Application of computers for experiment design, data acquisition, and analysis in the chemistry laboratory
by Ronald Paul Furstenau

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Chemistry
Montana State University
© Copyright by Ronald Paul Furstenau (1990)

Abstract:
The objective of this research project was to develop an introductory chemistry program which uses computers in the laboratory for experiment design, data acquisition, and data analysis. The project used the Montana State University (MSU) laboratory interface system. The system is an integrated hardware and software package which allows for a wide variety of measurements (pH, temperature, time, voltage, current, etc.) totally under the control of the user. The MSU lab interface system was designed to allow students to participate in the process of science. The hardware and software contain components which allow students to design experiments, acquire data in methods which they choose, and organize and analyze the data to draw conclusions.

To meet the objective, we developed and accomplished the following: (1) we developed a model which explains how computers in the laboratory can improve a student's overall understanding of chemistry and laboratories; (2) we developed a laboratory program which successfully taught students how to use the MSU laboratory interface system to design their own experiments; and (3) we developed, tested, and evaluated experiments designed to utilize the capabilities of the MSU lab interface system.

We successfully integrated the MSU laboratory interface system into our general chemistry laboratories. Our students were able to acquire the conceptual knowledge, lab skills, and computer skills necessary to complete an independent design project using the MSU lab interface system. Students overwhelmingly supported the concept of final projects and found the computers useful for learning chemistry in the laboratory. Our approach to using computers in the chemistry laboratory is unique in the country. A comparable integrated hardware/software system and set of curriculum materials simply does not exist elsewhere on any scale, large or small. Computers are no longer viewed as a novelty or as something "neat" to have in the laboratories at MSU; they are an integral part of the chemistry labs.

APPLICATION OF COMPUTERS FOR EXPERIMENT DESIGN, DATA ACQUISITION, AND ANALYSIS IN THE CHEMISTRY LABORATORY

by

Ronald Paul Furstenau

A thesis submitted in partial fulfillment
of the requirements for the degree

of

Doctor of Philosophy

in

Chemistry

MONTANA STATE UNIVERSITY
Bozeman, Montana

May 1990

D378
F9835

APPROVAL

of a thesis submitted by

Ronald Paul Furstenau

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

May 9, 1990
Date

John R. Edmond
Chairperson, Graduate Committee

Approved for the Major Department

May 10, 1990
Date

Edwin H. Abbott
Head, Major Department

Approved for the College of Graduate Studies

May 24, 1990
Date

Henry S. Parsons
Graduate Dean

STATEMENT OF PERMISSION TO USE

In presenting this thesis in partial fulfillment of the requirements for a doctoral degree at Montana State University, I agree that the Library shall make it available to borrowers under rules of the Library. I further agree that copying of this thesis is allowable only for scholarly purposes, consistent with "fair use" as prescribed in the U.S. Copyright Law. Requests for extensive copying or reproduction of this thesis should be referred to University Microfilms International, 300 North Zeeb Road, Ann Arbor, Michigan 48106, to whom I have granted "the exclusive right to reproduce and distribute copies of the dissertation in and from microfilm and the right to reproduce and distribute by abstract in any format."

Signature Ronald P Furstenau

Date 10 May 90

ACKNOWLEDGMENTS

I would like to thank the Air Force Institute of Technology of the Department of the Air Force for sponsoring my PhD program at Montana State University. I would also like to acknowledge the support given by the Montana Commissioner of Higher Education and the Montana Office of Public Instruction for the MSU laboratory interface project.

I would especially like to thank the superb people at Montana State University with whom I have had the privilege to work with on this project. Pat Hermanson, Dora Anderson, Joan Johnson, Peggy Tombre, and Elaine Howald were all instrumental in building the interface boxes and associated equipment. Bruce Ivey, Dr Reed Howald, and Glenn Howald all made critical contributions to the design of the software. I also had the pleasure of sharing an office with Bruce Ivey, who always patiently answered my endless computer questions, such as "Where's the on switch?". Ray Larsen and Dallas Johnson provided a wealth of advice and suggestions on laboratory experiments.

I must single out the members of the group with whom I had the closest association: Dr John Amend, my advisor, and Kathleen Tucker, the head programmer on the interface project. These two people provided the knowledge, professionalism, guidance, "can do" attitude, and leadership essential for making a project as large as this successful. I have truly been awed and impressed by their talents.

