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### Research Article

## Utilizing python for potentiometric redox titrations: A study on ferrous ion detection with potassium permanganate

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### Abstract

Instrumental chemical analysis offers a powerful approach for qualitative and quantitative methods estimating various parameters. An open-source programming language is used to automate potentiometric redox titrations. Modern methods are preferred over conventional methods as they are useful in identifying linear dynamical systems and they also have low computational complexity leading to accurate results. Potentiometric redox titrations are powerful analytical chemistry tools for quantifying the concentration of analytes based on their redox properties, and they find widespread use in various industries, including environmental monitoring, pharmaceuticals, and chemical process control. The aim of this work is to integrate instrumental chemical analysis with artificial intelligence. Artificial Intelligence in potentiometric titrations can further encourage innovations in the field of industry. The purpose of this study is to develop and implement a Python-based approach for automating potentiometric redox titrations, specifically focusing on ferrous ion detection using potassium permanganate as the titrant. By integrating Python with instrumental chemical analysis, the study aims to enhance the precision, efficiency, and accessibility of potentiometric titrations in analytical chemistry. Python is used effectively to simulate and analyse such titrations. NumPy for numerical operations, Matplotlib is used in plotting; the results were comparable with regular instrumental analysis and obtained satisfactory report.

### Keywords

programming language, potentiometric redox titrations, Artificial intelligence, Python, simulate, NumPy, Matplotlib

### Abbreviations

AI – artificial intellect; FAS – ferrous ammonium sulphate; EMF – electromotive force; SCE – saturated calomel electrode;

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## Introduction

Potentiometric titrations are analytical techniques which are based on measuring changes in electrode potential during a redox reaction (Szabadváry et al. 2016). These titrations typically depend on pH electrode or redox electrode to determine the equivalence point (Burns et al. 2014).

Nernst equation is the principle behind potentiometric redox titrations. The equation gives the relationship between the measured electrode potential to the concentrations or activities of the oxidizing and reducing species involved in the titration. As the titrant is added to the analyte solution, the electrode potential changes until it reaches a maximum or minimum value indication end point or equivalence point of the reaction (Compton and Sanders 1996).

Potentiometry is used when titrimetric methods, such as acid-base and redox titrations, require a measurement of a cell's EMF. The apparatus utilized includes a potentiometer (a device for measuring potential), a reference electrode, and an indicator electrode.

The reference electrode has a fixed half-cell potential and is not affected by the solution being analysed. In potentiometric titrations, the saturated calomel electrode is commonly employed as the reference electrode. In addition to the reference electrode, a working electrode or indicator is utilized to detect variations in the concentration of the solution (Skoog et al. 1998).

During cell construction, reference electrodes, indicator electrodes, and the test solution are combined. This cell is then titrated against a standard solution. A graph is drawn to depict the varying cell potentials as the titration process proceeds. The endpoint of the titration is determined from this graph, allowing for the calculation of the concentration of the test solution.

The present study is likely to explore the application of Python programming in analysing potentiometric redox titrations, specifically for detecting ferrous ions using potassium permanganate as the titrant. By employing Python, the study may aim to enhance the precision and efficiency of potentiometric titrations, replacing traditional manual methods of endpoint detection and offering automated data analysis. The work can

serve as an educational resource, showing how modern computational tools like Python can complement traditional laboratory techniques, enhancing both the learning experience and the practical application of potentiometric titration methods in fields such as chemistry, environmental analysis, and quality control.

## Materials and Methods

### Potentiometric titrations - $\text{Fe}^{2+}$ against standard $\text{KMnO}_4$ .

**Principle.** The saturated calomel electrode is the reference electrode utilized in this setup. In order to install it, mercury metal is coated with a mixture of  $\text{Hg} + \text{Hg}_2\text{Cl}_2 \downarrow$ , followed by a saturated solution of  $\text{KCl}$ , and then connected by a platinum wire. The electrode's reduction potential is recorded at 0.242V. In this system, the saturated calomel electrode operates as the Anode.

