GChem: Learning Basic Concepts in Chemistry Using MS Excel VBA

Borhannuddin Arifin
Faculty of Applied Sciences, Universiti Teknology MARA, 40450 Shah Alam, Malaysia
borhan545@salam.uitm.edu.my

***Abstract*—GChem is an Excel VBA (Visual Basic for Application) program that has been developed to assist chemistry students learn basic concepts in chemistry. Two modules are included: electrochemistry and acid base calculations. For the electrochemistry module, users can calculate the cell potential of an electrochemical cell, the free energy change (ΔG) and the equilibrium constant (K) of a chemical reaction. It can also determine the spontaneity of the cell reaction and display the cell notation. Glossary of terms, quiz and application of Nernst equation are also included in this module. For the acid-base module, users can calculate the pH of a strong or weak acid and a strong or weak base. Users can also answer questions in the quiz section and the scores are also displayed. The visual basic editor in Excel is used to write all the programming codes. The application is user friendly and it is easily accessible without the need to purchase sophisticated software. Students can conveniently use it from a laptop or personal computer even without the Internet connection. It is hoped that this application will motivate students to enhance their understanding of the basic concepts of electrochemistry and acid base calculations. A preliminary survey on students at the Faculty of Applied Sciences shows that students find this application helpful in their study.**

Keywords-Visual Basic; Electrochemistry; Acid-base; pH

I. INTRODUCTION (HEADING 1)

Over the years, there has been a growing understanding of the important role on the use of computers in higher education [1]. New models of education are becoming available by integrating Web-based technologies [2]. Several studies have indicated that information processing, inquiry-based learning, and exploring resources via networks, are beneficial for science education [3]. Barak and Dori [4] found that incorporating information and communication technology (ICT) into freshmen courses can enhance students' understanding of chemical concepts, theories, and molecular structures. Another study showed that ICT-enhanced learning had a positive affect on students' chemistry achievements, provided the students were actively engaged in these environments [5]. A study by Akcay [6] found that significant and positive changes were found on students' attitudes toward analytical chemistry. The results also showed no significant differences in attitudes toward analytical chemistry in traditional teaching method. Other studies [7,8] also show similar results. There are many chemistry software that have been developed to be used in research and teaching. Some examples of chemistry software that are available in the internet are Chemix, Chemit and HSC. Some of the websites require users to register and the software can be used over a certain period of time. There are many reasons for using computers in chemistry. Calculating and predicting molecular properties, drawing chemical structures, searching a chemical from a database, drug design, simulation and molecular modeling are just some examples. Many years ago, developing computer applications require very good knowledge of programming. Now, one does not need a computer science background to develop a simple application because help can be obtained easily from self-learning books, internet sources and also from specialized training. The author [9] had previously developed an application containing three topics or modules which are molecular weight calculator, conversion of units and electrochemistry using MS Visual Basic 6.0. The module for electrochemistry was improved using MS Excel VBA [10]. Programming codes in visual basic are written using the visual basic editor of MS Excel. The ease of storing and retrieving data from worksheets make MS Excel more attractive than using MS Visual Basic. In this work the author has added another module, the pH calculation of acid and base to the existing electrochemistry module using Microsoft Excel VBA. Although there are many application software, MS Excel is chosen because it is easily available and it is one of the programs available in Microsoft Office. In this application, the necessary databases are stored in the Excel worksheets and the visual basic editor is used to write visual basic codes that will utilize these databases. The primary aim of developing this application is to assist students of general chemistry in learning electrochemistry and acid base calculations, specifically, the calculation of pH or pOH. The presentation of this paper is as follows: Basic computing requirements are described in Section II. Section III describes some general features of this application. Section IV contains the relevant equations in electrochemistry and acid base calculations that are used in this application. Screenshots and descriptions of the application are discussed in Section V. A preliminary results of survey is mentioned in Section VI. Conclusion and recommendations are in the last Section.

II. SYSTEM REQUIREMENTS

In order to develop or use this application, it is necessary to have a personal computer or laptop with reasonable storage size and speed. At least a Windows XP operating system is required. The application works with a computer with Windows Office 2003 or 2007. The completed application has a file size of less than 1 MB.

