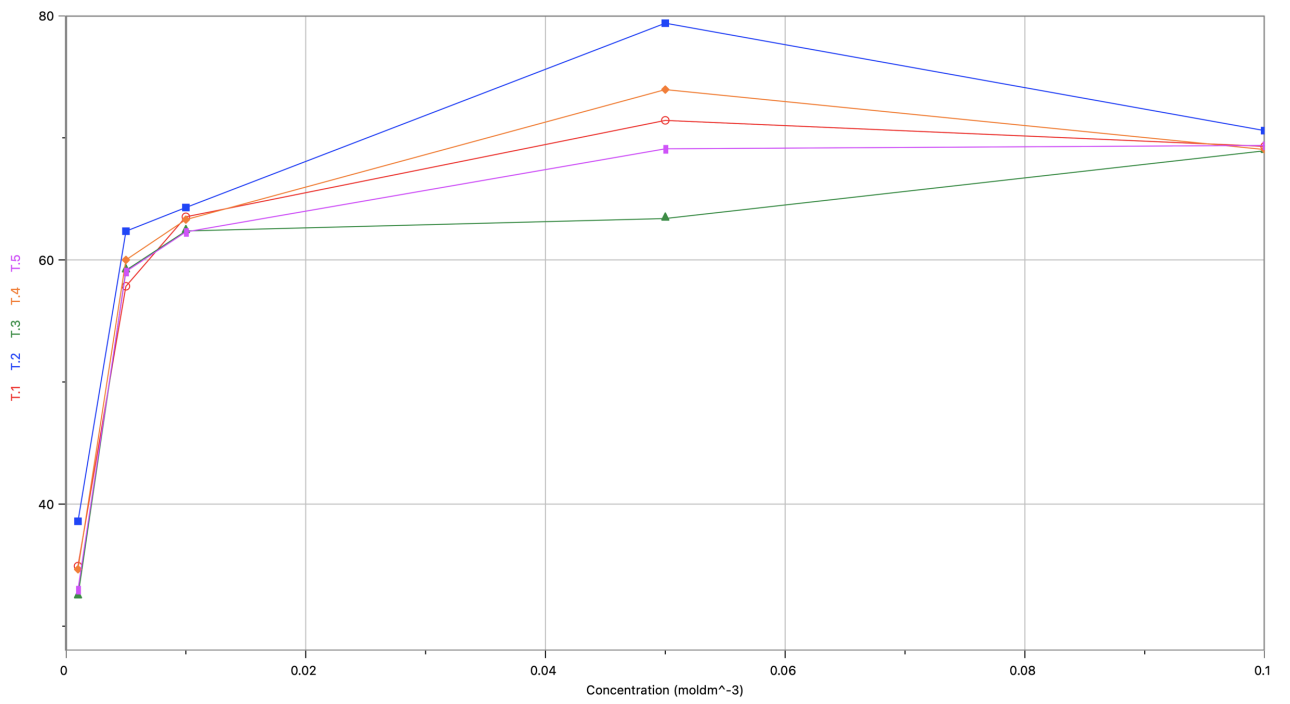


Figure 9: Inhibition Efficiency of Caffeine at 50°C.

INVESTIGATION of the CORRELATION

The correlation between the inhibition efficiency and molarity of solutions is measured via

regression (R), which has the formula:
$$\frac{\Sigma(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\Sigma(x_i-\bar{x})^2\Sigma(y_i-\bar{y})^2}}$$
.

| VARIABLES | | | | | | |
|--|---------|----------------|-------|-------|-------|-------|
| X-Variables (Molarity) (mol ^{dm} ⁻³) | | 0.1 | 0.05 | 0.01 | 0.005 | 0.001 |
| Y-Variables (Inhibition Efficiency Percentages) (gh ⁻¹) | Trial.1 | 75.93 | 69.11 | 66.99 | 57.72 | 75.93 |
| | Trial.2 | 75.29 | 72.32 | 55.19 | 52.72 | 75.29 |
| | Trial.3 | 76.07 | 70.82 | 63.44 | 54.26 | 76.07 |
| | Trial.4 | 77.15 | 72.12 | 58.51 | 54.13 | 77.15 |
| | Trial.5 | 75.25 | 69.27 | 60.63 | 53.65 | 75.25 |
| Regression (R-coefficient) | Trial.1 | ≈ 0.711 | | | | |
| | Trial.2 | ≈ 0.810 | | | | |
| | Trial.3 | ≈ 0.747 | | | | |
| | Trial.4 | ≈ 0.798 | | | | |
| | Trial.5 | ≈ 0.776 | | | | |