Platinum electrodes, also known as indicator electrodes, respond quickly to oxidation and reduction reactions and sense potential by detecting the ratio of reactants to products. Ferrous-Ferric couple serves as cathode in this case, with Pt electrode attached to it as described by (Harvey et al. 2019).

Cell representation

$(-)\text{Pt}, \text{Hg}(1), \text{Hg}_2\text{Cl}_2(\text{s}), \text{KCl}(\text{sat.}) / \text{Fe}^{3+}, \text{Fe}^{2+}, \text{Pt}(+)$

Cell reactions

Anode:  $2 \text{Hg} + 2 \text{Cl}^- \rightarrow \text{Hg}_2\text{Cl}_2 + 2 \text{e}^-$

Cathode:  $2 \text{Fe}^{3+} + 2 \text{e}^- \rightarrow 2 \text{Fe}^{2+}$

Cell E.M.F:  $E_{\text{cell}} = E^\circ (\text{Fe}^{3+}/\text{Fe}^{2+}) + 2.303RT/F \times \log [\text{Fe}^{3+}] [\text{Fe}^{2+}] - E_{\text{SCE}}$

Figures 1 and 2 are generated according to cell potential measurements taken throughout the reaction. This titration endpoint is determined from these figures, enabling the calculation of the concentration as described by Hach Company (2014) and Svehla (1979).

**Requirements.** Potentiometer, platinum plate electrode, saturated calomel electrode, beakers, Burette (100mL), Pipette (20mL), Stirrer and Salt Bridge.

**Chemicals.** i) Ferrous ammonium sulphate (~N/80) Test solution; ii) Potassium permanganate (~N/40) solution.

## Methods

**Part A. Preparation of standard ferrous ammonium sulphate solution.** Accurately weigh Mohr salt (FAS) in a pristine weighing bottle and transfer it into a pristine 100 mL standard flask using a funnel. Next, dissolve it in approximately 1/2 test tube (around 10 mL) of dilute  $\text{H}_2\text{SO}_4$  to prevent hydrolysis. Ultimately, complete the solution by adding distilled water until it reaches the designated mark as described by (Svehla 1979). The solution is vigorously agitated to ensure its uniformity. The normality of the standard solution is determined based on the weight of FAS.

**Part B. Standardization of  $\text{KMnO}_4$  solution.** Transfer 20 mL of the standard FAS solution into a new conical flask using a pipette. Add around 10 mL (1/2 test tube) of diluted  $\text{H}_2\text{SO}_4$  (6N) to create an acidic environment. Slowly titrate the solution with  $\text{KMnO}_4$  from the burette until a pale pink colour appears and remains for at least a minute, indicating the end point. Record the titre value.

The repetition of the process continues until consistent titre values are achieved. The calculation of the normality of  $\text{KMnO}_4$  is derived from the data obtained through titration as described by (Svehla 1979).

**Part C. Estimation of  $\text{Fe}^{2+}$  in the given test solution.** The  $\text{Fe}^{+2}$  test solution is prepared by adding distilled water until it reaches the desired volume and achieving homogeneity.

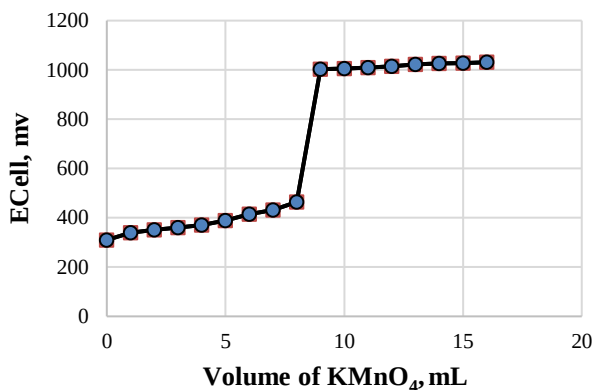
To establish a connection, attach the potentiometer to the A/C mains and activate it by switch on the instrument. Extract precisely 20 mL of the test solution using a pipette and transfer it into a pristine 100 mL beaker. Submerge the platinum electrode into the solution, resulting in the formation of a  $\text{Fe}^{2+}/\text{Fe}^{3+}$  couple. Finally, connect the electrode to the pH terminal.

