

Cloud Computing and Conduction of Electrochemical Titrations in Virtual Laboratory instead of Chemical Laboratory: Explanation by Potntiometric Titrations

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Abstract - University Education is nowadays conducted in Microsoft Teams, Google Meet, Zoom Cloud Meet and Cisco Webex Meet. Availability of Cloud Computing is useful for conduction of Electrochemical Titrations of Chemistry Laboratory in Virtual Laboratory. In this article, the explanation is provided by taking Potentiometric Titrations as examples. Advantages of virtual / online experimentations are unexpectedly high as price of Chemicals and apparatus are on the rise. As a result, online experiments are opted as beneficial complements to chemistry teaching. Virtual laboratory exercises for electrochemical titrations are examined in detail. Electrochemistry details measuring conductivity or electrode potential. There are a lot of electrochemical analytical titrations that are quite precise. Titrations based on conductometry and potentiometry are simple and accurate and are modeled easily into virtual laboratory exercises. In these titrations, the modeling of potentiometric titrations are not only providing readings and end points easily and minutely, but also wonderful graphs are produced simultaneously and the plots are dynamically provided in computer screen.

Index Terms - Cloud Computing, Titration, Colorimetry, Potentiometry, Virtual Laboratory, Chemical Laboratory.

I.INTRODUCTION

Online classes and laboratories are a growth and an advancement of our university education system. Student inflow to higher educational institutions and campus recruitment based job opportunities are huge in computer science and information technology courses in colleges and universities in India and Tamil Nadu. Online classes are easy to conduct in Computer and Internet based educational courses. Though

chemistry teaching is easy in online mode using power point slides and video demonstrations, its laboratory is more troublesome to carryout in online mode. But, some of the experiments can be done in online mode, ie, in virtual laboratory. For example, the quantitative analytical titrations can be conducted easily in online mode. Analytical laboratory with titrations are fundamental practical work in all chemistry courses and main part in engineering chemistry laboratory. So, its availability in online / virtual laboratory is very useful to chemists in recent times. Due to long Covid-19 Pandemic lockdown periods announced by both Indian and Tamil Nadu Governments, university chemistry is with long time online classes using Microsoft Teams, Google Meet, Zoom Cloud Meet or Cisco Webex Meet. Additionally, the high and unpredictable cost of Chemicals, Glasswares, Apparatus, Instruments and Equipments are on steep rise. So, virtual laboratory and online experimentations are advantageous additions to chemistry theory education [1-5].

In this article, analytical chemistry laboratory for engineering chemistry courses is analysed using virtual laboratory exercises for electrochemical titrations. Electrochemistry involves measurement of conduction of electric current (in terms of specific and molar conductivity), electrode and cell potential and p-values of acids and bases. Electrochemical analytical experiments are many and very accurate. Titrations based on conductometry and potentiometry are many and are very simple to conduct. These titrimetry is so important as industrial applications are many. In this paper, one typical titration is selected to analyze in detail the virtual laboratory concept. Indicator used in

titrimetry is replaced by conductance or potential in electrochemical titration. In these titrations, not only readings and end points are obtained easily and minutely, but also wonderful graphs are produced simultaneously and the plots are dynamically provided in computer screen. Figures 1 & 2 show the schematic of potentiometric titration and the plots used for analytical purpose.

End point in potentiometric titration is either the mid point of S-curve of E-V plot, or the peak value in the plot of $\Delta E/\Delta V$ versus V, or the mid point of wave in the plot of $\Delta^2 E/\Delta V^2$ versus V. Virtual Laboratory of Potentiometric Titration gives experimental set up, all three plots (E - V, $\Delta E/\Delta V - V$ and $\Delta^2 E/\Delta V^2 - V$), end point /equivalence point, colour change at equivalence point, and value of the unknown variable (mostly, concentration of the analyte) and dynamic and interactive results and plots [6-10].

