GChem: Assisting Students Learning in General Chemistry

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Abstract— **GChem is an Excel VBA (Visual Basic for Application) program that has been developed to assist chemistry students learn basic concepts in chemistry. This application which contains five modules: molecular-weight calculator, empirical formula, thermochemistry, electrochemistry and acid-base calculations, is an improvement from a previous version containing only two modules. For the electrochemistry module, users can calculate quantities such as the cell potential, the free energy change (ΔG) and the equilibrium constant (K) of a chemical reaction. 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. In the molecular-weight calculator module, users can determine the molecular-weight of a compound which can have up to five elements. The empirical formula and the molecular formula of a compound can be determined using the empirical formula module. The thermochemistry module will check whether a chemical equation is balanced or not. It will then calculate the standard thermochemical quantities. 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.**

Keywords- Visual Basic for Application; Electrochemistry; thermochemistry; empirical formula; molecular formula

I. INTRODUCTION

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.

Nico Rutten et al. [9] investigate the learning effects of computer simulation in science education. The reviewed literature provides robust evidence that computer simulations can enhance traditional instruction, especially as far as laboratory activities are concerned.

There are many chemistry softwares that have been developed to be used in research and teaching. Some examples of softwares for general chemistry are Chemix, Chemit and HSC. Some of the websites require users to register and the softwares can be used over a certain period of time.

There are many reasons for using computers in chemistry. Calculations and prediction of 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 from specialized training.

This work is an improved version of work done by the author [10,11,12]. In this work the author has added three more modules i.e thermochemistry, molecular weight calculator and determination of empirical formula for a chemical compound. The Microsoft (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 basic concepts in general chemistry. The presentation of the present report is as follows: Basic computing requirements are described in Section 2. Section 3 describes some general features of this application. Section 4 contains the relevant equations in this application. Sample screenshots and descriptions of the application are discussed in Section 5. 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 Windows XP operating system is required. The computer must have Windows Office 2007. The completed application has a small file size, less than 2 MB.

III. General features of the Application

This section describes the general features of the five modules; electrochemistry and pH calculation of acids and bases, empirical formula, molecular-weight calculator and thermochemistry.

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 calculations above have been done.

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

In addition to the above, this module 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.

C. Thermochemistry

This module will enable the users to:

- Balance a chemical equation
- Calculate the thermochemical quantities such as ΔG^o, ΔH^o and ΔS^o for a given chemical reaction

D. Molecular -Weight Calculator

This module will enable the users to:

- Calculate the molar mass of a compound
- Calculate the percentage by mass of each element in compound

E. Empirical Formula

This module will enable the users to determine the molecular formula and empirical formula of a given compound.

IV. Relevant Equations

The relevant equations used in the five 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

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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

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

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

C. *Thermochemistry*

The equations for the calculation of ΔG^o, ΔH^o and ΔS^o are:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \tag{10}$$

$$\Delta H^0 = \sum \Delta H_f^0(prod) - \sum \Delta H_f^0(react) \tag{11}$$

$$\Delta S^0 = \sum S^0(prod) - \sum S^0(react) \tag{12}$$

where

ΔG^0 = standard Gibb's free energy change

ΔH_f^0 = standard enthalpy change of formation

ΔS^0 = standard entropy change

D. *Molecular-Weight Calculator*

The molecular weight of a compound is the sum of the atomic masses of all the elements in that compound.

E. *Empirical Formula*

The empirical formula represents the simplest whole number ratio of atoms in a compound. For example, if the molecular formula is C_6H_6, the empirical formula is CH.

V. THE GCHEM APPLICATION

Figure 1 shows a screenshot of the main menu of the GChem application. Five modules are shown and the user needs to choose by clicking the desired module. The user can always go back to the main menu or exit the application. The instructions to use this application is given in a separate file.