A saturated calomel electrode is placed in a 100 mL beaker containing a saturated potassium chloride (KCl) solution. It is then linked to the R.E. terminal. The connection between the two solutions is established through a salt bridge to create the Galvanic cell (Anderson et al. 2020).

(-) Pt Hg (1),  $\text{Hg}_2 \text{Cl}_2(\text{s})$  KCl (sat)//  $\text{Fe}^{3+}, \text{Fe}^{2+}$  Pt (+)

Activate the device. Ensure that the current red switch is held down in the pressed position (mv

mode). The milli volt reading on the display indicates the electromotive force of the cell. Use the right side knob to adjust the initial EMF to the desired value.  $\text{KMnO}_4$  was introduced into the ferrous solution in 1 mL increments using a burette, followed by stirring, and the EMF was shown in Fig. 1.



**Figure 1.** Ecell vs Volume of  $\text{KMnO}_4$

Proceed with the titration until a noticeable shift in EMF is detected. Subsequently, document around 5 to 6 measurements following the alteration in 1 mL increments according to the method described by (Danilewicz et al. 2019; Rodrigues et al. 2018).

The estimated volume of  $\text{KMnO}_4$  needed is ascertained by conducting titrations. The titration process involves adding  $\text{KMnO}_4$  in increments of 0.1 mL near the end point (in 2 mL range) (Fig. 2).

A plot is created depicting the relationship between Ecell and the volume of  $\text{KMnO}_4$  added. The point of inflection on the graph provides an estimation of the approximate equivalence (Fig. 1) as per Whittemore et al. (1972).

## Results and Discussions

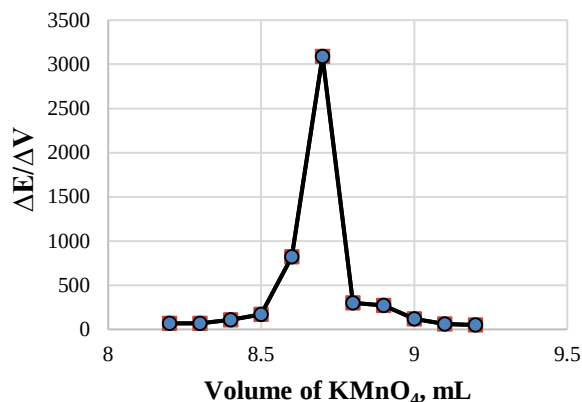
The differential graph is constructed by graphing the change in potential over the change in volume ( $\Delta E/\Delta V$ ) on the Y-axis against the volume of  $\text{KMnO}_4$  ( $v\text{KMnO}_4$ ) on the X-axis in order to observe a distinct peak, indicating the exact equivalence point of the titration as described by Fatibello-Filho et al. (2019) (Fig. 2).

**Results:** Amount of  $\text{Fe}^{2+}$  present in test sample.

**Part A.** Normality standard FAS. solution

Normality of FAS (N1) = 0.0122

**Part B.** Normality of  $\text{KMnO}_4$  solution ( $N_2$ ) =  $N_1V_1 = N_2V_2$



**Figure 2.**  $\Delta E/\Delta V$  vs Volume of  $\text{KMnO}_4$

Normality of  $\text{KMnO}_4$  solution = 0.024

```
def calculate_fe_weight (n_kmnO4 ,v_fe2):
```

```
# Equivalent weight of  $\text{Fe}^{2+}$ 
```

```
eq_weight_fe2 = 56
```

```
# Calculating normality of  $\text{Fe}^{2+}$ 
```

```
N_fe2 = (n_kmnO4*v_kmnO4)/v_fe2
```

```
# Calculating the weight of  $\text{Fe}^{2+}$ 
```

```
Weight_fe2 = n_fe2 * eq_weight_fe2
```

```
return weight_fe2
```