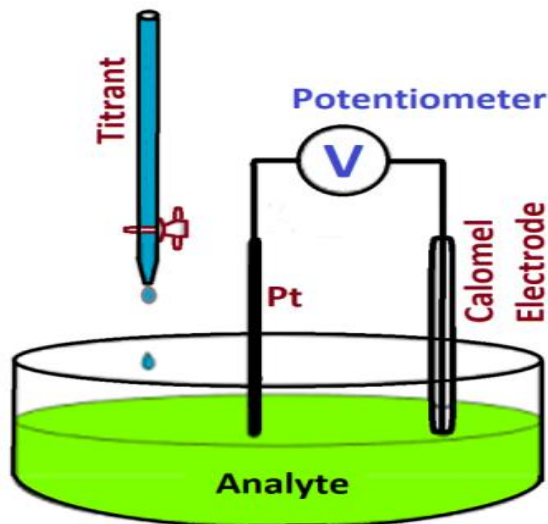


Figure 1: Potentiometry in Chemical Laboratory

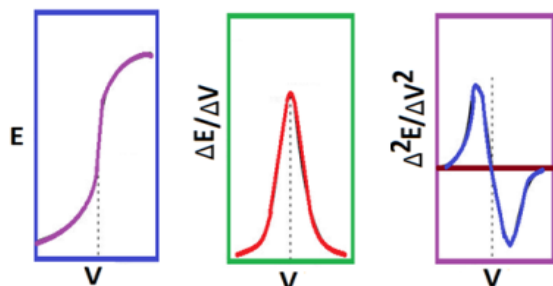


Figure 2: Potential & Derivatives X Titrant Volume

II. MATERIALS AND METHODS

In the beaker solution (see Figure 1), a known amount of analyte (ferrous ion solution, ie, a solution of

ferrous ammonium sulphate in water) is added. In the burette, the titrant solution of known concentration (either dichromate ion solution, ie, a solution of potassium dichromate in water, or ceric ion solution, ie, a solution of ceric sulphate in water) is taken. Indicator for this titration is cell potential of cell formed between the beaker solution with immersed platinum rod, and a saturated calomel electrode. Cell potential measurement is possible using multimeter, voltmeter and potentiometer [8-10]. In general, potentiometer is suitable for measuring accurately the potential during chemical titrations (see Figure 1).

In computational method of titrating the above solutions, the types of analyte ions and their concentration, the titrant ions and their added volume to analyte solution are followed mathematically. In potential manipulation, the Nernst equation is used to calculate the cell potential of an electrochemical cell at any given temperature, pressure, and reactant concentration. For example, electrode potential (E) of ferrous ions in ferrous ammonium sulphate of molar concentration $[Fe^{2+}]$ is equated to standard electrode potential (E°) and reaction temperature (Equation 1).

$$\text{For } M^{m+} + ne^- \rightarrow M^{(m-n)+}, E = E^\circ - \frac{RT}{nF} \ln \frac{[M^{(m-n)+}]}{[M^{m+}]} \quad (1)$$

where $Fe^{2+}=M^{(m-n)+}$, $Fe^{3+}=M^{m+}$, $m=3$ and $n=1$. Potential is measured for various volumes of titrant (dichromate ions or ceric ions) added to analyte containing beaker. In this process, the cell potential is followed for different volumes of titrant added or different concentrations of ferrous ions that got diluted by titrant additions. Plots are generated as per Figure 2, either all 3 plots, or 1&2 or only 1 is used for complete data analytics. Manipulation scheme for Titration I - Fe(II) versus Cr(VI) is adding a volume of dichromate ion to the solution of ferrous ion at an unknown initial concentration for the reaction gives concentration change as given in Table 1. When $V < V_{eq}$, the potential depends on the couple Fe^{3+}/Fe^{2+} and it is given in Equation 2. When $V > V_{eq}$, the species $Cr_2O_7^{2-}$ determines the potential and is given by Equation 3. The potential change at the equivalence point could be used to determine the equilibrium volume V_{eq} so the unknown concentration of ferrous ion can be calculated using the relation $C_{Fe} = V_{eq} \cdot C_{Cr_2O_7^{2-}} / V_{Fe}$ in mol/L.

Table 1: Virtual Laboratory Manipulations - Fe(II) versus Cr(VI)

$6Fe^{2+} + Cr_2O_7^{2-} + 14H^+ \rightarrow 6Fe^{3+} + 2Cr^{3+} + 7H_2O$				
	Fe^{2+}	$Cr_2O_7^{2-}$	Fe^{3+}	Cr^{3+}
V=0	$V_{Fe}C_{Fe}$	0	0	0
$0 < V < V_{eq}$	$C_{Cr_2O_7^{2-}}(V_{eq} - V)$	0	$C_{Cr_2O_7^{2-}} \cdot V$	$C_{Cr_2O_7^{2-}} \cdot V$
V=V _{eq}	0	0	$C_{Cr_2O_7^{2-}} \cdot V_{eq}$	$C_{Cr_2O_7^{2-}} \cdot V_{eq}$
V>V _{eq}	0	$C_{Cr_2O_7^{2-}}(V - V_{eq})$	$C_{Cr_2O_7^{2-}} \cdot V_{eq}$	$C_{Cr_2O_7^{2-}} \cdot V_{eq}$

