

LEARNING BASIC CONCEPTS IN CHEMISTRY USING VISUAL BASIC APPLICATIONS

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ABSTRACT

In the Information and Communication Technology (ICT) age, we use computers for a variety of reasons e.g to write reports, manage database, solve mathematical problems and to serve the internet for educational, personal or commercial purposes. Most of the time we will use application softwares to do a given task. There are softwares such as Visual Basic (VB) that can be used to create graphical user interface application programs to solve problems that are of interest to us. This work, which is still at its early stage of implementation, will demonstrate the use of VB by creating a simple application program known as ChemVB. Basic concepts in chemistry such as conversion of units and calculation of molecular weight of a compound will be demonstrated. This work can be expanded to include other topics in chemistry.

1. INTRODUCTION

We are living in the Information and Communication Technology (ICT) era and computers are used in many different fields by different groups of people. Some of us use computers to serve the internet, write reports, manage database while others especially in the scientific community use computers to do modeling, simulation, calculate molecular properties or solve complex problems. If you are a programmer, you can develop your own application softwares; otherwise we just buy a certain software that suits our requirement to do or solve a given task. There are also softwares that we can use to develop our own applications that suit our needs. One such application is the Microsoft Visual Basic for Applications or VBA for short. VBA is an object-oriented programming language that can be used to create graphical user interface (GUI). A GUI is a graphical (rather than purely textual) user interface to a computer. Elements of a GUI include such things as: windows, pull-down menus, buttons, scroll bars, iconic images, wizards, the mouse and probably many things that have not been invented yet. An application known as ChemVB has been developed using VBA.

The ChemVB has three programs

- a) Conversion of units
- b) Molecular weight calculator
- c) Periodic Table

The purpose of developing this application is to use VBA as a tool to assist students in learning basic concepts in chemistry. This work will demonstrate how to use ChemVB. Step by step instructions on how to run the application are given in the next section. Other concepts or topics in chemistry can also be developed. The author used (McKeown, 1999) as a reference for VBA programming and specific applications of VBA in chemistry can be found in (Sime, 2005). Incorporating VBA into Excel is described in (Billo, 2001). It is up to one's creativity to explore all the available features of VBA. With routine use and practice, one can design and create an application that is of professional quality.

The ChemVB

The ChemVB application was developed using MS Visual Basic 6.0. Basically three steps are involved when a programmer wants to develop an application.

- Creating the user interface (the form and its embedded controls)
- Setting the properties of the controls (caption, name, size, color and other properties)
- Writing the code (attaching the Visual Basic code to the controls)

Details for creating GUI will not be discussed here but the instructions on how to use ChemVB are as follows:

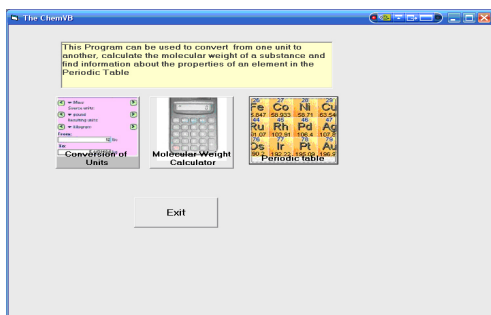


Figure 1: The ChemVB main window

Instructions to Open ChemVB

- Open ChemVB.exe
- A window similar to Figure 1 is displayed. It shows the three different programs available in ChemVB.
- Select any of the three programs.

Program 1: Conversion of Units

This program converts the following quantities.

Quantity	From	To
Temperature	°C	K and °F
Pressure	bar	atm and Pa
Volume	m ³	cm ³ and L
Energy	J	cal and Latm

Instructions

- Select The Conversion Program button.
- Fill the first column with values of the respective quantities. All four must quantities must be filled with values. The example in Figure 2 shows a value of 1 for each quantity.
- Click the calculate button.
- The screen will display the converted values in the next two columns for all four quantities.

- Click the clear button to repeat using different values.
- Click exit to go to the main ChemVB window.

Program 2: Molecular Weight Calculator

This program demonstrates the calculation of the molecular weight for a given compound that consists of up to three elements. This program will also calculate the percentage by mass of each element present in the compound.