**Part C.** Normality of  $\text{Fe}^{2+}$  Test solution ( $N_3$ )

$N_2V_2 = N_3V_3$

Normality of  $\text{Fe}^{2+}$  Test solution = 0.01044

Weight of  $\text{Fe}^{2+}$  present in given test solution =  $0.01044 \times 56 = 0.585 \text{ gms/Lt}$

$N_{\text{fe2}} = (n_{\text{kmno4}} \times v_{\text{kmno4}}) / v_{\text{fe2}}$

**Python program designed to calculate the weight of  $\text{Fe}^{2+}$  ion in a solution.** This is Python program designed to calculate the weight of  $\text{Fe}^{2+}$  ion in a solution using titration data in accordance with the recommendations of QuantInsti the program takes user inputs for the normality and volume of  $\text{KMnO}_4$  used in the titration, as well as the volume of the  $\text{Fe}^{2+}$  solution (Krishnamoorthy et al. 2021). The code can be executed in Google Colab for ease of use and accessibility (Adawadkar et al. 2017). The Python code consists of a function to perform the calculation and a section for user input and output, as described by (Sodhi et al. 2019; Sundaradasu et al. 2013).

Here, the function **calculate\_fe\_weight** calculates the weight of  $\text{Fe}^{2+}$  based on the provided normality and volumes.

**Equivalent weight of  $\text{Fe}^{2+}$ :** The variable **eq\_weight\_fe2** is set to 56, representing the equivalent weight of  $\text{Fe}^{2+}$ .

**Normality of  $\text{Fe}^{2+}$ :** The normality (**n\_fe2**) of the  $\text{Fe}^{2+}$  solution is calculated using the formula.

**Weight of  $\text{Fe}^{2+}$ :** The weight of  $\text{Fe}^{2+}$  in the solution is calculated using the formula.

```
# Taking inputs from the user
```

```
N_kmnO4 = float (input ("Enter the normality of kmno4(N): "))
```

```
V_kmnO4 = float (input ("Enter the volume of kmno4used in titration (mL) : "))
```

```
V_fe2 = float (input ("Enter the volume of  $\text{Fe}^{2+}$  solution (mL) : "))
```

```
# Calculating the weight of  $\text{Fe}^{2+}$ 
```

```
Weight_fe2+ = calculate_fe_weight (n_kmnO4, V_kmnO4, V_fe2)
```

```
# Printing the result
```

```
print (f "The weight of  $\text{Fe}^{2+}$  in the solution is : {weight_fe2+:.3f}grams")
```

Here, the program prompts the user to input the normality and volume of  $\text{KMnO}_4$ , as well as the volume of the  $\text{Fe}^{2+}$  solution. It then calculates and prints the weight of  $\text{Fe}^{2+}$ . As described by Lambert (2019):

