TITLE PAGE

COMPUTERIZATION OF LABORATORY QUANTITATIVE ANALYSIS

BY

JAMES ADE BELLOS

A PROJECT SUBMITTED TO THE DEPARTMENT OF MATHEMATICS/COMPUTER SCIENCE, FEDERAL UNIVERSITY OF TECHNOLOGY MINNA, IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF A POST GRADUATE DIPLOMA (PGD) IN COMPUTER SCIENCE

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APPROVAL PAGE

THIS RESEARCH PROJECT HAS BEEN READ AS HAVING MET THE REQUIREMENTS OF THE DEPARTMENT OF MATHS/COMPUTER SCIENCE, FEDERAL UNIVERSITY OF TECHNOLOGY, MINNA, FOR THE AWARD OF POST GRADUATE DIPLOMA IN COMPUTER SCIENCE.

DR. S.A REJU PROJECT SUPERVISOR	DATE
DR. S.A REJU H.O.D MATHS/COMPUTER DEPARTMENT	DATE
EXTERNAL EXAMINER	 DATE

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God Bless you all.

DEDICATION

To `Yemi, `Femi, `Ope, `Debo, and `Gbemi- most precious people

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ABSTRACT

Computation in the laboratory quantitative analysis by manual method is no longer adequate for the purpose of computation due to the problems of human error, time wastage, wrong results. Therefore computerization of the computation in quantitative analysis is necessary to eliminate these problems and make the process easier faster, error proof, mentally less tasking record keeping, retrieval and reproduction possible.

CHAPTER ONE

1.0 INTRODUCTION TO QUANTITATIVE ANALYSIS

1.1 Introduction

The study of science is so important that the National Policy on Education (1983) (NPC) advocated for a greater proportion of the education expenditure to be devoted to science and technology. This has led to the establishment of science secondary schools by different states of the federation and ultimately universities of technology to ensure continuity for the secondary school leavers.

For science to be meaningful at the secondary school level to the student, science activities needs to be integrated with theory and demonstration, to complement the cognitive knowledge acquired. Laboratory investigation is one of these activities, which add to the learning experiences of students. The NPC understood this when it went further to emphasize that students should be taught to have practical implication of basic ideas. In other words, students should be actively involved in the practice of science in order to achieve manipulative skills.

Chemistry is a science subject; and the then Federal Ministry of Education, Science and Technology in 1985 emphasized that chemistry curriculum should be an experimental science, with its roots in the laboratory. This is because in addition to understanding concepts, laboratory experiments develop the student's ability for critical thinking and better understanding of principles, theories and laws of chemistry.

The laboratory experiment includes such activities as demonstrations to prove theorems and laws; investigation of the composition of substances (components) and their quantity. That is the qualitative and quantitative investigation of substances. This work is concerned with the later, i.e. the computerization of the quantitative analysis of substances.

1.2 Quantitative Analysis

The analysis of substances to determine their quantitative composition is referred to as quantitative analysis. The analysis is based on volume measurements and it uses the titration method hence, it is also called volumetric analysis. Quantitative analysis establishes the attitude of careful handling of equipment, sharpens the observation ability of the student and builds the capacity of the student to make correct predictions about chemical reaction or phenomenon.

Quantitative analysis is usually an acid-base reaction, which is primarily a neutralisation reaction. It involves titrating the solution of the substance under investigation (usually an acid) with a standard solution of a suitable reagent (usually an alkali). A suitable indicator and the colour change during the titration marks the end-point or completion of the neutralisation process.

The experiment above and the analysis that follow is an investigative laboratory work. It deals with the investigation in quantitative form of the substances that are involved in a chemical reaction. In other words, it is the investigation of the amount of the reactants, that have reacted and the amount of the products formed in any given reaction. And sometimes it is used in the determination of percentage purity or percentage impurity of the substance under investigation. The 'amount' in quantitative form is expressed as Mole; concentration in Mol/dm³; concentration in g/dm³; or as % purity, % impurity.

This research is aimed at reducing the errors that are usually encountered in these determination and also reducing the time involved in the computation as well as increasing the efficiency of the system.

1.3 Objectives of the Study

Computer studies and the use of computers in solving problems is gaining wider acceptability in different areas of human endeavour, such as in production in the manufacturing industries, in decision making at management level; in the education sector. Computers and their usage have become an important and indispensable companion in the teaching-learning process in the educational enterprise, like solving mathematical problems identifying metallic substances and rocks (in chemistry and geology); predicting weather conditions, etc.

The world is moving towards computer controlled activities and hence the chemistry laboratory activities also needs to be aided by computers.

Computerisation of quantitative analysis has the following objectives:

- Encourage the use of computers in different activities of the chemistry laboratory.
- ii. Use of computers in analysing substances involved in chemical reactions.
- iii. Develop programmes that can be used in solving mathematical problems in quantitative analysis.
- iv. Speed up calculations in quantitative analysis.
- v. Eliminating errors associated with manual calculations in quantitative analysis.

1.4 Scope and Limitation of the Study

Laboratory activities are many and include record keeping; identification of gases, metallic radicals and acidic radicals – commonly referred to as qualitative analysis; determination of the amount of substances involved in chemical reactions as reactants or products – commonly called quantitative analysis and laboratory time allocation.