V_{Fe} - volume of the solution of ferrous ions (mL), C_{Fe} -unknown concentration of ferrous ion that we need to find (mol/L), $C_{Cr_2O_7^{2-}}$ -known concentration of dichromate ion (mol/L), V_{eq} -volume of dichromate ion used to reach equilibrium with ferrous ion

$$E = E_{Fe}^o + \frac{0.059}{1} \log_{10} \frac{[Fe^{3+}]}{[Fe^{2+}]} = E^o + \frac{0.059}{1} \log_{10} \frac{V}{V_{eq} - V} \quad (2)$$

$$E = E_{Cr_2O_7^{2-}}^o + \frac{0.059}{6} \log_{10} \frac{([Cr_2O_7^{2-}][H^+]^{14})^2}{[Cr^{3+}]}$$

$$= E^o + \frac{0.059}{6} \log_{10} \frac{V - V_{eq}}{V_{eq}} \quad (3)$$

Manipulation scheme for Titration II - Fe(II) versus Ce(IV) is adding a volume of ceric ion to the solution of ferrous ion at an unknown initial concentration for the reaction gives concentration change as given in Table 2. The following table also shows how to determine equivalence by colourimetry using the color of indicator, now the analyte solution colour. With the volume of ceric solution V (in mL) added to the solution of ferrous ion at the unknown initial solution of concentration C_{Fe} , we have the following results as per manipulation as given in Table 2. When $V < V_{eq}$, the concentration of the couple Ce^{4+}/Ce^{3+} is negligible, so the potential measured is that of the couple Fe^{3+}/Fe^{2+} and is given by Equation 4. When $V > V_{eq}$, the couple Ce^{4+}/Ce^{3+} determines the measured potential and is given by Equation 5. The change of the potential near the equivalence point can be used to determine the equilibrium volume V_{eq} . Then the unknown concentration can be calculated using $C_{Fe} = V_{eq}C_{Ce}/V_{Fe}$ in mol/L.

Table 2: Virtual Laboratory Manipulations - Fe(II) versus Ce(IV)

$Fe^{2+} + Ce^{4+} \rightarrow Fe^{3+} + Ce^{3+}$				
	Fe^{2+}	Ce^{4+}	Fe^{3+}	Ce^{3+}
V=0	$V_{Fe}C_{Fe}$	0	0	0
$0 < V < V_{eq}$	$C_{Ce}(V_{eq} - V)$	0	$C_{Ce}V$	$C_{Ce}V$
V=V _{eq}	0	0	$C_{Ce}V_{eq}$	$C_{Ce}V_{eq}$
V>V _{eq}	0	$C_{Ce}(V - V_{eq})$	$C_{Ce}V_{eq}$	$C_{Ce}V_{eq}$

V_{Fe} - volume of the solution of ferrpus ions (mL), C_{Fe} -unknown concentration of ferrous ion that we need to find

(mol/L), C_{Ce} -known concentration of ceric ion (mol/L), V_{eq} -volume of ceric ion used to reach equilibrium with ferrous ion

$$E = E_{Fe}^o + \frac{0.059}{1} \log_{10} \frac{[Fe^{3+}]}{[Fe^{2+}]} = E^o + \frac{0.059}{1} \log_{10} \frac{V}{V_{eq} - V} \quad (4)$$

$$E = E_{Ce}^o + \frac{0.059}{1} \log_{10} \frac{[Ce^{4+}]}{[Ce^{3+}]} = E^o + \frac{0.059}{1} \log_{10} \frac{V - V_{eq}}{V_{eq}} \quad (5)$$

As these titrations uses high level of computation and graphics, the results are displayed as dynamic plots. All variables (analyte concentration, analyte volume, titrant concentration, titrant volume, amount of acid and acid concentration) can be adjusted to get desired reading minutely and graphically [6,7].