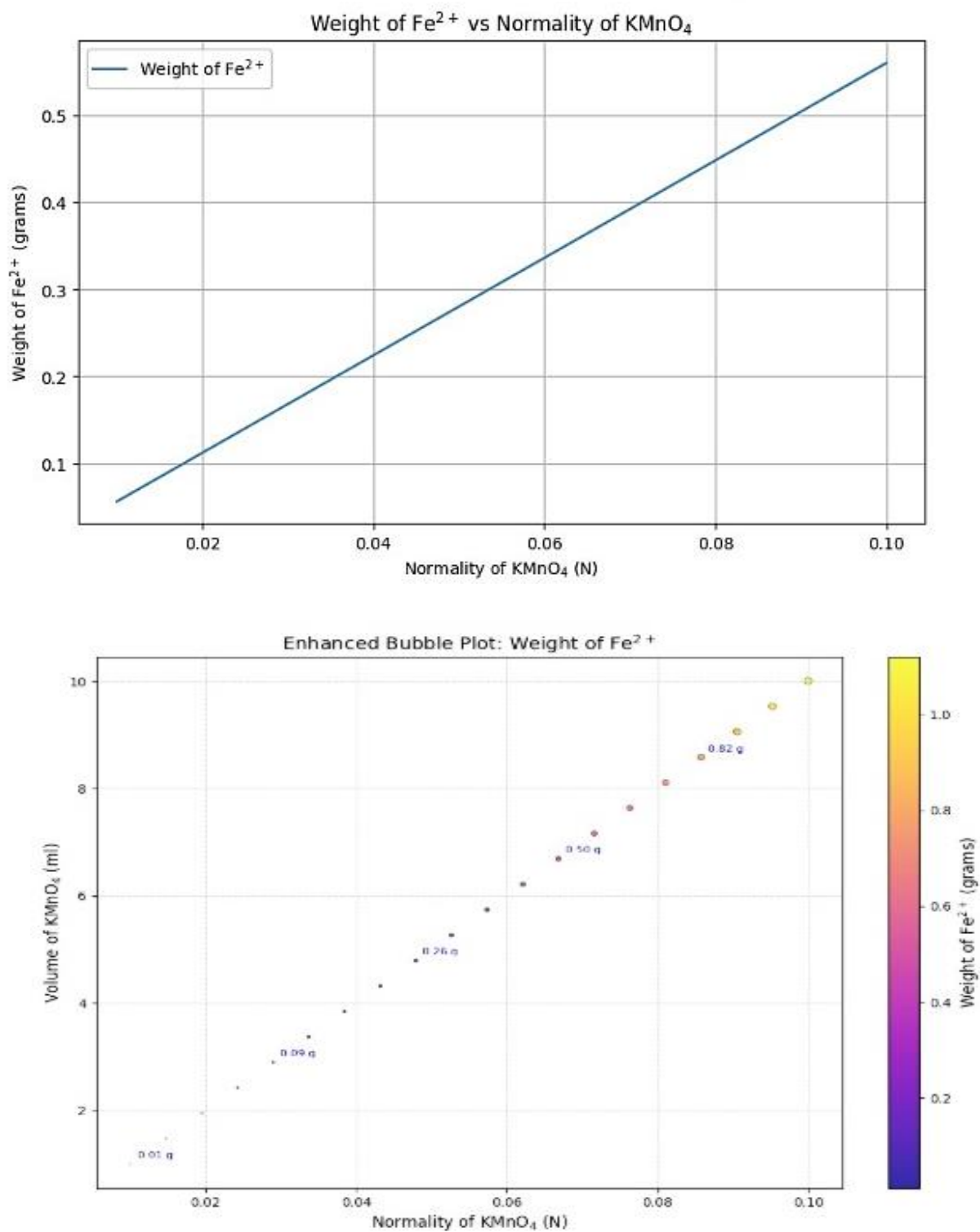
Enter the normality of  $\text{kmno}_4$  (N) : 0.024

Enter the volume of  $\text{kmno}_4$  used in titration (mL): 8.7

Enter the volume of  $\text{Fe}^{2+}$  solution (mL): 20

The weight of  $\text{Fe}^{2+}$  in the solution is: 0.585 grams

**Matplotlib for plotting and NumPy for data generation.** The Python code generates and plots graphs (Urban 2016) that show how the weight of  $\text{Fe}^{2+}$  ion in a solution varies with changes in three parameters: the normality of  $\text{KMnO}_4$ , the volume of  $\text{KMnO}_4$  used, and the volume of the  $\text{Fe}^{2+}$  solution. The code uses matplotlib for plotting and NumPy for data generation in accordance with the recommendations of Rougier (2023) and Harris et al. (2020).





**Observation:** The graph shows a linear relationship between the weight of  $\text{Fe}^{2+}$  and the normality of  $\text{KMnO}_4$ . As the normality of  $\text{KMnO}_4$  increases, the weight of  $\text{Fe}^{2+}$  also increases linearly.

**Implication:** This indicates that the amount of  $\text{Fe}^{2+}$  is directly proportional to the concentration of  $\text{KMnO}_4$  used in the titration. This makes sense because higher normality means more oxidizing power, leading to more  $\text{Fe}^{2+}$  being oxidized. The enhanced bubble plot, annotated heat map is customized to the gridlines for better visual structure and clarity.