Table 15: Regression values between Molarity of Solutions and Inhibition Efficiency of Caffeine in Trial.1, Trial.2 and Average, at 30°C.

| VARIABLES | | | | | | |
|--|---------|----------------|-------|-------|-------|-------|
| X-Variables (Molarity) (mol ^{dm} ⁻³) | | 0.1 | 0.05 | 0.01 | 0.005 | 0.001 |
| Y-Variables (Inhibition Efficiency Percentages) (gh ⁻¹) | Trial.1 | 69.3 | 71.43 | 63.53 | 57.84 | 69.3 |
| | Trial.2 | 70.59 | 79.39 | 64.29 | 62.35 | 70.59 |
| | Trial.3 | 68.94 | 63.39 | 62.37 | 59.15 | 68.94 |
| | Trial.4 | 69.04 | 73.95 | 63.3 | 60.00 | 69.04 |
| | Trial.5 | 69.38 | 69.1 | 62.29 | 59.05 | 69.38 |
| Regression (R-coefficient) | Trial.1 | ≈ 0.646 | | | | |
| | Trial.2 | ≈ 0.607 | | | | |
| | Trial.3 | ≈ 0.626 | | | | |
| | Trial.4 | ≈ 0.614 | | | | |
| | Trial.5 | ≈ 0.643 | | | | |

Table 16: Regression values between Molarity of Solutions and Inhibition Efficiency of Caffeine in Trial.1, Trial.2 and Average, at 50°C.

Calculated regression values signifying the correlation between inhibition efficiency and concentration of solution, are closer to 1 than it is to 0, indicating a positive relationship between the two variables.

| VARIABLES | | | | | | | |
|--|---------|----------|---------|---------|---------|-------------|---------|
| X-Variables (Molarity) (mol dm ⁻³) | 0.1 | 0.05 | 0.01 | 0.005 | 0.001 | 0 (absence) | |
| Y-Variables (Rate of Reaction) (gh ⁻¹) | Trial.1 | 0.00617 | 0.00792 | 0.00846 | 0.01083 | 0.01692 | 0.00617 |
| | Trial.2 | 0.00625 | 0.00700 | 0.01133 | 0.01196 | 0.01808 | 0.00625 |
| | Trial.3 | 0.00608 | 0.00742 | 0.00929 | 0.01163 | 0.01804 | 0.00608 |
| | Trial.4 | 0.00588 | 0.00717 | 0.01067 | 0.01179 | 0.01838 | 0.00588 |
| | Trial.5 | 0.00621 | 0.00771 | 0.00988 | 0.01163 | 0.01763 | 0.00621 |
| Regression (R-coefficient) | Trial.1 | ≈ -0.631 | | | | | |
| | Trial.2 | ≈ -0.721 | | | | | |
| | Trial.3 | ≈ -0.678 | | | | | |
| | Trial.4 | ≈ -0.713 | | | | | |
| | Trial.5 | ≈ -0.689 | | | | | |

Table 17: Regression values between Molarity of Solutions and Rate of Reaction in Trial.1, Trial.2 and Average, at 30°C.

| VARIABLES | | | | | | | |
|--|---------|----------|--------|--------|--------|-------------|--------|
| X-Variables (Molarity) (mol dm ⁻³) | 0.1 | 0.05 | 0.01 | 0.005 | 0.001 | 0 (absence) | |
| Y-Variables (Rate of Reaction) (gh ⁻¹) | Trial.1 | 0.0330 | 0.0308 | 0.0393 | 0.0454 | 0.0700 | 0.0330 |
| | Trial.2 | 0.0327 | 0.0229 | 0.0397 | 0.0419 | 0.0683 | 0.0327 |
| | Trial.3 | 0.0318 | 0.0374 | 0.0385 | 0.0418 | 0.0690 | 0.0318 |
| | Trial.4 | 0.0328 | 0.0276 | 0.0389 | 0.0424 | 0.0693 | 0.0328 |
| | Trial.5 | 0.0319 | 0.0322 | 0.0393 | 0.0426 | 0.0698 | 0.0319 |
| Regression (R-coefficient) | Trial.1 | ≈ -0.588 | | | | | |
| | Trial.2 | ≈ -0.566 | | | | | |
| | Trial.3 | ≈ -0.579 | | | | | |
| | Trial.4 | ≈ -0.332 | | | | | |
| | Trial.5 | ≈ -0.590 | | | | | |