Perhaps the most important support I have received during this project is from my wife Julie. I would never have attempted this work without her support. In addition, I would like to thank my parents, who have shown me throughout my life that "punt" is an unacceptable word in our vocabulary.

TABLE OF CONTENTS

Page

1. INTRODUCTION 1
Establishing a need for our work, plus a review of other aspects of using computers in chemistry.

What Chemistry Needs from Computers in the Laboratory 1
Computers in Chemistry: A Brief History 3
Review 3
KC?Discoverer 4
Some Commercial Software 5
Investigative 6
Computer Simulated Experiments 7
The Microcomputer-Based Laboratory 10
Basic Interfacing 13
Computer Gameport 14
External Circuitry 15
Data Analysis 17

2. STATEMENT OF THE PROBLEM TO BE SOLVED 19
A definition of the objective of this research project and the goals formulated to meet the objective.

The Objective of the Research Project 19
The Goals of the Research Project 19

3. A MODEL FOR USING COMPUTERS IN THE LABORATORY 21
The process of science provides the framework of our model for using computers in the chemistry laboratory.

The Model: Duplicating the Process of Science 21
The Process of Science in the Chemistry Laboratory 24
Integrating Computers into the Process of Science 25
Redistribution of Time 28
Necessary Components of the Model 30

Page

4. THE MSU LABORATORY INTERFACE HARDWARE AND SOFTWARE 32
The design of the hardware and software incorporates the steps in the process of science.

Hardware 33
The Interface as an Instrument 33
The MSU Lab Interface 34
Software 38
Design Principles 38
The MSU Lab Interface Software 40
Main Menu 41
Calibration 41
Builder 42
Runner 43
Spreadsheet 43

5. THE LABORATORY PROGRAM 47
The laboratory program develops conceptual, laboratory, and computer skills to allow students to fully participate in the process of science.

Workshops: The Foundation 48
Instructor Demonstrations 49
Instructor-Led Experiment Design Exercises 50
Performing Staff-Designed Experiments 51
Teachers Designing Experiments 52
A Pilot Program: The Framework 53
Going Full Scale: Involving All of the Students 57
The Overall Approach 57
Laboratory Instructor Training 59
The Computer Book 61
Lesson 1: Getting Started 61
Lesson 2: Designing a Basic Experiment 63
Lesson 3: Basic Measurements with a Photocell 65
Lesson 4: Changing the Display of Data 66
Lesson 5: Obtaining Data the Interface Can't Measure 68
Lesson 6: More Practice and Programming Tips 69
Lesson 7: More Graphing and Math Functions 69
The Laboratory Manuals 70
Chem 125/135 70
Chem 136 71
The Final Projects 74

Page

6. EXPERIMENTS 78
The speed, accuracy, and precision offered by the MSU lab interface system opens new doors to experimentation in the chemistry laboratory.

Thermometry 78
The Ag^+/Cl^- Reaction 82
Formation of Complex Ions of Cadmium 86
Acid/Base Titrations 91
The Strong Acid/Strong Base Titration 92
Weak Acids and Bases 97
Acetic Acid (Vinegar) 97
Phosphoric Acid 99
Carbonate Titration 101
Colorimetry 105
Quantitative Light Absorption 107
Kinetics 113
Nuclear Chemistry 119
Decay as a Random Process 119
Beta Radiation 121
Determining Half Lives 125

7. RESULTS AND SUMMARY 131
Computers are a useful tool for learning chemistry in the laboratory.

Preliminary Evaluations: The First Quarter 132
Evaluation of Our Approach, Methods, and Materials 135
Recommendations for Future Work 150

REFERENCES CITED 153

APPENDICES 161

Appendix A -- Chem 125/135 Final Projects 162
Appendix B -- Chem 136 Projects 202
Appendix C -- Experiment Programs for the MSU Lab Interface ... 230