This study is only focussed on the computerisation of the quantitative analysis, taking Government Secondary School, Nyanya – Abuja, as a Case Study. But the principle of quantitative analysis is the same in all secondary schools using the same chemistry curriculum in Nigeria, therefore, the study is relevant to all secondary schools – their teachers and students. And the program developed could be used in all secondary schools.

Limitations of the study are; it focuses on only the quantitative analysis which leaves other activities like; record keeping of time allocations, accidents, inventory, and quantitative analysis for future researchers. Also, lack of adequate finance and short duration of the time available for this research made it difficult to assess the attitude and full participation of the students in the execution of the programme.

CHAPTER TWO

2.0 LABORATORY QUANTITATIVE ANALYSIS CASE STUDY

2.1 Structure of the Laboratory

The chemistry laboratory is built on specifications. These specifications cover such areas as the length and width of the building; number of students – usually forty; space per student; arrangement of tables, position and location of doors and windows bearing in mind ventilation and safety. The absence of or wrong location, or arrangement of any of the items mentioned above could reduce the effective utilisation of a laboratory.

In GSS Nyanya, the laboratory is structured to accommodate equipment and materials (chemicals). Some of the equipment and materials are kept in a store attached to the laboratory, while others are kept on shelves standing on tables for students' use. A preparation room for teacher's experiment is also attached. The laboratory was designed for forty students and in the previous years, the facilities were adequate for this number of students. The space allocation per student was about 1.6 metres. This allows for free movement of students, reduced collisions and thus few accidents were recorded. Sufficient equipment and materials were available for demonstration experiments, investigative and verification experiments by both the teacher and the students. With increased population, the equipment and materials are no longer sufficient and this leads to crowding. Invariably, it affects the speed with which experiments can be carried out as well as the accuracy of the results obtained. Messy working environment and misplaced titre values all results in wrong calculations. These calls for the use of a method that will increase the speed of determination by calculation of the components of the substances. Computerisation of the calculations is therefore highly desirable.

2.2 Record Keeping

In the chemistry laboratory, different records are kept. These records are useful and necessary for a successful experimental work. These records help in making useful observations and drawing inferences. The records kept in the laboratory are:

- i. List of equipment/date supplied,
- ii. List of materials /date supplied,
- iii. List of consumables,
- iv. List of materials consumed,
- v. List of replaced materials,
- vi. List of broken/damaged equipment,
- vii. Record of accidents/treatments,
- viii. Record of laboratory class/period allocation,
- ix. Record of experiments/observation/inference,
- x. Record of titration figures and calculation.

Each of these records is useful in compiling reports, determination of time of last supply and time next supply is due. Information on type of equipment/materials available in the laboratory and type of experiments that can be carried out is readily obtained from these records.

In this study items (ix) and (x) are most useful. And these records deals with the type of the acid and base involved in the reaction, the indicator used, the titre value obtained, the molecular mass of the substance, the mole ratio from the Stoichiometry of the reaction, the given mass or concentration of the substances. All of these help the student in calculating the quantities of the substances that react or are produced.

2.3 Types of Activities in the Laboratory

There are different types of experimental activities that take place daily in the secondary school chemistry laboratory. These activities affect the cognitive domain as in recall of concepts, laws and relationship; affective domain as in handling of equipment and apparatus and psychomotor domain as in the attitude of students in manipulating equipment and making correct observation. These activities are demonstrated in the following experiments:

- i. Production of gases
- ii. Identification of gases
- iii. Production of 'new' substance
- iv. Identification of the 'new' substance
- v. Identification of the components of substances
- vi. Determination in quantitative terms of the volume and amount of components of substance.
- vii. Determination of the purity of substances.

These activities are usually for convenience grouped into two groups, that is qualitative and quantitative analysis. And each can be carried out as a demonstration, confirmatory or investigative experiments by both the teacher and the student.

Qualitative analysis involves the identification of gases, e.g. O_2 , H_2 , CO_2 , etc. by simple methods; identification of acid radicals e.g. NO_3^- , CI, $So_4^{2^-}$, etc and metallic radicals e.g. Ca^{2^+} , Cu^{2^+} , Fe^{3^+} , etc. While quantitative analysis which is the subject of this study is the determination of the relative proportion of the components of a substance by volumetric method. The volume, concentration, mass and percentage purity of such components or substances are determined in quantitative terms.

All of the experiments are designed to reinforce the understanding of the theoretical class-work, lay foundation for scientific investigation and independent thinking in each student.

2.4 Quantitative Analysis

Quantitative analysis is the determination of the relative proportions of the components of substances in a neutralisation reaction. It is often called volumetric analysis because it involves volume measurements of the reactants. Analysis is achieved by titrating a solution of the substance under investigation with a standard solution of a suitable reagent. Titration is carried out by using and manipulating apparatus such as pipette, burette, measuring cylinder, conical flask, beaker and retort stand. Before setting up the apparatus the following are undertaken:

- Washing and drying of all glass apparatus
- Rinse the pipette with the base
- Rinse the pipette with the acid
- Prepare the standard solution.