Table 18: Regression values between Molarity of Solutions and Rate of Reaction in Trial.1, Trial.2 and Average, at 50°C.

Calculated regression values signifying the correlation between reaction rate and concentration of solution, are closer to -1 than it is to 0, indicating a moderate negative relationship between the two variables.

QUALITATIVE OBSERVATIONS

Despite of the obtained quantitative results, several qualitative observations were made.

Initial observations were made in preliminary experiments. *Figure.10* below, shows the Zinc specimens that were held in HCl in *Preliminary Experiment.4* mentioned before. Greater deterioration was observed in Zn specimen that was held in HCl solution without caffeine content in it. This is due to the protective property of caffeine against corrosion.



Figure 10: Zn specimens waited inside HCl solutions with (Right) and without (Left) caffeine added.

It also was observed that the colours of the acid solutions, after metal specimens were immersed and kept waited in, vary with the caffeine concentration present inside the solutions. In solutions with higher concentrations of caffeine included, the colour of the solution remained approximately transparent whereas the lower the concentration of caffeine became, the darker the colour of acid turned out, as can be observed from *Figure.11*.

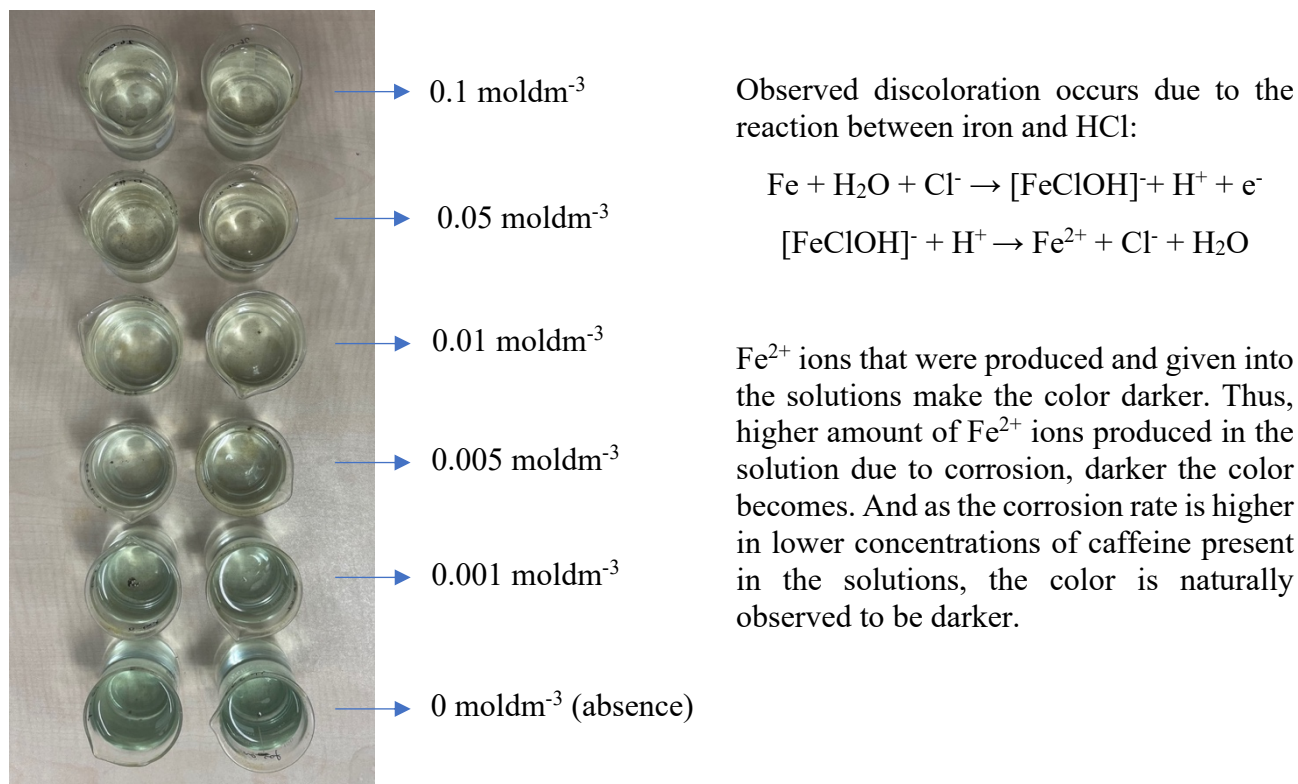


Figure 11: Acid solutions with different caffeine concentrations that metal specimens were immersed in at 50°C displaying the change of colour.

UNCERTAINTY / ERROR PROPAGATION

Uncertainty of Mass Loss

For each measured mass value, percentage uncertainty = $\frac{0.001}{mass} * 100$. Thus, for each calculated

$$mass\ loss\ value, \text{percentage uncertainty} = \frac{0.001+0.001}{mass} * 100 = \frac{0.002}{mass} * 100$$

