Research on the Application of Computer Technology in Data Processing of University Chemical Experiment

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Abstract. University chemistry is a subject based on experimental verification, which is inseparable from instruments and data analysis. However, with the increasing complexity of university chemistry experiments, we need to use modern instruments for analysis, which can record experimental data more accurately. However, there are clear requirements for the processing of experimental data. With the different purposes of the experiment, we need different graphics and data analysis, which needs the help of computer technology. Through the computer technology, we can realize the automation of chemical experiment instrument operation, which can also automatically collect and transmit test data. Therefore, computer technology not only promotes the development of modern chemical instrument technology, but also improves the processing of university chemical experiment data. First of all, this paper analyzes the main application software technology. Then, this paper puts forward some examples for MATLAB and origin respectively.

Keywords: Computer Technology, University Chemistry Experiment, Data Processing

1. Introduction
With the change of the requirements of university chemistry experiment, the university chemistry basic education curriculum of college students will be reformed, which will pay more attention to the exploration of learning process [1]. The correct recording, processing, induction and analysis of experimental data is the basis of forming experimental report, which is the basic requirement of chemical experiment teaching [2-4]. The traditional experimental data processing method is still manual processing, which will have many problems. However, the data processing process of university chemistry experiment is often ignored, which is difficult to accurately complete the experimental data mining [5]. Through computer technology, we can better mine the principles hidden in the experimental data. Through computer software, we can avoid the tedious data processing process, which will improve the accuracy of data [6]. We can find that computer software has been used in chemical experiment data processing, which has abandoned the traditional manual drawing method. Through computer technology, we can reduce the burden of students' experimental data processing, which will more quickly complete the complex mathematical problems of experimental data [7].
2. Computer technology applied in data processing of university chemistry experiment
The data processing of university chemistry experiment can be carried out through a variety of computer technologies. This paper mainly introduces the following common experimental data processing software, as shown in Figure 1.

![Diagram of Excel, Matlab, and Origin Software](image_url)

**Figure 1.** Experimental data processing software.

2.1. Matlab software
Matlab is a commercial mathematical software developed by MathWorks in 1984. Matlab is based on advanced matrix language to process experimental data. Matlab can realize many functions, such as matrix operation, drawing function and data, realizing algorithm, creating user interface, connecting programming language program, etc., which can be applied in many fields, such as image processing, signal processing and communication, engineering calculation, financial modeling, University and so on. Matlab can write its own program, which can achieve data processing. The numerical calculation and drawing analysis of MATLAB are all realized by program language, which makes it easy to operate and the program is not complicated. The written program can be stored in the software and called repeatedly, which can directly call the original program to obtain data processing results. Matlab contains more than 600 kinds of functions, which can draw a variety of graphics, such as stereogram, three-dimensional rendering, animation and so on.

2.2. Origin Software
Origin is a professional drawing and data analysis software released by Originlab in 1992. It is easy to use and intuitive. Origin does not need to write program code, which can directly call the function for data analysis and drawing. Compared with the experimental results calculated by programming, origin can display more parameters in nonlinear fitting, which will make the fitting results more accurate. Origin's data analysis includes a variety of perfect mathematical analysis functions, such as data statistics, drawing graphics, curve fitting, signal processing and peak analysis. Origin's drawing function is based on the original template, which includes a large number of 2D and 3D drawing templates. Origin provides a variety of interfaces, which can easily connect with various databases.

2.3. Excel software
Excel has powerful function calculation function. Excel contains more than 300 functions, including text function, logic function, trigonometric function, logarithmic function, statistical function, search function, etc. We can process and analyze the data in most fields through various operations, such as data statistical summary, sorting and filtering, calculation and analysis, and searching at any time. Through the macro and visual basic custom function, we can meet the special requirements of customers. Excel software supports the call, edit, copy and paste of formula, which can perform advanced operation on the recorded data. Through mixed operation, Excel software improves the efficiency and accuracy of manual calculation. Although excel has powerful data analysis function, it
can be used as the basic unit of data processing. By making the basic unit into an electronic template, we can call out the corresponding template to complete the parameters of the experimental drawing.

### 3. Application of origin

#### 3.1. Data processing method

Through Excel, we can make the data processing template for the corrosion experiment of steel bars in concrete determined by the tow electrode method. In the corresponding position of the template, we can enter the original data of the first line. By activating the corresponding cells, we can get the original data spreadsheet, as shown in Table 1.

| Wire position | Day first | Day second | Day third | Day forth | Day Fifth | Day six | Day seven | Day eight | Day nine |
|---------------|-----------|------------|-----------|-----------|-----------|--------|-----------|-----------|---------|
| 3cm           | 0.27047   | 0.31193    | 0.3728    | 0.38493   | 0.40603   | 0.41177| 0.4465    | 0.4531    | 0.4701  |
| 5cm           | 0.14327   | 0.13937    | 0.16063   | 0.17153   | 0.22427   | 0.2141 | 0.26597   | 0.2446    | 0.2751  |
| 7cm           | 0.18033   | 0.1663     | 0.20473   | 0.21763   | 0.21297   | 0.19033| 0.21537   | 0.2103    | 0.2333  |

#### 3.2. Data processing results of origin experiment

To open origin, we can select Open excel in the file menu, which can open the table in the way of origin worksheet. At the same time, we can choose time t and self corrosion potential E to plot. By selecting layer contents, we can synthesize all the data, which will be drawn on the same graph, as shown in Figure 2.