The thermochemistry module is shown in Figure 2. Users can choose the reactants and products for a chemical reaction. Then the user can try to balance the equation and check whether it is correct by clicking the appropriate button. A statement will be displayed to indicate whether the equation is balanced or not. The number of atoms for each element for the reactants and products are also displayed. Based on the balanced equation, the thermochemical quantities can be calculated. Spontaneity of the reaction of the reaction will then be determined.

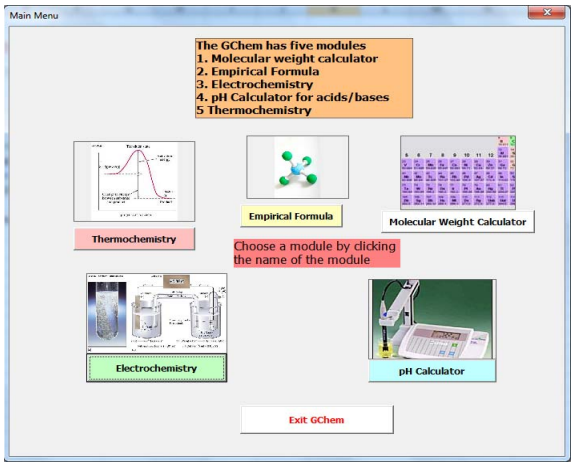

Figure 1. Main Menu

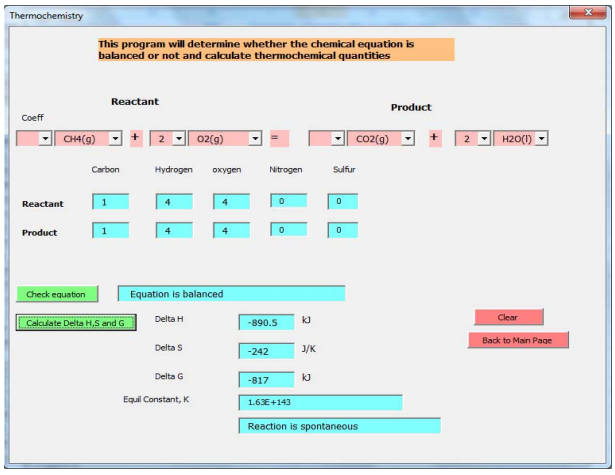

Figure 2. The Thermochemistry module.

The molar mass or molecular weight of a compound is just the sum of the atomic masses of all the elements in that

compound. Figure 3 shows the molecular-weight calculator module. The user can choose up to five elements for the compound. Input of the number of atoms is also required before it calculates the molar mass of the compound. The percentage by mass of each element will be shown on the application.

Figure 4 shows a screenshot of the empirical formula module. The user can select up to four elements for the compound. Percentage by mass of each element in the compound is required. The result will show the mole ratios, the empirical formula and the molecular formula if the molar mass of the compound is known.