LIST OF TABLES

Table		Page
1.	Table of Contents for *Using Computers in the General Chemistry Laboratory*	62
2.	Chem 125 Laboratory Schedule	72
3.	Chem 135 Laboratory Schedule	72
4.	Chem 136 Laboratory Schedule	73
5.	Chem 125/135 Final Projects	74
6.	Chem 136 Projects	75
7.	Equilibrium Constant Data for Cadmium Iodide Complex Ions	87
8.	Thermodynamic Values for Cadmium Iodide Complex Ions	88
9.	Determination of Beta Radiation Penetration Using the Standard Deviation Method	124
10.	Examples of Experiments Designed for the MSU Lab Interface	130
11.	Comments from the Chem 125/135 Final Project Critique: Autumn 1989	134

LIST OF FIGURES

Figure — Page

1. The Microcomputer-based Laboratory (MBL): Laboratory Interfacing 11
2. The Process of Science 22
3. The Process of Science in the Laboratory 24
4. The Personal Computer in the Laboratory 27
5. Time Allocation in a Traditional Chemistry Lab 28
6. Time Allocation in the MSU Computer-based Chemistry Lab 30
7. Components of a Laboratory Instrument 33
8. The Computer as Part of an Instrument System 34
9. The MSU Laboratory Interface 35
10. Block Diagram of the MSU Lab Interface Electronics 36
11. MSU Lab Interface Software Flowchart 40
12. Screen Photo of the **Main Menu** Options 41
13. The Menu Structure of the **Builder** Subprogram 42
14. The **Spreadsheet** 45
15. Simple Program to Measure Temperature and Display the Value on the Screen 50
16. A Cadmium Sulfide (CdS) Photocell 51
17. Student Graph Illustrating Beer's Law for Cu^{2+} Solutions 56

LIST OF FIGURES -- continued

Figure		Page
18.	Flowchart for the Introductory Chemistry Laboratory, Chem 125	58
19.	Photocell/Lights Experiment	69
20.	Student at a Laboratory Station	76
21.	A Photograph of a Thermistor	79
22.	Resistance Versus Temperature for a 5-kohm Thermistor	80
23.	Ln(R) Versus 1/T for a 5-kohm Thermistor	81
24.	Experiment Program to Obtain Thermistor Operating Characteristics	82
25.	Ag^+/Cl^- Thermometric Titration	85
26.	Experiment Program for Thermometric Titrations	85
27.	Appearance of the **Spreadsheet** in the **Analysis** Mode	86
28.	Determination of Cd^{2+}/I^- Complex Ion Formation	89
29.	Manual titration to Determine Cd^{2+}/I^- Complex Ion Formation	90
30.	Experimental Set-up for Acid/Base Titration	93
31.	pH Versus Volume for a HCl/NaOH Titration	94
32.	pH Versus Volume Curve for HCl/NaOH with Derivative	95
33.	Temperature and pH versus Volume for the HCl/NaOH Titration	96
34.	Temperature and Derivative Curves Superimposed	96
35.	pH and Temperature Curve for Vinegar Titration	98
36.	Temperature and Derivative Curve for Vinegar Titration	98
37.	Temperature and pH Curves for a Manual Vinegar Titration	99
38.	Phosphoric Acid pH/Temperature Titration Curves	100

LIST OF FIGURES -- continued

Figure		Page
39.	Sodium Carbonate pH/Temperature Titration Curves	101
40.	Program to Obtain pH and Temperature Values for a Timed Titration	103
41.	Program to Obtain pH and Temperature Values for a Manual Titration	104
42.	Cut-away View of the Colorimeter Box	106
43.	Principle Behind Beer's Law	106
44.	Transmission Currents for Co^{2+} Calibration Curve	108
45.	**Spreadsheet** Calculations and Graph for the Transmittance of Co^{2+} Samples	109
46.	Linear Regression Analysis of the Transmittance Data	110
47.	Beer's Law: Absorbance Versus Concentration for Co^{2+} Solutions	111
48.	Experiment Program to Obtain Transmission Current Data	112
49.	Changing Bromine Concentration During the Br_2/HCOOH Reaction	115
50.	Test for a First Order Reaction: $\ln[Br_2]$ Versus Time	116
51.	Least Squares Plot for First Order Relationship	116
52.	Test for Second Order in Br_2 on the Br_2/HCOOH Reaction	117
53.	Program for the Br_2/HCOOH Kinetics Experiment	118
54.	Counts from a Uranium Sample Over a 30-Second Time Period for Twenty Experiments	120
55.	Counts Data with Lines Indicating +/- One and Two Standard Deviations of the Mean	121
56.	Experiment Program to Determine Beta Radiation Penetration	122