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| no caffeine | 0.325 | 0.329 | 0.328 | 0.324 | 0.332 |
| 0.1 moldm ⁻³ | 1.35 | 1.33 | 1.37 | 1.42 | 1.34 |
| 0.05 moldm ⁻³ | 1.05 | 1.19 | 1.12 | 1.16 | 1.08 |
| 0.01 moldm ⁻³ | 0.985 | 0.735 | 0.897 | 0.781 | 0.844 |
| 0.005 moldm ⁻³ | 0.769 | 0.697 | 0.717 | 0.707 | 0.717 |
| 0.001 moldm ⁻³ | 0.493 | 0.461 | 0.462 | 0.454 | 0.473 |

Table 19: Percentage Uncertainty of Mass Loss due to Corrosion at 30°C.

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| no caffeine | 0.0774 | 0.0749 | 0.0815 | 0.0786 | 0.0801 |
| 0.1 moldm ⁻³ | 0.252 | 0.255 | 0.263 | 0.254 | 0.261 |
| 0.05 moldm ⁻³ | 0.271 | 0.364 | 0.223 | 0.302 | 0.259 |
| 0.01 moldm ⁻³ | 0.212 | 0.21 | 0.217 | 0.214 | 0.212 |
| 0.005 moldm ⁻³ | 0.184 | 0.199 | 0.2 | 0.197 | 0.196 |
| 0.001 moldm ⁻³ | 0.119 | 0.122 | 0.121 | 0.12 | 0.12 |

Table 20: Percentage Uncertainty of Mass Loss due to Corrosion at 50°C.

Uncertainty of Concentration

Uncertainty of 1000 cm³ Volumetric Flask = ± 0.3 cm³

From the equation: $c_1V_1 = c_2V_2 \rightarrow 12 \times V_1 = 1 \times 1000$

V_1 (volume of 12 moldm⁻³ to dilute HCl) = 83.3 cm³

This amount was measured by using 100 cm³ beaker with uncertainty value ± 0.5 cm³

$$\text{Overall percentage uncertainty} = \frac{0.5}{83.3} * 100 + \frac{0.3}{1000} * 100 = 0.6\%$$

Uncertainty of Time

Rate of reaction was calculated by referencing hours, as the duration was 24 hours and was too long to calculate in seconds. Expression of time is in following form:

00.00.00 (hours.minutes.seconds) Thus, the uncertainty of time during which the mass loss was calculated is equal to: $\frac{0.01}{24 \times 3600} = 1.15 \times 10^{-7}$

Uncertainty of Reaction Rate

Formula of reaction was: *(initial mass – final mass) / change of time (hours)*.