III. RESULTS AND DISCUSSION

This article contains its brain nested over six important topics such as, cloud computing, chemistry cloud, online education, virtual laboratory, online titrations and virtual potentiometry. Cloud Computing, in general, is a set up of softwares, big data, computer storage, and work groups. It makes computing and related activities very fast and cheap [1]. Chemistry Cloud is an essential requirement for business and industrial growth. Because, there are more than 30,00,000 chemicals in the world today and above 1,000 are heavily bonded to our life-support. Formula, reactions, hazards, prices, etc associated with chemicals are really very big. Big data, private cloud, etc are essential to support chemists and industries [2,4]. Online Education in university scheme is organized due to two major reasons. University education is mainly a job-oriented computer science and information technology based. Now, online courses and teaching have spread to all courses due to Covid-19 Pandemic lockdown [3]. Virtual Laboratory, in short, is an alternate and the best chemical

laboratory. Computers and Internet replace the costly hazardous chemicals and fragile glass apparatus [5]. Online Titrations such as the alkalinity of water sample, hardness of water sample, dissolved oxygen in water sample and many other titrations are available free of cost in www.vlab.co.in. Virtual Potentiometry, as a classical example, is the potentiometric titration of Ferrous Ion solution by Dichromate solution, or the potentiometric and colourimetric titration of Ferrous Ion solution by Ceric Ion solution. These titrations and some other titrimetries are available free of cost in www.wolfram.com. Data, Graph and Calculation are modeled by using input data to various variables and using all equations discussed in “Materials and Methods” (Equations 1-5). Using Equation 1, electrode potential is calculated and saturated calomel is reference for cell formation. For calculation purpose, Table 3 shows the numerical values taken from internet database for a titration of ferrous ammonium sulphate, $\text{FeSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4$ against potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$), and for $\text{FeSO}_4 \cdot (\text{NH}_4)_2\text{SO}_4$ versus ceric sulphate (Ce_2SO_4). Virtual laboratory calculates electrode potential (E) values for various input titrant volumes (V_{titrant}) and plots the graph of E versus V_{titrant} . S curve middle point is end point (Figures 3-12). Internet database is very good for this virtual experiment.

Table 3: Electrode potential for selected ions

Electrode	E° (Volt)
$\text{Fe}^{3+}/\text{Fe}^{2+}$	+0.767
Calomel $\text{Hg}_2^{2+}/\text{Hg}$	+0.241
$\text{Ce}^{4+}/\text{Ce}^{3+}$	+1.7
Dichromate $\text{Cr}^{6+}/\text{Cr}^{3+}$	+1.33

Advent of virtual laboratory is essential for successfully teaching courses in online mode. As far as chemistry laboratory is concerned, virtual laboratory is cutting the cost associated with chemicals and apparatus. Risk associated with handling

hazardous chemicals is zero [8-10]. In virtual laboratory mode, potentiometric titration is explained in this research paper. Similarly, in internet, colourimetry, flame photometry, alkalinity of water, hardness of water, dissolved oxygen in water and EDTA titrations are available for free access (www.vlab.co.in).

Table 4 gives ranges / data for various variables for virtual potentiometry. For Titration I, ie, Fe(II) versus Cr(VI) or Potentiometric titration of ferrous ion against dichromate ion with $C_{\text{Fe}}=0.1\text{mol/L}$, $V_{\text{Fe}}=15\text{mL}$, $C_{\text{H}}=0.05\text{mol/L}$ and $C_{\text{Cr}}=0.1\text{mol/L}$. Figures 3-7 give plots for various extents of reaction / titration that are fixed at $V_{\text{Cr}}=5, 10, 15, 20 \& 30\text{mL}$. Similarly, for Titration I, ie, Fe(II) versus Ce(IV) or potentiometric titration of ferrous ion against ceric ion with $C_{\text{Fe}}=0.1\text{mol/L}$, $V_{\text{Fe}}=15\text{mL}$ and $C_{\text{Ce}}=0.1\text{mol/L}$. Figures 8-12 give plots for various extents of reaction / titration that are fixed at $V_{\text{Ce}}=5, 10, 15, 20 \& 30\text{mL}$. For making explanation easy for both Titrations I & II, analyte volume is taken as 15mL, analyte concentration as 0.1M, titrant concentration as 0.1M, example graphs are given for titrant volumes (extent of titration) of 5, 10, 15, 20, 30mL so that end point always appears at 15mL. Being the demonstration of virtual experimentation concepts via potentiometric titrations, the potential (E) versus volume of titration (V) is plotted for 5 different values of extent of the titration (Figures 3-7 for Titration I and Figures 8-12 for Titration II). Otherwise, Figures 7 & 12 are sufficient to explain Titrations I & II. As the virtual titrimetry is computer simulation, end point can be plotted apriori in the plot before data point reaches the end (equivalence point). Large green dot at the centre of E-V plot in Fe(II)-Cr(VI) titration and large red dot at the center of Fe(II)-Ce(IV) titration show end point of titrations.