After setting up the apparatus then, measure accurately 25cm³ each of a standard solution of the alkali into three different clean and dry conical flasks labelled 1, 2, and 3 respectively. Fill the burette with the acid and adjust the burette to the zero mark or level. Add two drops of a suitable indicator to the conical flask 1. Run the acid carefully from the burette into the conical flask 1 until there is a colour change in the solution. This marks the end point. Record the reading on the burette. Repeat the titration similarly using alkali in conical flask 2 and record the volume of the acid used on each occasion. The average of the two closest readings is taken and used as the volume of the acid that has reacted with the

alkali. And it is this volume that is used in various calculations that may be required. It is recorded as below:

	Burette Reading in cm3		
	1	2	3
Final Reading	25.55	24.50	24.50
Initial Reading	0.00	0.00	0.00
Volume of acid used	25.55	24.50	24.50

Average titre value =
$$24.50 + 24.50 \text{ cm}^3$$

2
= 24.50 cm^3

The concentration of the acid is calculated from the formula

$$Ca = \frac{C_b V_b n_a}{V_a n_b}$$

Where C_a = Concentration of acid

V_a = Volume of acid (titre value)

C_b = Concentration of base

 V_b = Volume of base

 $\underline{n_a}$ = Mole ratio of acid and base from the

n_b Stoichiometry of the reaction.

Other calculations can be done similarly using the appropriate formula, thus mass of the substance = conc. $Mol/dm^3 \times Molar Mass$.

% purity/impurity = Mass of pure substance x 100%

Mass of given substance

Quantitative analysis does not involve only the determination of components and substances, but it is a useful teaching-learning tool in chemistry. For any effective teaching - learning process to take place the three domains of learning must be involved. These domains are the cognitive, affective and psychomotor. The cognitive domain relates to the ability to recall. Quantitative analysis is an experimental work designed to verify theoretical class work, concepts, laws, ability to write equation and remember relationships. All of these help the student to remember (recall) what he/she has been taught. Learning in the psychomotor domain relates to the ability to handle and use equipment. Quantitative analysis involves handling of apparatus such as burette, pipette, measuring cylinder - all of which are used in measurement. The success of volumetric analysis and the result depends on the manipulative ability of the student. This therefore help learning in The affective domain relates to the attitude of the the psychomotor domain. student in recalling handling and manipulating the equipment to achieve an accurate analysis of the substances under investigation. An extra drop of the indicator or a drop of the acid wasted could affect the result obtained in volumetric analysis, hence the attitude developed by students in manipulating and handling of equipment is very important in analysis. It is a well known fact that without the right attitude, it is difficult to develop an investigative mind, undertake experiment, make correct and useful observation of the minutest detail and arrive at conclusions that are of significance to science. Quantitative analysis teaches all of these.

CHAPTER THREE

PROGRAM DESIGN

3.10 Study of the existing system

3.0

In the existing system, the analysis of substances by volumetric method and the computations are carried out manually. First titration is carried out for the purpose of obtaining accurately the volume of the test solution under investigation. Then the volume obtained is used in various calculations to determine in quantitative terms the component and composition of the test substance.

The result of the computation is arrived at by imputing the volume of the test solution, its mole and other data into the appropriate formula for the determination of he concentration, purity, molar mass or mole. These data are entered into a calculating machine for a final output which could be used in making inference and drawing conclusion as regards the test substance. Some times a four figure mathematical table is used for such calculations.

This methods is tedious, time consuming and often leads to loss of the result obtained; moreover the result cannot be reproduced easily.

3.20 Requirement of the New System

By the close of the 20th century, people have become aware of the benefits of using an electronic calculator to speed up complex calculations. The computer is even faster and more efficient at doing lengthy and complex analysis on data in a very short time.

The computerization of the laboratory quantitative analysis of substances would require the following, PC, Appropriate Software, a designed program and training of users.

3.21 System Analysis

The objective of the system was analysed. Its limitation and constraints were also analysed. The procedure was considered as well. The following problems were identified:

- (i) It is tedious
- (ii) It is time wasting
- (iii) Process of calculation is cumbersome
- (iv) Result (output) is not always accurate due to calculator error or human error arising from incorrect mathematical table reading.
- (v) Hence result many not always be reliable.
- (vi) Record (of result) easily lost with loss of student laboratory notebook
- (vii) Records cannot be stored
- (viii) Record are not easily retrievable.
- (ix) Result cannot be easily printed or reproduced in large quantity.

3.22 Feasibility Study

The existing system was studied very studiously and the various alternative solutions were considered in this project for the computerization of the laboratory quantitative analysis. The following feasibility studies were undertaken:

- Operational feasibility:- the workability or otherwise of the proposed system was considered.
- (ii) **Technical feasibility:-** in this feasibility, the specification of the equipment needed together with the appropriate software and personnel requirement was established.
- (iii) **Economic feasibility:-** the feasibility of the cost implication for the management was also undertaken.