Uncertainty of reaction rate = $\frac{0.002}{\text{mass loss}} + 1.15 \times 10^{-7} + \frac{0.6}{100}$

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| no caffeine | 0.00925 | 0.00930 | 0.00928 | 0.00924 | 0.00932 |
| 0.1 moldm ⁻³ | 0.0195 | 0.0193 | 0.0197 | 0.0202 | 0.0194 |
| 0.05 moldm ⁻³ | 0.0165 | 0.0179 | 0.0172 | 0.0176 | 0.0168 |
| 0.01 moldm ⁻³ | 0.0159 | 0.0134 | 0.0150 | 0.0138 | 0.0144 |
| 0.005 moldm ⁻³ | 0.0137 | 0.0130 | 0.0132 | 0.0131 | 0.0132 |
| 0.001 moldm ⁻³ | 0.0109 | 0.0106 | 0.0106 | 0.0105 | 0.0107 |

Table 21: Percentage uncertainty of reaction rate at 30°C.

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| no caffeine | 0.00677 | 0.00675 | 0.00682 | 0.00679 | 0.00680 |
| 0.1 moldm ⁻³ | 0.00852 | 0.00855 | 0.00862 | 0.00854 | 0.00861 |
| 0.05 moldm ⁻³ | 0.00871 | 0.00964 | 0.00823 | 0.00902 | 0.00859 |
| 0.01 moldm ⁻³ | 0.00812 | 0.00810 | 0.00817 | 0.00814 | 0.00812 |
| 0.005 moldm ⁻³ | 0.00784 | 0.00799 | 0.00800 | 0.00796 | 0.00796 |
| 0.001 moldm ⁻³ | 0.00719 | 0.00722 | 0.00721 | 0.00720 | 0.00719 |

Table 22: Percentage uncertainty of reaction rate at 50°C.

Uncertainty of Inhibition Efficiency

Formula of inhibition efficiency was: $E_f = (R_i - R_0) / R_0 \times 100$

Thus, percentage uncertainty is: $\frac{\text{percentage uncertainty } R_i + \text{percentage uncertainty } R_0}{R_i - R_0}$

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| 0.1 moldm ⁻³ | 1.48 | 1.50 | 1.50 | 1.48 | 1.52 |
| 0.05 moldm ⁻³ | 1.46 | 1.49 | 1.47 | 1.45 | 1.50 |
| 0.01 moldm ⁻³ | 1.46 | 1.62 | 1.50 | 1.53 | 1.56 |
| 0.005 moldm ⁻³ | 1.55 | 1.67 | 1.63 | 1.60 | 1.67 |
| 0.001 moldm ⁻³ | 2.32 | 2.76 | 2.70 | 2.70 | 2.69 |

Table 23: Percentage uncertainty of Inhibition Efficiency of caffeine at 30°C.

| | Trial.1 | Trial.2 | Trial.3 | Trial.4 | Trial.5 |
|---------------------------|---------|---------|---------|---------|---------|
| 0.1 moldm ⁻³ | 0.205 | 0.195 | 0.219 | 0.209 | 0.213 |
| 0.05 moldm ⁻³ | 0.201 | 0.186 | 0.232 | 0.202 | 0.214 |
| 0.01 moldm ⁻³ | 0.218 | 0.208 | 0.235 | 0.222 | 0.230 |
| 0.005 moldm ⁻³ | 0.235 | 0.213 | 0.245 | 0.232 | 0.240 |
| 0.001 moldm ⁻³ | 0.372 | 0.326 | 0.423 | 0.381 | 0.408 |

Table 24: Percentage uncertainty of Inhibition Efficiency of caffeine at 50°C.

Standard Error

As standard error (SE) is calculated with the formula: $\frac{\sigma}{\sqrt{n}}$, where σ is standard deviation and n is the sample number; standard error values are as following. (Values are calculated by using Microsoft Excel.)

| | SE |
|---------------------------|----------|
| no caffeine | 1.13E-04 |
| 0.1 moldm ⁻³ | 6.64E-05 |
| 0.05 moldm ⁻³ | 1.69E-04 |
| 0.01 moldm ⁻³ | 5.04E-04 |
| 0.005 moldm ⁻³ | 1.93E-04 |
| 0.001 moldm ⁻³ | 2.53E-04 |

Table 25: Standard error of reaction rate at 30°C for each trial.