III. General features of the Application

This section describes the general features of the two modules; electrochemistry and pH calculation of acids and bases.

A. Electrochemistry

This module will calculate the following:

- the cell potential under standard conditions
- the cell potential using Nernst equation
- the equilibrium constant of the reaction
- change in Gibb's free energy.

The following will also be displayed when the above calculations have been done.

- Cell notation
- Cell reaction
- Spontaneity of cell reaction.

In addition to the above, this module also contains

- Self Quiz (True/False questions)
- Glossary of terms
- Multiple choice questions.

B. pH Calculation of Acids and Bases

This module will calculate the following:

- pH of strong acid or base
- pH of weak acid or base

This module also contains quiz and glossary sections.

IV. Relevant Equations

The relevant equations used in the two modules are described below. These equations are also on display in the worksheet named 'Equation' when the user opens the GChem application.

A. Electrochemistry

For the electrochemistry module, the symbols that are used in the equations below have the following meanings:

E^o_{cell} = standard cell potential

E^o_{red} = standard potential for reduction half reaction

E^o_{oxid} = standard potential for oxidation half reaction

ΔG^o = standard free energy change

n = number of moles of electrons

F = Faraday's constant = 96485 C/mol

K = equilibrium constant

Q = reaction quotient

The calculation of the standard cell potential is

$$E^0_{cell} = E^0(red) - E^0(oxid) \tag{1}$$

The change in Gibb's energy is determined from

$$\Delta G^o = -nFE^o_{cell} \tag{2}$$

The equilibrium constant is

$$\log K = \frac{nE^o_{cell}}{0.059} \tag{3}$$

The Nernst equation is

$$E = E^o_{cell} - \frac{0.059}{n}\log Q \tag{4}$$

A negative sign of ΔG^o indicates that the cell reaction is spontaneous. A positive sign means the cell reaction as written is not spontaneous but the reverse reaction is spontaneous.

B. pH Calculation of Acids and Bases

The following symbols are applicable in the equations for the pH calculations of acids and bases.

$[H^+]$ = the concentration of the hydrogen ion in Molar.

$[OH^-]$ = the concentration of the hydroxide ion in Molar.

K_a = acid dissociation constant

C = molar concentration of the weak acid

The pH value is defined as

$$pH = -\log[H^+] \tag{5}$$

Similarly the pOH is defined as

$$pOH = -\log[OH^-] \tag{6}$$

and

$$pH + pOH = 14 \tag{7}$$

For strong acids or strong bases are the $[H^+]$ and $[OH^-]$ are equal to the molar concentrations of the acids and bases respectively. Weak acids and bases are only partially ionized, so the calculation of $[H^+]$ requires information of the acid dissociation constant, K_a. The $[H^+]$ for a weak acid can be solved using the following quadratic formula

$$[H^+] = \frac{-K_a \pm \sqrt{K_a^{\ 2} + 4K_aC}}{2} \tag{8}$$

where C = molar concentration of the weak acid. An approximation of the value of $[H^+]$ can be obtained from

$$[H^+] = \sqrt{K_aC} \tag{9}$$

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provided that the value of $100[H^+]/C$ is less than 5%. Similar formula are used for the calculations involving weak base.

V. THE GCHEM APPLICATION

Figure 1 shows a screenshot of the application after opening the GChem file. It is necessary to enable the macro before running the application. Clicking the 'Start application' button will open the application. An introductory note is also shown in this worksheet. Users can send feedback about this application to the author using the e-mail address stated on the welcome page.