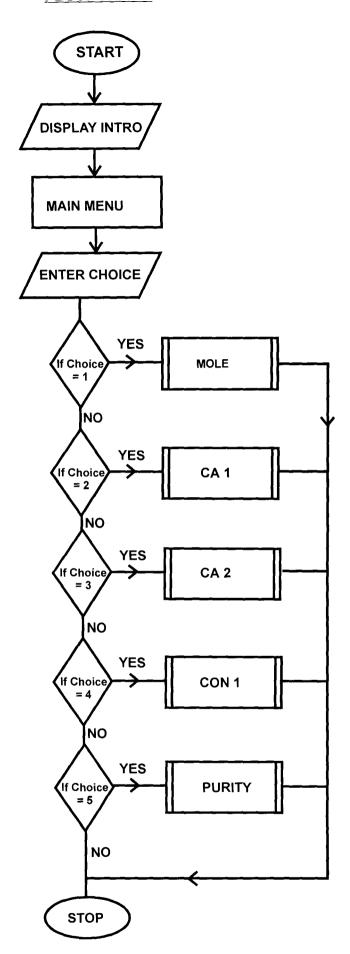
3.3 Program Structure of the New System

The new programme for the computerization of the computations of the laboratory quantitative analysis is designed in a modular form using the Pascal programming language. Since the computation depends on the requirement of each analysis therefore, the program is structured in such a way that it offers the user options. The user is required to choose from these options.

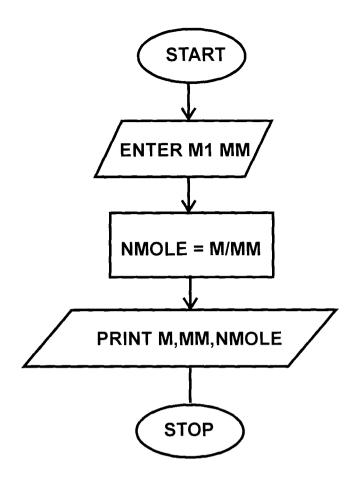
3.31 Flow Chart

The design of the algorithm in the development of the flow charts for these program was done in modules using structured English. The algorithm shows the introduction, main menu, choice of programme to execute, in the main programme. While the sub-programmes or modules shows how each is called and used in the different choices offered in the main menu.

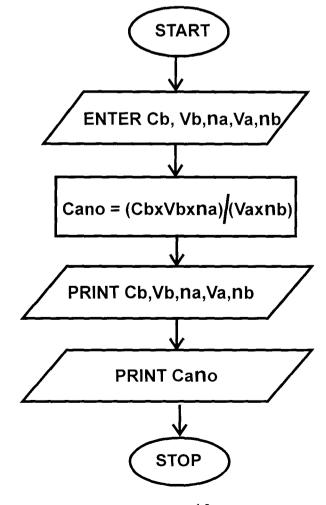
FLOW CHART

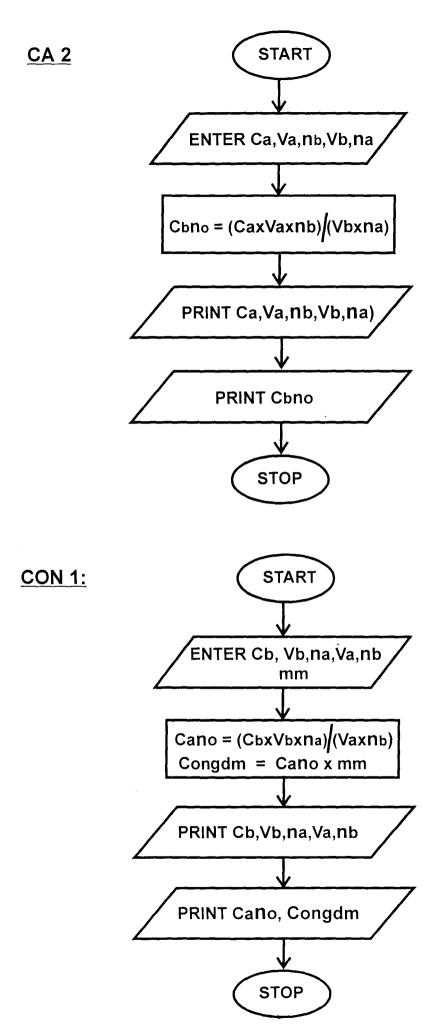


MOLE

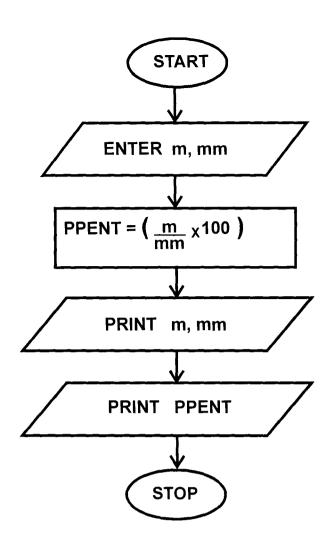


CA 1









3.4 Choice of Programming Language

The programming language used for this project is Pascal. And it was chosen because it has certain features which make it very relevant for this project. The Pascal programming language has to its advantage the use of structured language because it is also structured. It allows the design and use of programmes in modules. It combines these advantages with the following features:

- (i) **Maintenability:-** with the Turbo Pascal windows debugging feature maintenance of the system becomes very easy.
- (ii) **Readability:-** the choice of the language i.e. the Turbo Pascal windows aids in the coding of the system thereby allowing for proper program documentation to ease debugging and maintenance of the program.
- (iii) **User friendliness:-** the programming language's user friendly nature allows novice to be able to use the program. And its menu driven capability makes this possible and easy.
- (iv) **Portability:-** the program is not written for a single user environment alone. The choice of the language has made it possible to run on a multiuser environment, this can be achieved if run on multi-user operating system e.g. windows NT, loaded on a main central processing unit called the sever to several other client terminals.