| | SE |
|---------------------------|----------|
| no caffeine | 1.54E-04 |
| 0.1 moldm ⁻³ | 2.63E-03 |
| 0.05 moldm ⁻³ | 2.41E-03 |
| 0.01 moldm ⁻³ | 2.07E-04 |
| 0.005 moldm ⁻³ | 6.62E-04 |
| 0.001 moldm ⁻³ | 3.03E-04 |

Table 26: Standard error of reaction rate at 50°C for each trial.

| | SE |
|---------------------------|-------|
| 0.1 moldm ⁻³ | 0.345 |
| 0.05 moldm ⁻³ | 0.680 |
| 0.01 moldm ⁻³ | 2.02 |
| 0.005 moldm ⁻³ | 0.851 |
| 0.001 moldm ⁻³ | 1.03 |

Table 27: Standard error of inhibition efficiency at 30°C for each trial.

| | SE |
|---------------------------|-------|
| 0.1 moldm ⁻³ | 0.297 |
| 0.05 moldm ⁻³ | 2.64 |
| 0.01 moldm ⁻³ | 0.375 |
| 0.005 moldm ⁻³ | 0.751 |
| 0.001 moldm ⁻³ | 1.08 |

Table 28: Table 27: Standard error of inhibition efficiency at 50°C for each trial.

Absolute Uncertainty

By calculating absolute uncertainty, the reason of error can be estimated. Formula for absolute uncertainty is:
$$\frac{\text{maximum value in sample} - \text{minimum value in sample}}{2}$$

| | absence | 0.1 mol dm^{-3} | 0.05 mol dm^{-3} | 0.01 mol dm^{-3} | 0.005 mol dm^{-3} | 0.001 mol dm^{-3} |
|----------------------------------|----------|-----------------------------|------------------------------|------------------------------|-------------------------------|-------------------------------|
| Rate of reaction at 30°C | 3.13E-04 | 1.88E-04 | 4.58E-04 | 1.44E-03 | 5.63E-04 | 7.29E-04 |
| Rate of reaction at 50°C | 4.50E-03 | 6.46E-04 | 7.25E-03 | 6.25E-04 | 1.81E-03 | 8.75E-04 |
| Inhibition efficiency at 30°C | - | 0.949 | 1.609 | 5.901 | 2.503 | 2.741 |
| Inhibition efficiency at 50°C | - | 0.826 | 8.001 | 1.002 | 2.253 | 3.071 |

Table 29: Absolute uncertainty values for reaction rate and inhibition efficiency at 30°C and 50°C.

CONCLUSION

The research subject for this essay was “An investigation on the inhibitory effect of different concentrations (0, 0.1 mol dm^{-3} , 0.05 mol dm^{-3} , 0.01 mol dm^{-3} , 0.005 mol dm^{-3} , 0.001 mol dm^{-3}) of caffeine solutions prepared with pure caffeine (C₈H₁₀N₄O₂) and 1mol dm^{-3} hydrochloric acid (HCl) on the corrosion of carbon steel (ST 37), measured by mass loss, observed in 30°C and 50°C environment.” Based on the data and the results obtained as a result of the given experiment and a deep literature research on this area, caffeine was expected to decrease the corrosion rate of metal surfaces, by creating cathodic adsorption. In conclusion, as can be observed from *Table.13 and Table.14*, inhibition efficiency of caffeine increased with the increasing concentration, which supported my initial hypothesis.

The relationship between different concentrations of caffeine in caffeine-HCl solutions and inhibition efficiency observed in 30°C and 50°C were previously given in *Tables 15&16* and the correlation between different concentrations of caffeine in caffeine-HCl solutions and the rate of reactions for the two given temperatures were given in *Tables 17&18*. Overall, a positive

and relatively strong relationship is observed between the variables, depending on the regression coefficients calculated which was used as the statistical method.

Limitations & Strengths Assessment

It was stated that several preliminary trials were had to be done before reaching to the functioning method. Some of the reasons why preliminary experiments failed were impurity of caffeine and possible side reactions occurred; improper choice of metal (e.g., Aluminium's capability to form a stable oxide layer, which prevents its possible corrosion and disable caffeine to adsorb onto the surface) and acids (e.g., H₂SO₄ usage caused SO₂ gas to be produced which was harmful and the reaction occurred very slow, thus no observation could be made) changed the reaction dynamics; insufficient sanding of metal surfaces preventing caffeine to adsorb onto the surface and inhibit corrosion. However, the optimum and functioning method was provided once obstacles were eliminated, and several improvements and alterations were made, and repetition of the experiment made the results credible.