**Observation:** This graph also shows a linear relationship between the weight of  $\text{Fe}^{2+}$  and the volume of  $\text{KMnO}_4$  used. As the volume of  $\text{KMnO}_4$  increases, the weight of  $\text{Fe}^{2+}$  increases proportionally.

**Implication:** The weight of  $\text{Fe}^{2+}$  is directly proportional to the volume of  $\text{KMnO}_4$  solution used. This is because increasing the volume of  $\text{KMnO}_4$  increases the number of moles of  $\text{KMnO}_4$

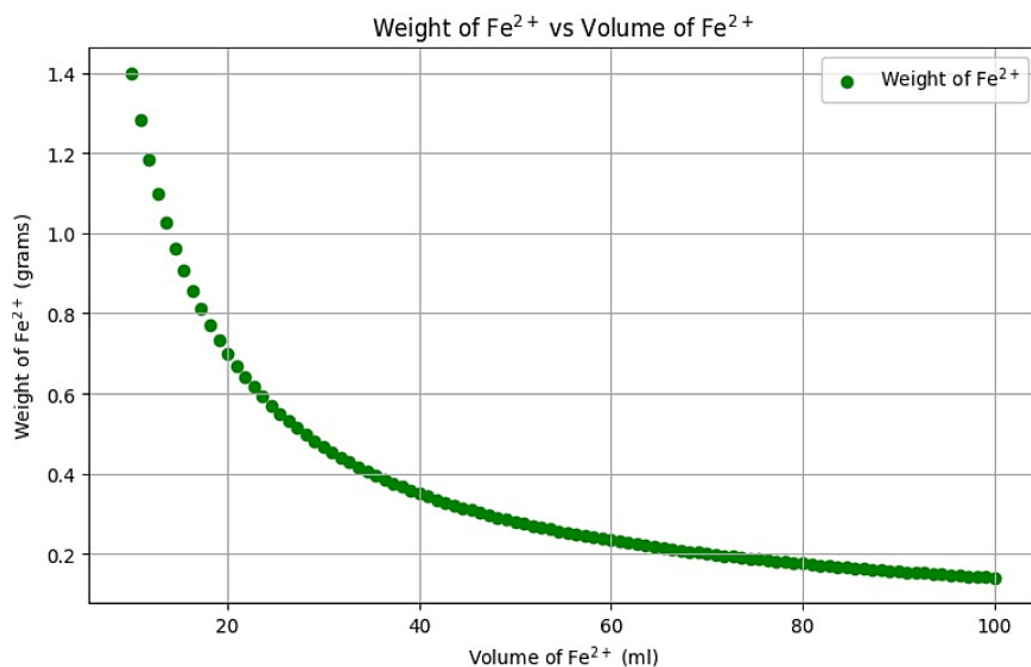
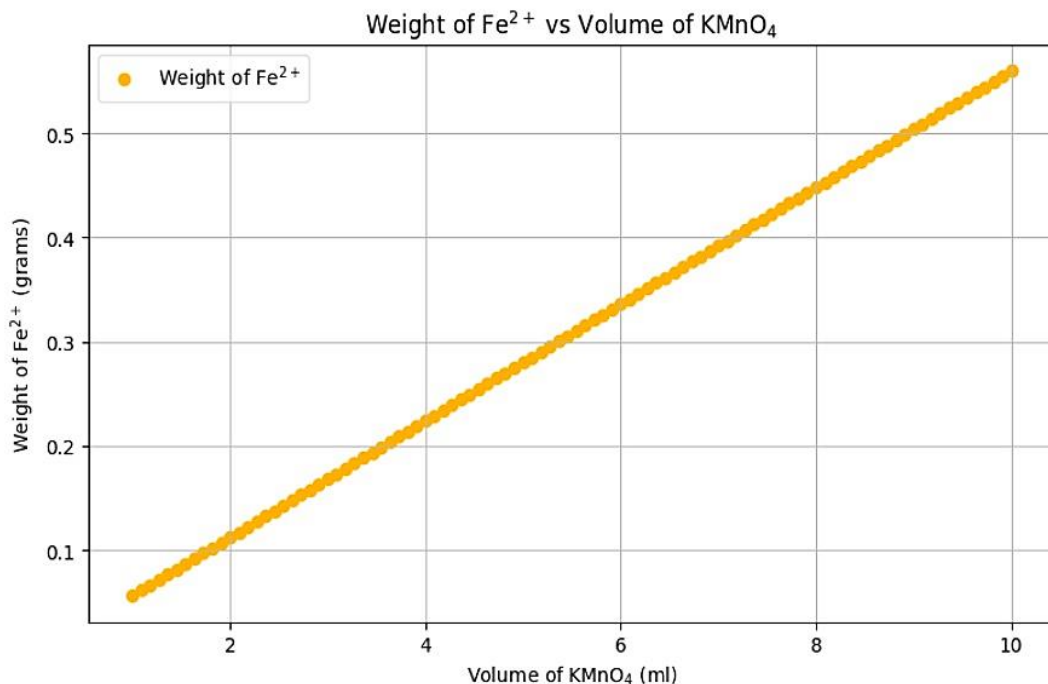
available to react with  $\text{Fe}^{2+}$ , thus increasing the amount of  $\text{Fe}^{2+}$  oxidized.