CHAPTER FOUR

4.0 PROGRAM IMPLEMENTATION

4.10 Introduction

In this chapter the process of implementation of the new program is discussed. To implement the program, the various aspects of the choice of program, analysis, design are brought together to make the actual implementation possible.



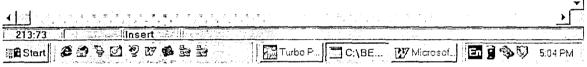
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BY
J.A. BELLOS
REG. NO: PGD/MCS/98/99/860
DEPARTMENT OF MATHS / COMPUTER SCIENCE
FEDERAL UNIVERSITY OF TECHNOLOGY MINNA, NIGER STATE

Press enter key to continue...



This is the introduction to the program. It states the topic, programmer, programmer identify number, the department, the university and instruction to the user of the program.



As you press enter key, the main menu appears on the screen. The main menu is the different modules of the program and it offers the user various choices of the calculations that it can perform. The choice is made by selecting any of the numbers listed 1= to 5=7. the user can also exit by selecting 6= if none of the choices offered is suitable.

CALCULATE NUMBER OF MOLES OF SUBSTANCE

Enter mass of the subtance :4 Enter molar mass of the subtance :40

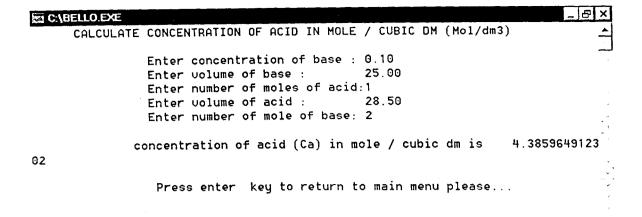
Number of mole of the subtance is 1.0000000000E-01

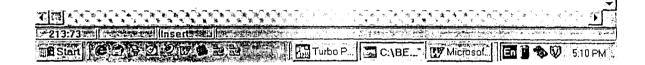
Press enter key to return to main menu please...



The choice of module 1= calculates the mole of a substance. This input the mass and molar mass of the substance the computation is done by the computer giving the output above.

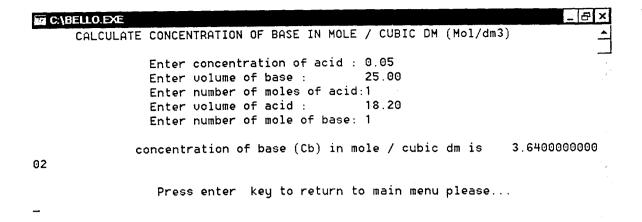
The formular is $n = \frac{m}{M}$ where $n = n\underline{o}$ of mole m = mass of substance the example in the output above is for NaOH.

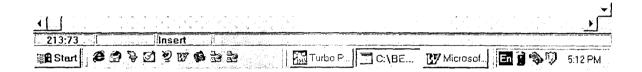




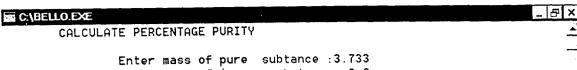
On returning to main menu, choice 2= offers the user to calculate concentration of acid in mol/dm³.

The formula is given in chapter 2. Note that the number of mole in this case is obtained from the stoichiometry of the reaction (see appendix I)





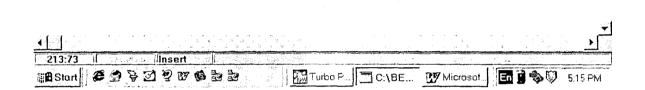
Choice 3= is used in calculating the concentration of the base in mol/dm³. This gives the quantity of the substance present in 1dm³ (1000cm³) of the solution. The formula for this is stated in chapter 2 (see appendix I for sample question)



Enter mass of impure substance :6.3

5.9253968254E+01 The percentage of purity is

Press enter key to return to main menu please...



To calculate (the degree of) percentage purity, choice 5= gives the correct option. The mass of the pure substance and the molar mass of the substance are input into the computer. The output gives the percentage of the purity of the substance. The formula for percentage purity is stated in chapter 2.

Note that at the completion of each computation, that is execution of each module, the "press enter key" returns the program to the main program. This has enhanced the overall efficiency of the program. It also means that other modules could added to or removed from the main program without affecting it in any way.

CHAPTER FIVE

SUMMARY AND CONCLUSION

5.1 Introduction

5.0

This chapter deals with the Summary of the project, the cost and benefit analysis of the project and conclusion giving areas where complimentary project could be carried out in the chemistry laboratory.

5.2 **Summary**

It has been found that the use of manual method in performing complex computations in science is not only time wasting, cumbersome, error prone but also often produces unreliable results. And with the availability of the computer, such computations have been performed very fast, with ease and producing accurate and reliable results.