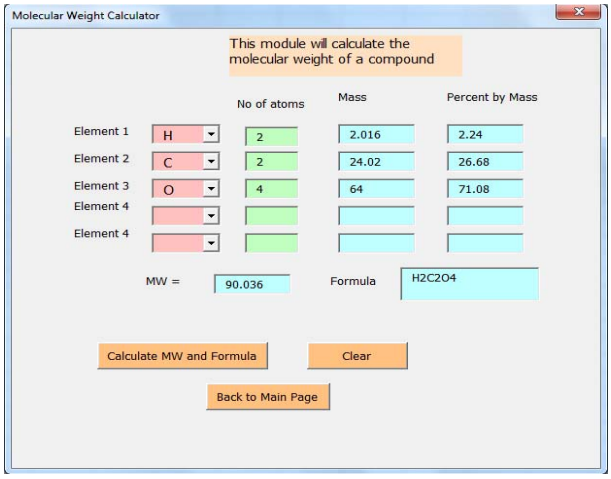

Figure 3. Calculating the molecular-weight of oxalic acid, $H_2C_2O_4$

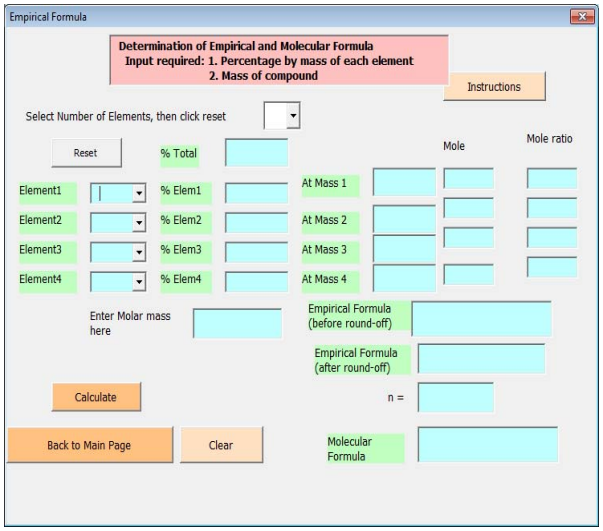

Figure 4. The Empirical Formula module

A screenshot of the pH calculator module is shown in Figure 5. The user will select a weak acid and enter the concentration of the acid in Molar (M). After clicking the calculate button, the pH of the acid and the molar hydrogen ion, $[H^+]$ of the acid will be displayed.

Figure 6 shows the quiz page for the acid-base module. Click the display question button, and a question will randomly be chosen from the questions database 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 is also displayed.

In this application the clear button can be used to clear all entries so that the user can try answering different questions or calculations.

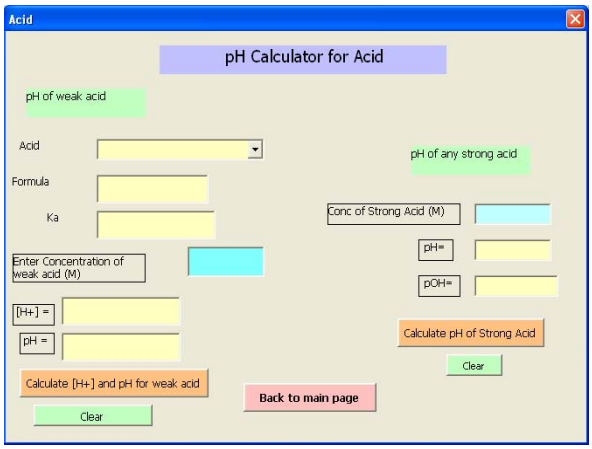

Figure 5. pH Calculator for weak acid

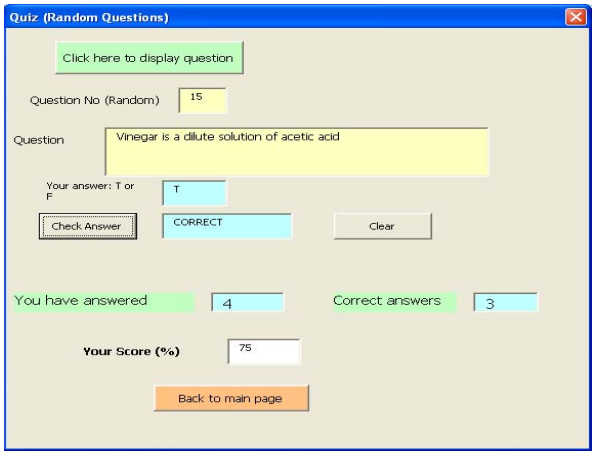

Figure 6. Quiz page

VI. CONCLUSIONS

The author has successfully added three more modules to the GChem application, which is a learning tool for students of general chemistry. Students can use this application to revise their understanding of electrochemistry and pH calculation of acids and bases, thermochemistry, molecular-weight calculation and empirical formula determination.

An ongoing survey is being conducted to determine the effects of computer-based learning on students achievements in the five modules covered in this application.

Additional topics such as gas laws, conversion of units, chemical equilibrium and stoichiometry will be considered for further work. Topics that include plotting of graphs such as kinetics, acid-base titration and phase diagrams will be also be helpful to students.

It is also hoped that students will 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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