Weaknesses concerning the experimental procedure were originating from the difficulties of standardising the materialistic and environmental conditions which created an obstacle in front of reaching to expected results. Furthermore, the corrosion and the inhibition of caffeine were only measured with mass loss and supported with existing information in literature, rather than making closer observation on the adsorption of caffeine with advanced equipment, which limited the extent of knowledge that can be reached to and weakened the thesis.

In order to strengthen the experiment and carry it out in the most efficient way given variables were intentionally chosen due to specific reasons. Reason given concentration values and temperature of environments were selected was to provide the optimum environmental conditions caffeine shows its impact in. Research and experimentation concerning this subject in literature showed that solubility of caffeine at approximately 30°C in 100 grams of water is

2.2 grams, approximately $10^{-2} \text{ moldm}^{-3}$. This is due to its heterocyclic structure and its hydrophobic characteristics. Therefore, the concentration that caffeine is most dissolved and creates the optimum adsorption is $10^{-2} \text{ moldm}^{-3}$ with temperature 30°C .

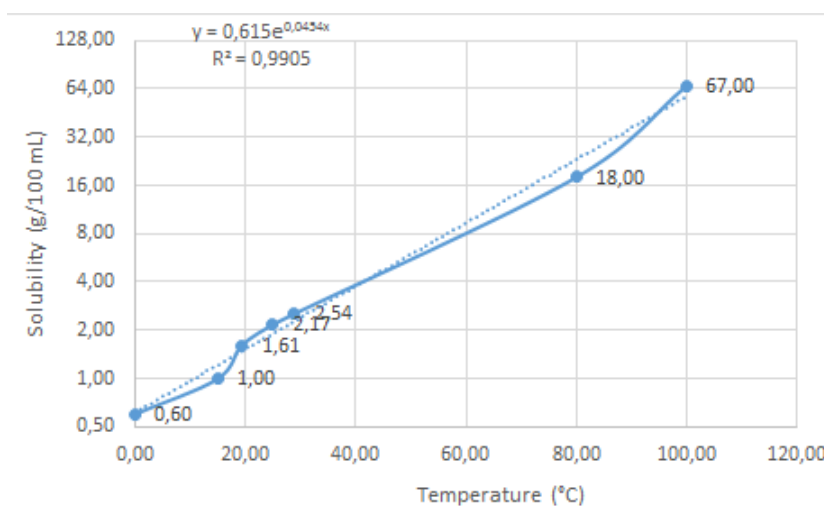


Figure 12: Caffeine solubility at different temperatures.

The range of temperature and concentration is determined accordingly.

Percentage uncertainty, absolute uncertainty and standard error was calculated for raw and processed data. It is known that if standard error of a sample is greater than the absolute uncertainty, this would indicate the presence of systematic error; whereas, if standard error is smaller than absolute uncertainty, this would indicate presence of random error. When compared, absolute uncertainty values are higher than standard error; showing that experiment is highly affected by random error.

The random error may have occurred due to parallax error during the preparation of solutions. Minimalistic alterations of measured mass may have caused error to occur as the measurements were made at milligram level, which is very precise and small. Even a smallest breeze may have caused values to be read different. Additionally, oversight and inattention may be a source of random error that took place.

Further Investigation & Extension

Preliminary experiments have shown that standardization of all materials was critical. Thus, sufficient and equal sanding, precise measurement with a single apparatus, impurity of materials and all other experimental components should be considered accordingly through the procedure for the further investigation.

As for extension concerning the experiment, expanding of the research area could be provided by using different metals to be investigated and observe whether the inhibitory impact of caffeine is variable depending on the metal surfaces. Organic compounds other than caffeine can be used with a single chosen metal and acidic environment and the inhibitory effect of these compounds can be observed and compared. Additionally, the difference in the colour of used acid solutions, which was previously mentioned in the qualitative observations section, can be measured spectrophotometrically, and expressed quantitatively.