In the computerization of the laboratory quantitative analysis, the computation procedures were reduced to simple form that could be performed by even a novice. Moreover the choice of Pascal as the programming language and its development and conversion to executable form in a windows environment has a combined effect of making the computation to be easy.

5.3 Cost and Benefit Analysis

The cost and benefit analysis of the project is as analysed, thus

A.	<u>Equ</u>	ipment Costs	N	K
	(i)	2 No. Personal Computer	250,000 =	
	(ii)	1 No. Printer (LaserJet)	75,000 =	
	(iii)	Computer Furniture	50,000 =	
	(iv)	Ancillary Equipment e.g. UPS	60,000 =	

	(v)	1 No. Air Conditioner (1.5 HP)	45, 000=
	(vi)	Fire proof Cabinet	20,000=
	(vii)	Fire extinguisher	<u>21,000</u> =
		Sub Total	<u>522,000</u> =
B.	Insta	llation Costs	
	(i)	Partitioning of new office	
		Including burglary proof, blind, etc	50,000=
	(ii)	Fiting of Air Conditioner, fire	
		Extinguishers	15,000=
	(iii)	Installation of computer system	
		software, UPS and Printer	25,000=
		Sub Total	91,000=
C.	Perso	onnel and development cost	
C.	Perso	onnel and development cost Staff training	45,000=
C.			45,000=
C.	(i)	Staff training	45,000= 25,000=
C.	(i)	Staff training Acquisition, development and	
C.	(i) (ii)	Staff training Acquisition, development and customization of software	25,000=
C.	(i) (ii) (iii)	Staff training Acquisition, development and customization of software Consultancy fees	25,000= 30,000=
C.	(i) (ii) (iii)	Staff training Acquisition, development and customization of software Consultancy fees Miscellaneous	25,000= 30,000= <u>10,000=</u>
C.	(i) (ii) (iii) (iv)	Staff training Acquisition, development and customization of software Consultancy fees Miscellaneous	25,000= 30,000= <u>10,000=</u>
	(i) (ii) (iii) (iv)	Staff training Acquisition, development and customization of software Consultancy fees Miscellaneous Sub Total	25,000= 30,000= <u>10,000=</u>
	(i) (ii) (iii) (iv)	Staff training Acquisition, development and customization of software Consultancy fees Miscellaneous Sub Total	25,000= 30,000= 10,000= 110,000=

(iv) Computer maintenance 35,000=

(v) Electricity Costs 30,000=

(vi) Contingency costs 40,000=

Sub Total <u>145,000=</u>

Grand Total <u>868,000=</u>

5.4 Benefit of the Project

The benefits of the computerized system of computation of the laboratory quantitative analysis are;

- (i) Calculations are fast
- (ii) Correct and accurate results are obtained
- (iii) Reliable results are obtained
- (iv) Valid inferences and conclusion can be made from result obtained.
- (v) Human error in computation is eliminated
- (vi) Result can be retrieved easily and quickly
- (vii) Result can be reproduced quickly and into many copies
- (viii) Several calculations can be performed at the shortest time
- (ix) Result can be stored.

5.5 Change Over

The method of changing from the old manual system to the new computerized system is referred to as change – over. The method of changing from the manual system of calculations in quantitative analysis to the computerized method of computation in laboratory quantitative analysis is the parallel change – over method. As it may be argued by some, this method, is time consuming and

expensive but for the purpose of this project it is the most preferred method for the following reasons;

- (i) It allows the concurrent use of both the old manual method and the new computerized method;
- (ii) Comparism of results obtained from the two methods (if the same) helps in building confidence of the user in the new system;
- (iii) It reduces the risk of complete failure of the system;
- (iv) It provides the system Analyst the opportunity to learn from mistakes in the new system and make corrections;
- (v) It enhances the effective participation of all the users, i.e. staff and students;
- (vi) It confers integrity on the new system.

5.6 Staff Training

The training of staff to handle the daily operation of this new system was identified and considered vital by the system Analyst. The training involved three different groups of the users. And because the project was undertaken in the secondary school chemistry laboratory, those involved in the training were teachers, laboratory assistants and the students.

The training was organized for two chemistry teachers, two laboratory assistants and five students each in SSII and SSIII. The training covered the input – output format of the new system, comparing the result obtained with that of the manual system. This is possible because the two systems were run in parallel.

The different groups were trained to use the new system as a complement to each other. In otherwords, any one of them present in the laboratory during the

conduct of experiments in quantitative analysis will ensure the correct and effective use of the new method of computation.

The training also highlighted error detection. Part of the motivation for those trained was the ease, speed and accuracy with which the result of otherwise complex and tedious computations were carry out by the new system.

The training is designed to be embarked on yearly because of transfer of staff, graduation of the SSIII students and the promotion of students SSI to SSII

5.7 System Testing

The new system was tested with known data and the result of the computation were compared. Moreover since the conversion method used was the parallel change – over the testing was thus made much easier. The data used on the two methods and the results were easily compared for confirmation of their correctness or otherwise. Thus mistakes were easily detected, corrected and avoided.

5.8 Documentation

Documentation is very important in the development of any new system, because it helps in the maintenance and modification of the program in its lifetime.