Table 4: Virtual Laboratory for Potentiometric Titration Examples

Titration I-Fe ²⁺ versus Cr ⁶⁺			Titration II-Fe ²⁺ versus Ce ⁴⁺		
Variable	Data Range	For Example	Variable	Data Range	For Example
C_{Fe}	0.1-0.15 mol/L	0.1M	C_{Fe}	0.1-0.15 mol/L	0.1M
V_{Fe}	10-15 mL	15mL	V_{Fe}	10-15 mL	15mL
C_{H}	0.0001-0.1 mol/L	0.05M	C_{Ce}	0.1-0.15 mol/L	0.1M
C_{Cr}	0.1-0.15 mol/L	0.1M	V_{Ce}	0.1-30 mL	5,10,15,20,30
V_{Cr}	0.1-30 mL	5,10,15,20,30	End Point	Analyte Colour : Red→Green	

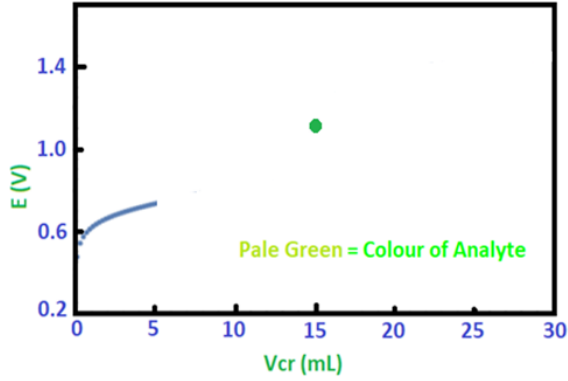


Figure 4: E versus Vcr (Extent of titration=5mL)

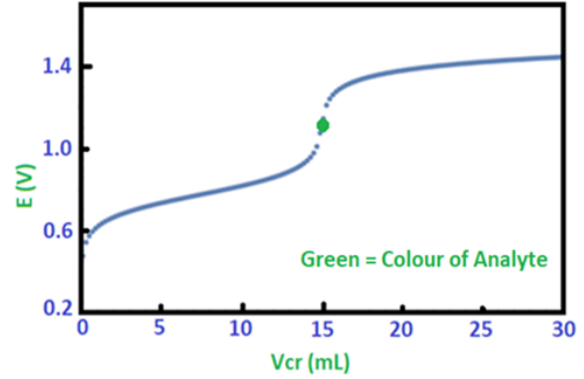


Figure 7: E versus Vcr (Extent of titration=30mL)

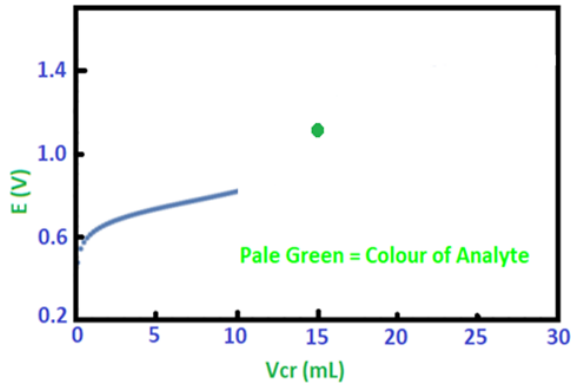


Figure 4: E versus Vcr (Extent of titration=10mL)

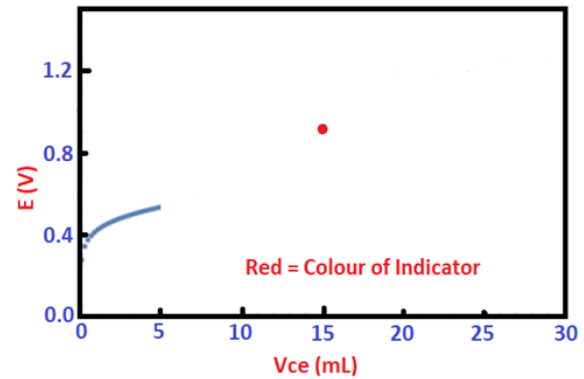


Figure 8: E versus Vce (Extent of titration=5mL)