**Observation:** This graph shows an inverse relationship between the weight of  $\text{Fe}^{2+}$  and the volume of  $\text{Fe}^{2+}$  solution. As the volume of  $\text{Fe}^{2+}$  solution increases, the weight of  $\text{Fe}^{2+}$  decreases sharply at first and then levels off.

**Implication:** The weight of  $\text{Fe}^{2+}$  is inversely proportional to the volume of the  $\text{Fe}^{2+}$  solution. Initially, a small volume of  $\text{Fe}^{2+}$  solution means high concentration, leading to a high weight of  $\text{Fe}^{2+}$  being titrated. As the volume increases, the concentration of  $\text{Fe}^{2+}$  decreases, reducing the weight of  $\text{Fe}^{2+}$  titrated.

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# Define the calculation function
def calculate_fe_weight (n_kmno4, V_kmno4, V_fe2+):
    Eq_weight_fe2+ = 56
```



```
n_fe2+ = (n_kmnO4 * V_kmnO4) / V_fe2+
weight_fe2+ = n_fe2+ * eq_weight_fe2+
return weight_fe2+

# Generate data for 3D plot
n_kmnO4_values = np.linspace(0.01, 0.1, 50)
```

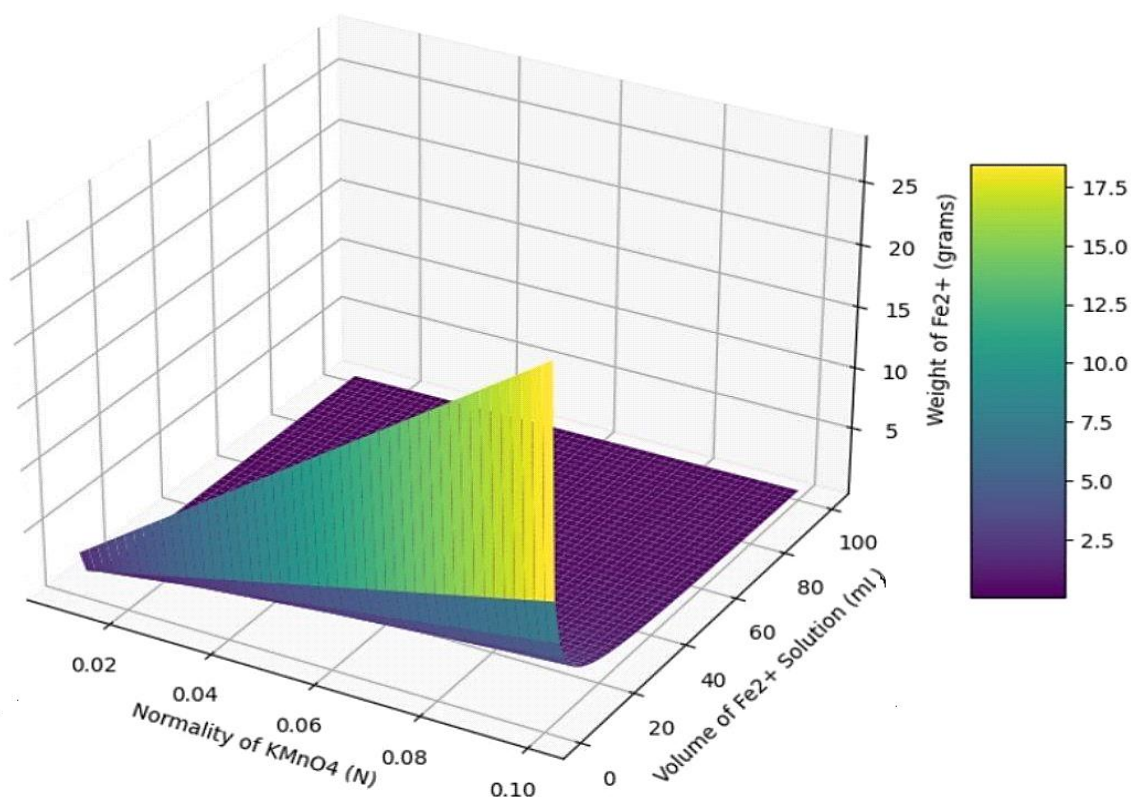
```
v_fe2+_values = np.linspace(1, 100, 50)
v_kmnO4_constant = 5 # mL