![Figure 2](image_url)

**Figure 2.** The average potential of the wire is negative.

Through the powerful data analysis and tabulation function of Excel, we can make chemical experiment data processing template. Then, we can directly import the data needed for mapping into origin mapping, which is a simple, fast and accurate process. Through origin mapping, we can draw detailed and beautiful graphics. The processing of experimental data by origin not only stimulates students' enthusiasm for learning physical chemistry experiments, but also saves a lot of time. Through origin, we can cultivate students' ability to learn chemical experiments by means of modern technology.
4. Matlab software

4.1. Data processing method
In the potentiometric titration analysis of analytical chemistry, we need an accurate method to get the titration end point. Several groups of (E, V) data measured in the experiment are used to draw E-V curve, which requires the first derivative (Δ E / Δ V) value and second derivative (Δ 2E / Δ V2) value of e to V of each group to draw curve. Through the curve, we can better determine the titration end point. In traditional calculation, the inflection point of titration jump can be calculated by interpolation method, which will increase the corresponding volume of titrant. Traditional calculation requires manual drawing on coordinate paper with calculator, which generally takes 2-3 hours, which will lead to the accuracy of reading titration end point. Through the function "diff" of MATLAB software, we can get the differential of E and V, as shown in Table 2. Then, we can get the first derivative and the second derivative.

| V/ml     | 22.00 | 23.00 | 24.00 | 24.10 | 24.20 |
|----------|-------|-------|-------|-------|-------|
| E/V      | 0.1230| 0.1380| 0.1740| 0.1830| 0.1940|
| V/ml     | 24.30 | 24.40 | 24.50 | 24.60 | 25.00 |
| E/V      | 0.2330| 0.3160| 0.3400| 0.3510| 0.7500|

4.2. Matlab experimental data processing results
Through this program, we can draw three kinds of potentiometric titration curves, as shown in Figure 3. According to the line ratio, we can calculate the titration end point (VEP = 24.34ml) by interpolation.

5. Excel software

5.1. Data processing method
A group of experimental data is obtained through the demonstration experiment, and the experimental data is entered into the excel table, as shown in Table 3.
Table 3. Statistical table of experimental data for exploring the law of temperature change.

| NO. | Volume V / ml | Pressure P / PA | NO. | Volume V / ml | Pressure P / PA | NO. | Volume V / ml | Pressure P / PA |
|-----|---------------|-----------------|-----|---------------|-----------------|-----|---------------|-----------------|
| 1   | 20            | 75.2            | 6   | 15            | 100.8           | 11  | 10            | 149.8           |
| 2   | 19            | 79.2            | 7   | 14            | 107.8           | 12  | 9             | 166.4           |
| 3   | 18            | 83.8            | 8   | 13            | 116.4           | 13  | 8             | 188.4           |
| 4   | 17            | 88.4            | 9   | 12            | 126.4           | 14  | 7             | 212.2           |
| 5   | 16            | 94.4            | 10  | 11            | 137.2           | 15  | 6             | 245             |

5.2. Nonlinear fitting
According to the experimental data, the fitting result of power function is the best, as shown in Figure 4.

![Figure 4. Nonlinear fitting.](image)

6. Conclusion
Through computer technology, we can reduce the burden of students' experimental data processing, which will more quickly complete the complex mathematical problems of experimental data. Computer technology has greatly improved the efficiency of laboratory work, which provides a strong support for the development of chemistry.

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References
[1] Gong LiNbO, Wang Congling, Xie Yin, et al. Application of Origin Software in analytical chemistry teaching [J]. College chemistry, 2008, 23 (3): 36-39.
[2] Hao Pingjiao, Li Shiyu. Application of MATLAB in chemical calculation [J]. Computer and applied chemistry, 2012, 2 (2): 98-104.
[3] Ling Yu Zhao. Using Origin6.1 software to process experimental data of automatic potentiometric titration [J]. Agriculture and technology, 2004, 24 (6): 166-169.
[4] Tan Jiangcheng. Application of Origin Software in data processing of physical chemistry experiment [J]. Guangzhou chemical industry, 2016, (9): 177 – 179.
[5] Xia Chunlan. Application of Origin Software in data processing of physical chemistry
experiment [J]. University chemistry, 2003. (2): 44-46.

[6] Xing Lin, Yang Wei, Yu Lin Po, et al. Application of Origin Software in experimental data and graphics processing [J]. Science and technology horizon, 2014, (13): 54 – 55.

[7] Zhao Ma. Application of Origin6.0 software in data processing of analytical chemistry [J]. Journal of Zhengzhou Institute of light industry: Natural Science Edition, 2006, 21 (3): 25-28.