LIST OF FIGURES -- continued

Figure		Page
57.	Determination of Beta Penetration Limit Through Index Cards	123
58.	Bar Graph of the Beta Penetration Data Using Index Cards	125
59.	Decay Curve for Tl-207	126
60.	Program to Determine Half Lives Using a Demonstration for Counter Input Data	127
61.	Ln(N_t) Versus Time for Tl-207 to Determine Half Life	128
62.	Chem 125, #1: Do you feel that doing projects in Chem 125 is a good idea?	135
63.	Chem 125, #2: The Chem 125 projects were challenging	136
64.	Chem 125, #3: The Chem 125 weekly laboratories (not the projects) were challenging	136
65.	Chem 125, #4: In the role of designing experiments, acquiring data, and analyzing data, do you believe that computers are useful for learning chemistry in the laboratory?	137
66.	Chem 125, #5: Are you more comfortable with computers as a result of taking Chem 125?	138
67.	Chem 125, #6: Based on your experience in Chem 125, were the laboratory computers easy to use?	138
68.	Chem 125, #7: Was the Chem 125 lab book easy to read and understand?	139
69.	Chem 125, #8: Was the book "Using Computers in the General Chemistry Laboratory" easy to read and understand?	140
70.	Chem 135, #1: Do you feel that doing projects in Chem 135 is a good idea?	141
71.	Chem 135, #2: The Chem 135 projects were challenging	141
72.	Chem 135, #3: The Chem 135 weekly laboratories (not the projects) were challenging	142

LIST OF FIGURES -- continued

Figure Page

73. Chem 135, #4: In the role of designing experiments, acquiring data, and analyzing data, do you believe that computers are useful for learning chemistry in the laboratory? 142

74. Chem 135, #5: Are you more comfortable with computers as a result of taking Chem 135? 143

75. Chem 135, #6: Based on your experience in Chem 135, were the laboratory computers easy to use? 143

76. Chem 135, #7: Was the Chem 135 lab book easy to read and understand? 144

77. Chem 135, #8: Was the book "Using Computers in the General Chemistry Laboratory" easy to read and understand? 144

78. Chem 136, #1: Do you feel that doing projects in Chem 136 is a good idea? 145

79. Chem 136, #2: The Chem 136 projects were more challenging than the Chem 135 projects 146

80. Chem 136, #3: The Chem 136 weekly laboratories (not the projects) were more challenging than the Chem 135 laboratories 146

81. Chem 136, #4: In the role of designing experiments, acquiring data, and analyzing data, do you believe that computers are useful for learning chemistry in the laboratory? 147

82. Chem 136, #5: Are you more comfortable with computers as a result of taking Chem 135 and Chem 136? 148

83. Chem 136, #6: Based on your experience in Chem 135 and Chem 136, were the laboratory computers easy to use? 148

84. Chem 136, #7: Was the Chem 136 lab book easy to read and understand? 149

85. Experiment Program to Determine Heat Capacity of Materials 232

86. Experiment Program for the Comparison of Insulation Materials 233

LIST OF FIGURES -- continued

Figure		Page
87.	Experiment Program to Measure Sediment Concentration in Water	234
88.	Experiment Program to Measure Sedimentation Rates	235
89.	Experiment Program to Measure Hamster Activity	236
90.	Program to Measure Reaction Time for an Unanticipated Event	237
91.	Program to Measure Reaction Time for an Anticipated Event	238
92.	Program to Measure the Growth Curve of a Yeast Colony	239
93.	Experiment Program for Finding an Unknown Resistance	240
94.	Experiment Program for Determining Planck's Constant	241
95.	Program to Check Photogate Alignment	242
96.	Program to Determine the Acceleration Due to Gravity	243
97.	Program to Measure the Voltage of a Designed Battery	244
98.	Program for the Timed Titration of Toilet Bowl Cleaner	245
99.	Program for Determining Beta Radiation Penetration	246

ABSTRACT

The objective of this research project was to develop an introductory chemistry program which uses computers in the laboratory for experiment design, data acquisition, and data analysis. The project used the Montana State University (MSU) laboratory interface system. The system is an integrated hardware and software package which allows for a wide variety of measurements (pH, temperature, time, voltage, current, etc.) totally under the control of the user. The MSU lab interface system was designed to allow students to participate in the process of science. The hardware and software contain components which allow students to design experiments, acquire data in methods which they choose, and organize and analyze the data to draw conclusions.