# Plotting the 3D surface plot
fig = plt.figure(figsize = (10, 8))
ax = fig.add_subplot(111, projection = '3d')
```

```
surface = ax.plot_surface (n_kmno4_grid, V_
fe2+_grid, weight_fe2+_grid,cmap = 'viridis')
ax. set_ x label ('Normality of kmno4(N)')
ax. set_ y label ('Volume of Fe2+ Solution (mL)')
ax. set_ z label ('Weight of Fe2+ (grams)')
```

```
ax. set_ title ('3D Surface Plot of Weight of Fe2+')
fig. colorbar (surface, ax=ax, shrink = 0.5, aspect
= 5)
plt.show ()
```

3D Surface Plot of Weight of Fe<sup>2+</sup>



## Conclusions

**Observation:** For low values of both the normality of KMnO<sub>4</sub> and the volume of Fe<sup>2+</sup> solution, the weight of Fe<sup>2+</sup> is minimal (around 2.5 grams).

As the normality of KMnO<sub>4</sub> increases (moving along the x-axis), the weight of Fe<sup>2+</sup> also increases.

Similarly, as the volume of the Fe<sup>2+</sup> solution increases (moving along the y-axis), the weight of Fe<sup>2+</sup> increases.

The highest weight of Fe<sup>2+</sup> (around 25 grams) is observed when both the normality of KMnO<sub>4</sub> and the volume of Fe<sup>2+</sup> solution are at their highest values.

The Python program effectively demonstrates the relationships between the normality of KMnO<sub>4</sub>, the volume of KMnO<sub>4</sub>, and the volume of the Fe<sup>2+</sup> solution in determining the weight of Fe<sup>2+</sup>. By visualizing these relationships through graphs, the program provides valuable insights into the stoichiometry of the titration process with the recommendations of [Johansson et al. \(2019\)](#) which can be useful for educational purposes and practical applications in analytical chemistry ([López et al. 2019](#)). In conclusion, the use of AI in conjunction with potentiometric redox titrations techniques is a revolutionary enhancement of contemporary analytical chemistry as it offers higher accuracy and

efficiency in the analytical processes and higher predictive potential. This collective cross-pollination is important for improving food science, biotechnology quality control, and innovation as a whole, leading to enhancement of product safety and consistency.

This study confirms that the code automates the calculation of the weight of  $\text{Fe}^{2+}$ , minimizing the risk of human error. It quickly computes the result, saving time compared to manual calculations. Available through Google Colab, the code can be accessed from any device with internet access, eliminating the need for local installation. The code helps students and professionals understand the relationship between normality, volume, and weight in titration experiments.

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