In computation involving the concentration, purity of substances, molar mass of substances, the documentation covers system specification manual, program manual and the operational manual.

System specification manual:- this include;

- (i) Introduction to quantitative analysis
- (ii) Problem of the manual system
- (iii) Benefits of the new system
- (iv) Implementation of the new system.

Program Manual:- details of the program as a whole and the modules including the line codes on the modules in specified.

Operating manual:- this manual contain the various step description of the working of the system. In other words it contains the outline of how the system can be operated. The details are:

- (i) Activate the computer loaded with windows 95, 98 or 2000 software;
- (ii) Click the start button on the task bar:
- (iii) Click on icon labeled "program"
- (iv) Insert the floppy disk press enter key:
- (v) Click on Windows Explorer then click on floppy disk drive A icon (twice)or once and press enter key;
- (vi) Introduction appears press enter key the main menu appears;
- (vii) Make a choice, press enter key, the program guides the user from here

5.9 System Limitation

The computerization of the laboratory quantitative analysis is limited to only computations in volumetric analysis. That is the result does not cover qualitative analysis; moreover the computation is now automated and can only be operated by a number of staff trained to handle it.

5.91 Handover

At the completion of this project the computerized computations of the laboratory quantitative analysis was handed over to the school authority of government secondary school, Nyanya.

The handing over was necessary to signify the official completion and takeover of the project. However continued support and periodic monitoring of the project was solicited for by the school management and agreed to by the system analyst.

5.92 Conclusion

In today's world "automation" is the word. Hence the increase in awareness, knowledge and the use of computers. As demonstrated in this project computation has been made easier and faster with the development of software to handle the various aspect of laboratory quantitative analysis. Other aspects of laboratory activities should also be computerized. These activities are:

- (i) The laboratory qualitative analysis
- (ii) Inventory of consumables
- (iii) Inventory of laboratory equipment
- (iv) Computerization of allocation of periods in the Chemistry laboratory

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APPENDIX I

A is a solution containing 6.3g /dm³ of impure ethanedioic acid. B is
 0.10 mol/dm³ sodium hydroxide solution.

Put A into the burette and titrate with 25.00cm³ portions of B using phenolphthalein as indicator. Record volume of your pipette.

From your result and information provided calculate the,

- (i) Concentration of A in mol/dm³.
- (ii) Concentration of A in g/dm³.
- (iii) Percentage purity of ethanedioic acid

Equation of reaction is,

$$H_2 C_{22 (aq)} + 2NaOH_{(aq)} \rightarrow Na_2C_2O_{4 (aq)} + 2H_2O_{(l)}$$

A is a solution containing 10.9g/dm³ of an acid H₂Y. Solution B containing
 1.0 mol/dm³ of sodium trioxocarbonate (iv);

If 22.55cm³ of solution A neutralizes 25.00cm³ of 0.10 mol/dm³ of sodium trioxocarnate (iv). Calculate;

- (i) Concentration of solution A in mol/dm³.
- (ii) Molar mass of the acid H_2Y .

Equation of reaction is

$$H_2Y_{(aq)}$$
+ $Na_2CO_{3(s)} \rightarrow NaY$ + H_2O + $CO_{2(g)}$

- 3. A is a solution containing O.050 mol/dm³ of tetraoxosulphate (vi) acid. B is a solution of anhydrous sodium trioxocarbonate (iv).
 - (a) Put A into the burette and titrate with 25.00cm³ portions of B using methyl orange indicator. Record the volume of your pipette.

- (b) From your results and information provided calculate the,
 - (i) Concentration of solution B in mol/dm³

Equation of reaction is;

$$Na_2CO_{3(aq)} + H_2 \; SO_{4\;(aq)} \rightarrow Na_2 \; SO_{4\;(aq)} + H_2O_{(I)} + \; CO_{2(g)}$$