To meet the objective, we developed and accomplished the following: (1) we developed a model which explains how computers in the laboratory can improve a student's overall understanding of chemistry and laboratories; (2) we developed a laboratory program which successfully taught students how to use the MSU laboratory interface system to design their own experiments; and (3) we developed, tested, and evaluated experiments designed to utilize the capabilities of the MSU lab interface system.

We successfully integrated the MSU laboratory interface system into our general chemistry laboratories. Our students were able to acquire the conceptual knowledge, lab skills, and computer skills necessary to complete an independent design project using the MSU lab interface system. Students overwhelmingly supported the concept of final projects and found the computers useful for learning chemistry in the laboratory. Our approach to using computers in the chemistry laboratory is unique in the country. A comparable integrated hardware/software system and set of curriculum materials simply does not exist elsewhere on any scale, large or small. Computers are no longer viewed as a novelty or as something "neat" to have in the laboratories at MSU; they are an integral part of the chemistry labs.

CHAPTER 1

INTRODUCTION

This thesis represents the compilation of the methods and efforts used to integrate computers into the general chemistry laboratories at Montana State University (MSU). In Chapter 1, I set the stage for the purpose and details of our work by examining the role of computers in the laboratory, detailing some of the history behind the use of computers in chemistry, and discussing some of the basics behind computer interfacing. This chapter lays the foundation for the approach taken in our effort. Chapter 2 highlights the specific objectives of this thesis project. In Chapter 3, I describe a model for using computers in the chemistry laboratory, based on the process of science. This chapter establishes our method and rationale for using computers in the laboratory. Chapter 4 summarizes the hardware and software capabilities of the MSU lab interface system. This system is the focal point for our laboratory development. In Chapter 5, I detail the development of our general chemistry laboratory program, starting with workshops and a pilot program and finally going full scale. Chapter 6 follows with a discussion of several experimental methods which illustrate the capabilities of the MSU laboratory interface system. Finally in Chapter 7, I summarize the results of our computer-based laboratory program, with the emphasis on student feedback.

What Chemistry Needs from Computers in the Laboratory

No one can argue the fact that computers are playing an increasingly important role in chemistry and society in general. The impact of computers on today's chemistry laboratories is overwhelming. Almost all modern chemical instrumentation

is now computerized in one way or another. Designers of mass spectrometers, nuclear magnetic resonance spectrometers, and scores of other instruments find computers invaluable for acquiring data quickly and analyzing the data once it's obtained. Computer-controlled signal processing and detectors have dramatically increased instrument precision and sensitivity. Moreover, computers have greatly assisted the users of such instrumentation by increasing the control of experiment variables.

Chemistry certainly benefits greatly by the creativity which computers can help foster in the laboratory. In a manner which will be discussed later in this thesis, computers can assist in the design of experiments. The power of rapid (or slow) data acquisition and versatile data analysis allow the experimenter to do research more quickly and to discover scientific relationships not previously possible without the computer.

It may appear from the first two paragraphs of this section that the computer has become a tool only for the modern chemical researcher . . . *this is not true!* Computers can also significantly improve the manner in which students learn chemistry. Through the interfacing of personal computers with experiments, computers can better involve students in the process of science. Computers can allow students to accomplish laboratory tasks which could not be done otherwise. In short, chemistry needs computers in the student laboratory to provide new opportunities for learning modern experimental methods and experiment design. The majority of this thesis will describe the development of a chemistry laboratory program at Montana State University (MSU) involving the use of computer-experiment interfacing. I will focus on the *development of a model* explaining how computers in the laboratory can improve a student's overall understanding of chemistry and laboratories, the *organization of the laboratory program*, and the *development of experiments* using the MSU laboratory interface system.

Before I begin discussing the details of my research project, I will use the introduction to discuss the historical role of computers in the chemistry laboratory, some basic interfacing concepts and systems, and the role of data analysis in computer interfacing. This background material will lead into the statement of my research problem in Chapter 2.