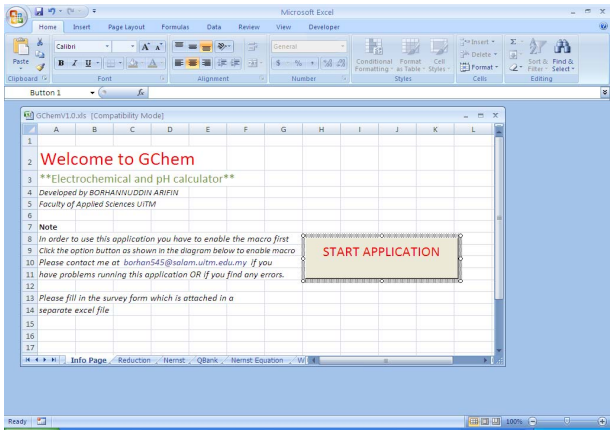

Figure 1. Welcome page

After clicking the 'Start Application' button in the welcome page, a main screen showing the two modules, electrochemistry and pH calculator for acids and bases will be displayed (Fig. 2). The user can exit the application or choose any of the two modules.

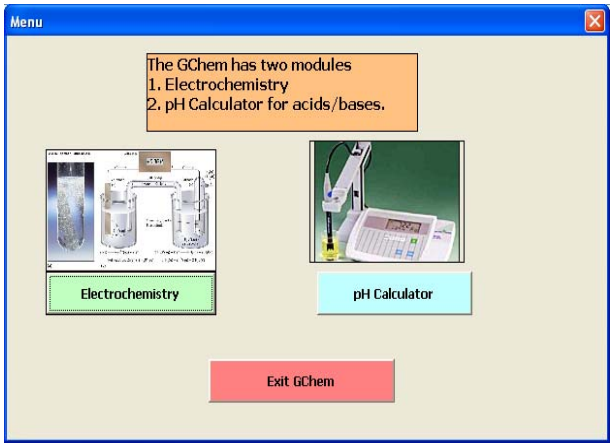

Figure 2. Main page showing the two modules.

Figure 3 shows an example for the $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$ cell reaction in the electrochemistry module. There are over 30 reduction and oxidation reactions and their respective potentials available in this module. The potentials can be selected from a drop-down list. The user must first select one reduction half reaction and one oxidation half reaction. The user also needs to enter the correct value of n i.e the number of moles of electrons. A message will be displayed to show whether the value of n entered by the user is correct or not. If the user is not sure of the value of n, he can click the hint button for assistance. Clicking the appropriate buttons will display the value of ΔG^o, equilibrium constant, cell notation and cell reaction. Based on the sign of ΔG^o, the cell reaction can be either spontaneous, non-spontaneous or at equilibrium. For this example, the value of E^o_{cell} is 1.10 V and the value of the equilibrium constant is very large (> 10^{30}) indicating that the cell reaction favours the formation of products. Other sub-menus shown as command buttons on this page are clear, self-quiz, applying the Nernst equation and glossary.

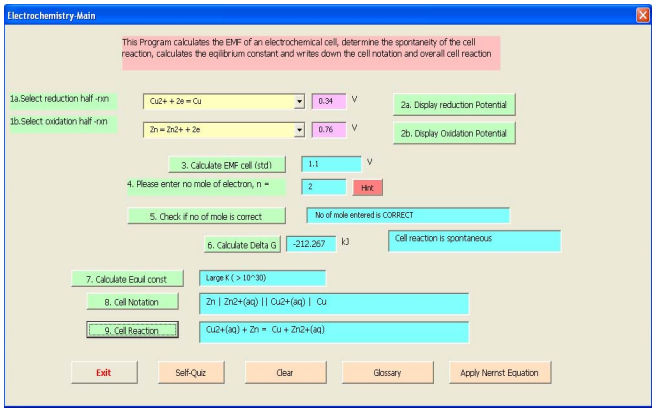

Figure 3. An example for $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$ reaction in the electrochemistry module

If the glossary button is clicked, the screenshot as in Fig. 4 will be shown. A user selects a word or term and after clicking the appropriate button the meaning of the term will be displayed. In order to find the meaning of a different term, press the 'clear' button to empty all earlier entries. Then repeat the same process by clicking another term and also the button that will display its meaning.