Instructions

- Molecular weight for compounds with 3 elements e.g H₃PO₄
 - Click the Molecular Weight Calculator button in the ChemVB main window.
 - Click the down arrow of combo box for the first element. Choose H
 - Click the down arrow of combo box for the second element. Choose P
 - Click the down arrow of combo box for the third element. Choose O (Figure 3).
 - In the next column, insert the number of atoms for that element, 3 for H, 1 for P and 4 for O.
 - Click the Calculate MW button. It will display 157.92 as the molar mass for H₃PO₄ and also the percentage by mass for each element. The formula for the compound is also displayed.
 - Click the clear button to repeat the calculation for a different compound.

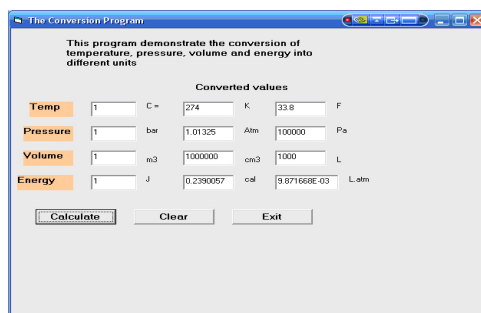


Figure 2: The Conversion Program

- B. Molecular weight for compounds with two elements (e.g CO₂)
1. Choose C for the first element and insert 1 for number of element for C
 2. Choose O for the second element and insert 2 for number of element for O
 3. Since there are only 2 elements (C and O), for the third element select X. This is a dummy atom that has mass of 0. So that its total mass regardless of number of atoms is 0. You must also insert a number for number of the third element.
 4. Click the Calculate MW button. It will display 44.01 as the molar mass for CO₂. (Figure 4)
 5. Click the clear button to repeat the calculation for a different compound.
 6. You can also view the instruction by clicking the Read Instruction button.
 7. Click the exit button to go to the main ChemVB window

Program 3: Periodic Table

This program allows the user to choose an element in the Periodic table and obtain a description of the element.

Instructions

1. Choose the Periodic Table window in the ChemVB main window. (Figure 5)
2. Choose an element by clicking on the icon of that element. For example click Na. A description of the element Na is shown the empty box at the bottom right of the window.
3. Repeat by choosing other elements
4. Click the exit button to go back to the main ChemVB window.

CONCLUSIONS

Simple concepts involving conversion of units, calculations of molar mass and the Periodic Table using VBA have been demonstrated. The programs are quite easy to use and the instructions quite simple and straight forward. These programs can be modified to make it more attractive and other topics can be included to cover other areas of chemistry.

REFERENCES

- E. J. Billo, (2001), Excel for Chemists 2nd. Ed., John Wiley and Sons.
- P. G. MvKeown, (1999), Learning to program with Visual Basic, John Wiley and Sons
- R. J. Sime, (2005), Physical Chemistry Calculations with Excel, Visual Basic for Applications, Pearson Education

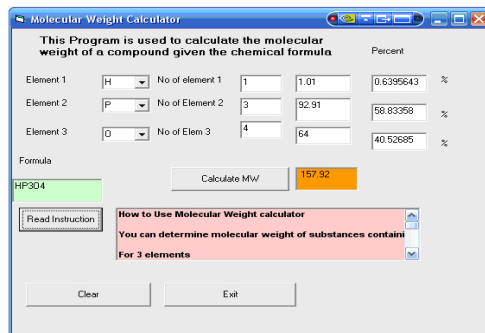


Figure 3: Results for the molecular weight of H₃PO₄

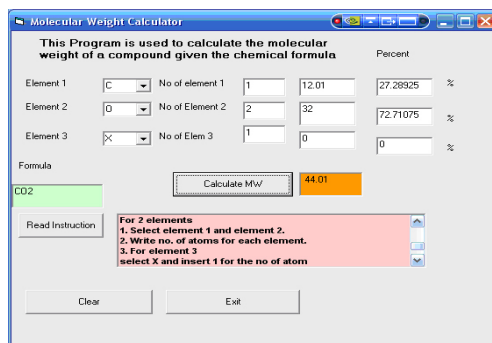


Figure 4: Results for CO₂ (For two elements in the compound)

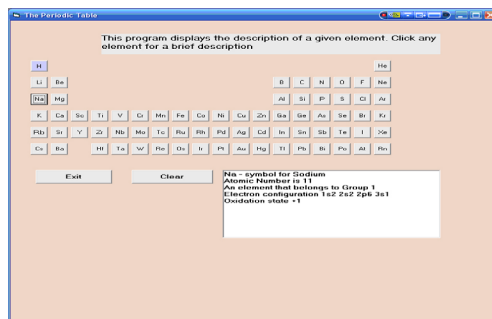


Figure 5: Information about sodium from the Periodic Table program