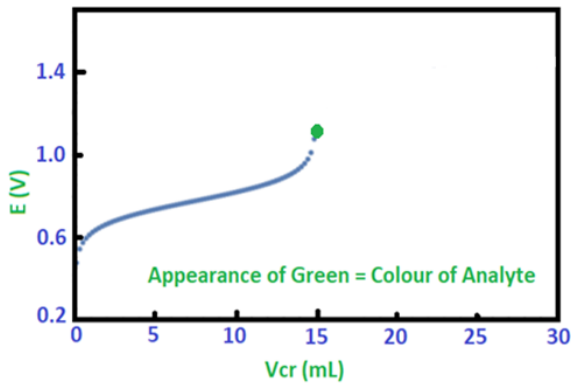


Figure 5: E versus Vcr (Extent of titration=15mL)

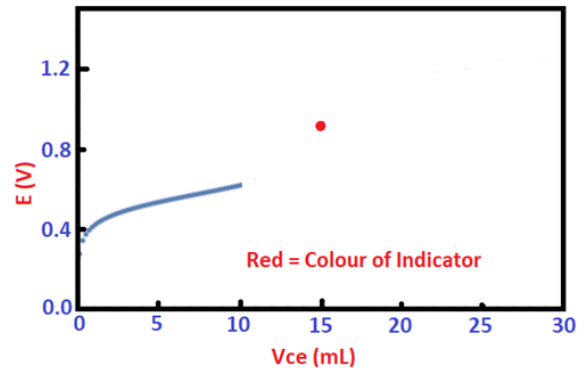


Figure 9: E versus Vce Extent of titration=10mL)

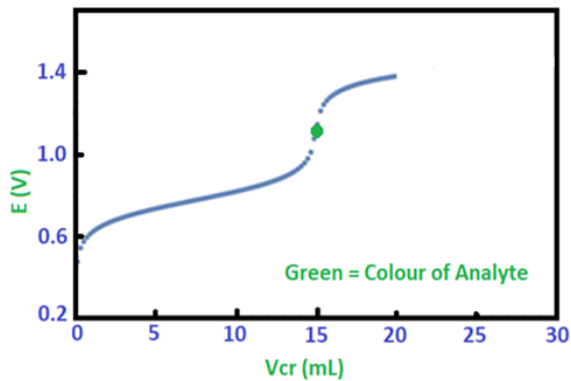


Figure 6: E versus Vcr (Extent of titration=20mL)

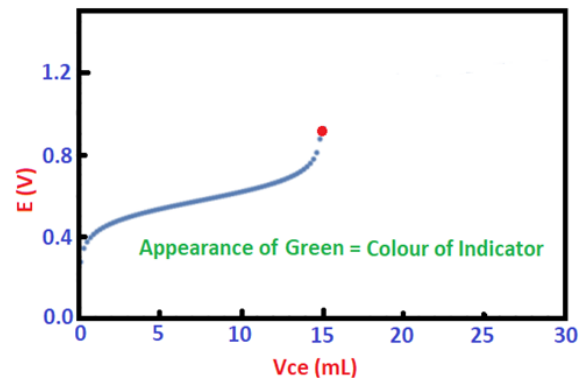


Figure 10: E versus Vce (Extent of titration=15mL)

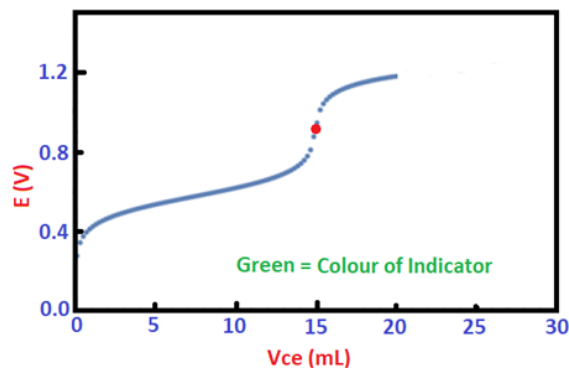


Figure 11: E versus V_{ce} (Extent of titration=20mL)