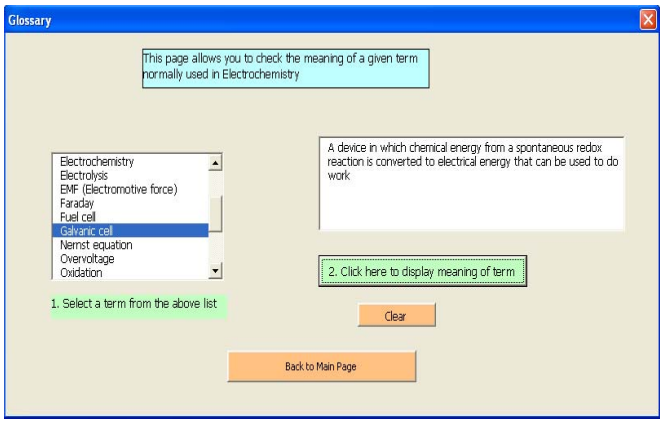

Figure 4. The glossary page to find the meaning of terms

The Nernst equation can be used to find the cell potential when the concentration of the ions involved in the cell reaction are not under standard conditions. The user can click the 'Apply Nernst Equation' button in Fig. 3 to learn more about how this equation can be applied.

The electrochemistry module has a quiz section which allows the user to answer questions (true or false) that are selected randomly. Click the 'display the question' button as in Fig. 5 and a question will be shown. Answer the question in the space provided by typing T (true) or F (false). The user can check whether the answer given is correct or incorrect by clicking the 'check answer' button. The application also keep track of how many questions have been answered and how many of those answered are correct.

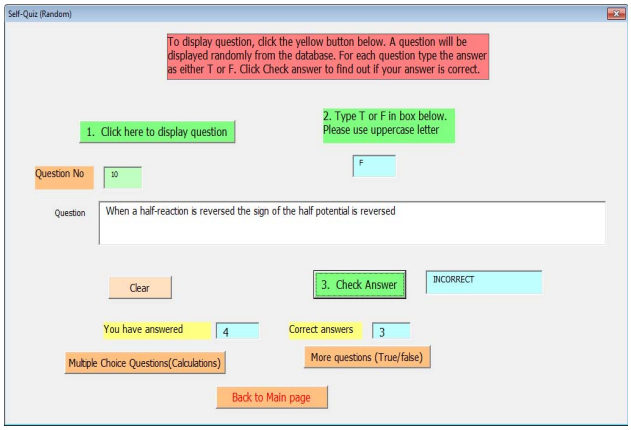

Figure 5. Quiz page for the electrochemistry module

Figure 6 shows a screenshot of the pH calculator for a strong or a weak acid. For a strong acid, the only input required is the concentration of the acid. For a weak acid, the user will select a weak acid and enter the concentration of the acid in Molar (M). After clicking the 'calculate' button, the formula of the weak acid, its K_a value, the hydrogen ion concentration and the pH of the acid will be displayed.

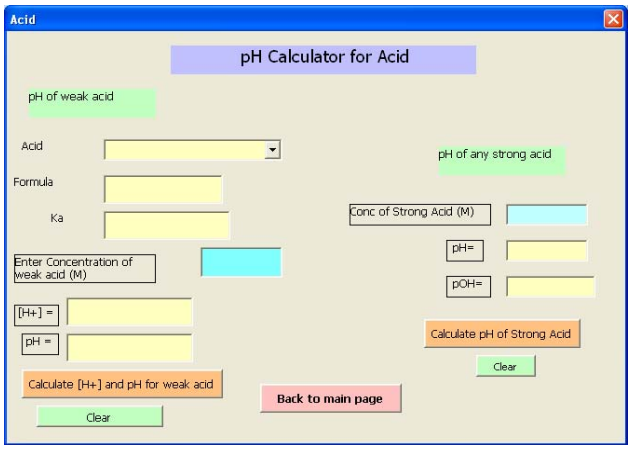

Figure 6. pH Calculator for strong or weak acid.

Similarly the user can calculate the pH and pOH of a strong or a weak base (Fig. 7). Selection of a weak base and the concentration of the base are the required input in order to calculate the pH and pOH.