APPENDIX II

```
program volanal;
this program is developed by J.A. Bellos, Reg. No.:PGD/MCS/98/99/860}
{ department of Maths/Computer Science, Federal University of Technology Minna, Niger state}
WinCrt; { Allows Writeln, Readln, cursor movement, etc. }
var
 i:integer;
procedure purity;
var
m,mm,ppent:real;
{this module computes the percentage of purity}
begin
   elrser.
                CALCULATE PERCENTAGE PURITY
   writeln('
                                                                         1);
   writeln:
   write('
                   Enter mass of pure subtance: '); Readln(m);
   write(1
                   Enter mass of impure substance: '); Readln(mm);
   ppent := (m / mm) * 100;
   writeln;
   writeln('
                   The percentage of purity is ',ppent);
   writeln:
   Writeln('
                      Press enter key to return to main menu please...');
   readln.
   ClrScr;
end:
procedure con1;
mm,cb,vb,na,va,nb,cano,congdm:real;
{this module computes the concentration in mole / cubic dm }
begin
   clrscr;
   writeln('
              CALCULATE CONCENTRATION IN G/CUBIC DM (g/dm3)
                                                                                 ');
   writeln:
                   Enter concentration of base : ');Readln(cb);
   write('
                   Enter volume of base:
   write('
                                              ');Readln(vb);
```

```
Enter number of moles of acid: ); Readln(na);
  write('
  write('
                   Enter volume of acid:
                                              ');Readln(va);
                   Enter number of mole of base: ');Readln(nb);
  write('
  write('
                   Enter molar mass:
                                             ');Readln(mm);
  cano := (cb*vb*na) / (va*nb);
  congdm := cano * mm;
   writeln:
                    concentration in mole / cubic dm is ',cano);
   writeln('
   writeln('
                    concentration in g / cubic dm is ',congdm);
   writeln:
   Writeln('
                      Press enter key to return to main menu please...');
   ReadIn:
   ClrScr;
end:
procedure ca2;
var
ca, vb, na, va, nb, cbno: real;
{this module computes the concentration of base in mole / cubic dm}
begin
   clrscr:
              CALCULATE CONCENTRATION OF BASE IN MOLE / CUBIC DM
   writeln('
(Mol/dm3) ');
   writeln;
   write(1
                   Enter concentration of acid: ');Readln(ca);
   write('
                   Enter volume of base:
                                               ');ReadIn(vb);
   write('
                   Enter number of moles of acid:');Readln(na);
  write('
                   Enter volume of acid:
                                               ');Readln(va);
  write('
                   Enter number of mole of base: ');Readln(nb);
  cbno := (ca*va*nb) / (vb*na);
  writeln;
  writeln('
                   concentration of base (Cb) in mole / cubic dm is ',cbno);
  writeln;
```

```
Writeln('
                      Press enter key to return to main menu please...');
   ReadIn;
   ClrScr;
end:
procedure cal;
var
cb, vb.na, va, nb, cano: real;
{this module computes the concentration of acid in mole / cubic dm}
begin
   clrscr;
               CALCULATE CONCENTRATION OF ACID IN MOLE / CUBIC DM
   writeln('
(Mol/dm3) ');
   writeln;
   write('
                   Enter concentration of base: ');Readln(cb);
   write('
                   Enter volume of base:
                                               ');Readln(vb);
   write('
                   Enter number of moles of acid:');Readln(na);
   write('
                   Enter volume of acid:
                                              ');Readln(va);
   write("
                   Enter number of mole of base: ');Readln(nb);
   cano := (cb*vb*na) / (va*nb);
   writeln;
   writeln('
                    concentration of acid (Ca) in mole / cubic dm is ',cano);
   writeln:
   Writeln('
                      Press enter key to return to main menu please...');
   Readln;
   ClrScr;
end:
```

```
ocedure mole:
 i,mm,nmole:real;
 his module computes the number of moles of base}
 egin
  clrscr;
  writeln('
                 CALCULATE NUMBER OF MOLES OF SUBSTANCE
                                                                               '):
  writeln;
  write('
                 Enter mass of the subtance :'); Readin(m);
  write('
                 Enter molar mass of the subtance: '); Readln(mm);
  nmole := m / mm;
  writeln:
  writeln('
                  Number of mole of the subtance is '.nmole):
  writeln:
  Writeln('
                    Press enter key to return to main menu please...');
  Readln:
   ClrScr:
end:
procedure mainmenu;
var chanteger;
begin
repeat
 writeln:
 writeln:
 writeln:
                     ***********MAIN MENU********
 writeln('
                                                                       1):
 writeln:
 writeln;
 writeln('
               1=> CALCULATE NUMBER OF MOLES OF SUBSTANCE
                                                                                 1):
               2=> CALCULATE CONCENTRATION ACID IN MOLE / CUBIC DM
 writeln('
(Mol/dm3) ');
 writeln('
               3=> CALCULATE CONCENTRATION BASE IN MOLE / CUBIC DM
(Mol/dm3) ');
               4=> CALCULATE CONCENTRATION IN G/CUBIC DM (g/dm3)
 writeln('
                                                                                  1);
               5=> CALCULATE PERCENTAGE PURITY
 writeln('
                                                                         ');
 writeln('
               6 => EXIT
                                                      ');
 repeat
   GotoXY(16,13);
   write('Enter your choice:'):
```

```
GotoXY(36,13);
 read(ch);
intil (ch \ge 0) and (ch \le 6);
case ch of
   Emole:
   2:cal;
   3:ca2;
   4:con1;
   5:purity.
 end:
 ntil ch = 6;clrscr;exit;
 id:
  ocedure intro;
  gin
  vriteln:
  vriteln;
  vriteln;
  vriteln;
  vriteln;
  vriteln:
                    COMPUTERIZATION OF LABORATORY QUANTITATIVE
  vriteln('
  NALYSIS
                   1);
                                                          1);
  vriteln('
                             BY
  vriteln('
                          J.A. BELLOS
                                                               ');
  vriteln('
                       REG. NO: PGD/MCS/98/99/860
                                                                        1);
  vriteln('
                      DEPARTMENT OF MATHS / COMPUTER SCIENCE
                                                                                       ');
  vriteln('
                   FEDERAL UNIVERSITY OF TECHNOLOGY MINNA, NIGER STATE
  ');
  vriteln;
  vriteln;
  vriteln;
  Vriteln('
                    Press enter key to continue...');
  teadln:
```

rScr;

d:

egin intro; mainmenu;

end.