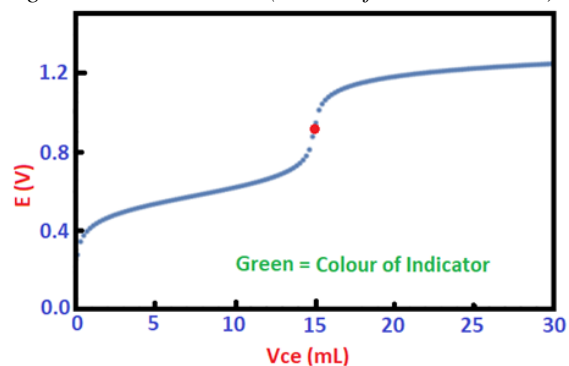


Figure 12: E versus V_{ce} (Extent of titration=30mL)

IV. CONCLUSION

Analytical laboratory containing titrations is a part of the chemistry practical exercises. Also, it is partially or fully essential for introducing virtual laboratory in recent years. In today's universities, online classes are taught using Microsoft Teams, Google Meet, Zoom Cloud Meet, or Cisco Webex Meet. In addition, prices of chemicals, glassware, apparatus, instruments and equipment are on the rise. Virtual laboratory is cutting fully cost associated with chemicals and apparatus. So, the advent of virtual laboratory is highly advantageous in this situation for teaching courses in online mode. In this article, a virtual laboratory exercise for electrochemical titrations is used to examine an analytical chemistry laboratory. Electrochemistry entails measuring electric current conduction (in terms of specific and molar conductivity), electrode and cell potential, and acid and base p-values. There are a lot of electrochemical analytical titrations that are quite precise. Modelling the conductometry and potentiometry and simulating the titrations are all easy to do and useful. Potentiometric titration is explained for the solutions of ferrous ammonium sulphate versus

potassium dichromate, and the solutions of ferrous ammonium sulphate versus ceric sulphate. These potentiometric titrations are freely available in the internet. There are many other titration experiments using virtual laboratory are freely available in internet.

REFERENCE

- [1] Jardim R R, Lemos E, Herpich F, Bianchim R, Medina R, Nunes F B. U-Lab Cloud : A Ubiquitous Virtual Laboratory Based on Cloud Computing. In: Proceedings of the 8th International Conference on Mobile Ubiquitous Computing, Systems, Services and Technologies, Rome, Italy, 2014
- [2] Kohlhoff K J, Shukla D, Lawrenz M, Bowman G R, Konerding D E, Belov D, Altman R B, Pande V S. 2014. Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. *Nature Chemistry*, Vol.6, pp.15-21, 2014
- [3] Dash S, Samadder S, Srivatsava A, Meena R, Ranjan P. Review of Online Teaching Platforms in the Current Period of COVID-19 Pandemic. *Indian Journal of Surgery*, 2021, <https://doi.org/10.1007/s12262-021-02962-4>
- [4] Xie C, Li C, Ding X, Jiang R, Sung S. Chemistry on the Cloud: From Wet Labs to Web Labs", *Journal of Chemical Education*, Vol.98, No., pp. 2840–2847, 2021
- [5] Pruthviraj U, Salian A B, Shetty S, Shetty A, Hegde A, Anand G, Rahul R K, Mantri S. Determination of hardness in water, National Institute of Technology, Surathkal, India, 2020, <http://vlabs.iitb.ac.in>
- [6] Culighin E. Potentiometric Titrations of Fe(II). Wolfram Research Incorporated, Illinois, USA, 2010, www.wolfram.com/knowledgebase
- [7] Trinh Q D. Potentiometric and Colorimetric Titration. Wolfram Research Incorporated, Illinois, USA, 2011, www.wolfram.com/knowledgebase
- [8] Vairam S, Suba R. Engineering Chemistry (Contents for Syllabus - Vel Tech Rangarajan Dr.Sagunthala R&D Institute of Science & Technology). Wiley India Private Limited, New Delhi, India, 2018

- [9] Skoog D A, Holler F J, Crouch S R. 2018, Principle of Instrumental Analysis. Cengage Learning & Brooks Cole, Belmont, USA
- [10] Mendham J, Denney R C, Barnes J D, Thomas M, Sivasankar B. Vogel's Textbook of Quantitative Chemical Analysis, Pearson Education, London, UK, 2009