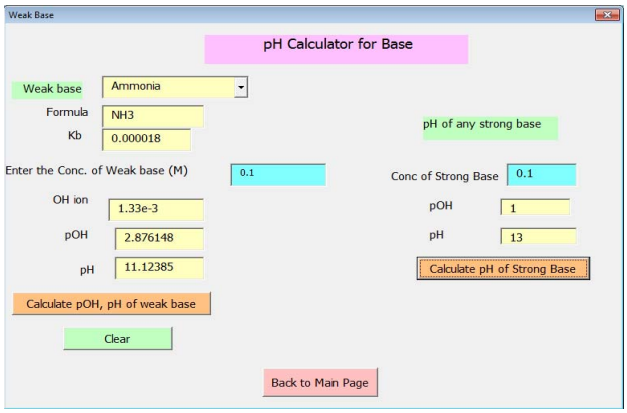

Figure 7. pH Calculator for strong or weak base

Figure 8 shows the quiz page for the acid base module. Click the 'display question' button, and a question will randomly be chosen from a database containing 50 questions stored in the Excel worksheet. After answering the question by typing T (true) or F (false), the user can check whether the answer is correct or incorrect. A percentage score based on the number of corrected answers from the total number of questions answered is also displayed. A 'clear' button can be used to clear all entries so that the user can try answering different questions.

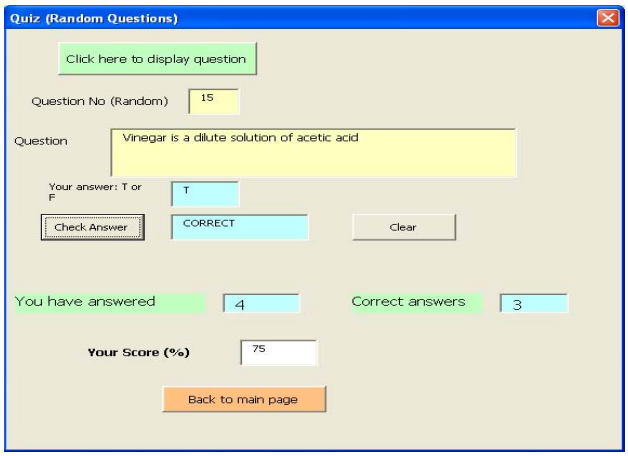

Figure 8. Quiz page in the acid base module

VI. SURVEY RESULTS

A perception survey for the electrochemistry module [10] was conducted on Year 2 students of the Faculty of Applied Sciences, University Technology MARA. A total of 44 students have responded to this survey. A more recent survey on 14 students of Year 1 Applied Chemistry students were conducted for this application. The questions in the survey are divided into three main categories: computer literacy,

electrochemistry and acid base and the software itself. Generally, students give positive response to the questions in the survey. About 78 % of the students considered themselves computer literate, 71% said they use computers mostly to communicate with friends, 71% have used Excel before. 71% have used on-line tutorials before. Other results are; they like the glossary section (85%), the instructions are clear and easy to follow (71%), the application is easy to use (85%), good study guide (85%). Regarding the software, 92% of the students said they will use this software again, 71% said they will recommend this application to their friends and 64% find this application helpful for their revision.

VII. CONCLUSIONS

The author has successfully developed a learning tool for students of general chemistry. The GChem application using Excel is quite easy to use and being stand-alone does not require any internet connection. Students can use this application to revise their understanding of electrochemistry and pH calculation of acids and bases.

Preliminary results on the perception of Year 1 Applied Chemistry students at the Faculty of Applied Sciences Shah Alam, Selangor show that students give positive feedback and find this application helpful in studying electrochemistry and pH calculation of acids and bases. A detailed analysis is still required to determine the effects of computer-based learning on students achievements towards electrochemistry and also acid base calculations. Respondents from different academic background and from different institution will be considered in future work.

A more complete package of this application would be more useful for the students with the addition of more topics such as thermochemistry, chemical equilibrium, kinetics and other suitable topics in general chemistry. It is also hoped students will also be motivated to learn how to develop these applications themselves probably as part of their final year projects. Instead of being users, we can now develop our own modules and applications and this should be an added-value for our science graduates with computer programming skills.

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