Computers in Chemistry: A Brief History

Computers have found many roles in the teaching of chemistry over the years. The role of the computer can be split into two general categories: review and investigative. *Review* refers to the use of tutorial and drill software programs for better understanding chemical concepts. *Investigative* refers to using computers to perform calculations, simulate experiments, acquire data, analyze data, and design experiments.

Review

Having computers in the laboratory implies that the computers are available to help not only in the experimental portion of chemistry, but the conceptual part as well. Tutorial and drill software has long been available for a variety of purposes. Castleberry and Lagowski (1) were probably the first to use computers for tutorials on a large scale back in 1970. Tutorial and drill programs are basically used as a method of providing individualized instruction. In chemistry, *tutorial* programs are used as a step-by-step method of teaching about chemical concepts. For example, a gas law tutorial may begin by presenting written information on the screen, and perhaps actively illustrating the basic concepts behind Boyle's and Charles' laws. The user of the tutorial may then literally "page" through the information, much like a book. A computer tutorial has the advantage over a book, however, of being able to "demand" interaction by asking questions. A gas law tutorial may then lead the user into combining the gas laws into the ideal gas law, perhaps eventually requiring the student

to solve gas law problems. The tutorial may now become a *drill* program, posing a series of problems which the student may answer. Most drill programs provide a variety of problems on a subject. Some drill programs explain to the users how they are doing problems incorrectly and what must be done to get on the right track. Since most tutorials contain components of drill programs and visa-versa, I will now refer to tutorial and drill programs collectively as tutorials.

It has only been in the past 10 years, coinciding with the proliferation of personal computers, that the variety and quality of tutorial software has made it a viable option for teaching and learning chemistry in almost any school. In almost every chemistry department in every major college and university, some faculty member has been involved with their own development of tutorial software for their chemistry undergraduates. Since 1981, the Journal of Chemical Education has had no less than 50 articles pertaining to new developments in computer-assisted instruction (CAI) in general, physical, organic, and biochemistry.

The commercialization of many tutorials has done much to make CAI a viable teaching tool. Companies such as HRM Software, COMPress, and Intellectual Software have done a great deal in ensuring that well-tested, debugged tutorials are making their way to general availability. The importance of quality control that is obtained through commercialization cannot be overestimated. Easy to run, "idiot-proof" software is a must for wide-spread use of tutorial software in a chemistry curriculum. No professor would consider using a poorly proofread, error-riddled book in a course; likewise, users have a right to expect the best out of commercially available software. To illustrate the potential usefulness of tutorial software for teaching chemistry, I will discuss a few of the highest quality, most widely used tutorials that are currently available.

KC?Discoverer. Project SERAPHIM, a clearinghouse for information about the use of personal computers in chemical education, has been instrumental in

providing software to interested users at nominal fees (2). Sponsored by the National Science Foundation and the Department of Education, Project SERAPHIM has become a center for the collection, development, and distribution of chemistry software. Perhaps the best product to date to come out of Project SERAPHIM is the multipurpose KC?Discoverer tutorial (3,4). KC?Discoverer allows users to explore the periodic table by graphing and tabulating numerous properties of the elements. Periodic trends in properties such as electronegativity and atomic radius can be seen graphically, quickly and easily. This computerized "CRC Handbook" allows anyone with an interest in chemistry to "dig in" to the periodic table. In fact, we (at MSU) have integrated KC? Discoverer into our introductory chemistry laboratory program to compare with experimental values for electrical conductivity (5).

Because of the clearinghouse function of Project SERAPHIM, it is not possible to thoroughly test and debug all of the software which they distribute. Much of the software has little or no documentation. Project SERAPHIM provides an extremely useful function, but the software distributed is often not usable on a large scale. Commercial software is beginning to provide the quality of programs needed for undergraduate chemistry.

Some Commercial Software. In my opinion, the best tutorial software now available for general chemistry has been developed by Dr Jack Weyh and co-workers at Western Washington University. Included in their bank of software is the "Tools of Chemistry" series, a set of tutorials dealing with such topics as scientific notation and significant figures (6). Much of the reason for Weyh's success lies in the philosophy behind the development of his software. As Dr Weyh puts it, "Drill and practice has a negative reputation. [We must] develop something that the students will enjoy" (7). The big advantage of Weyh's tutorials is that they emulate the paper and pencil logic that students already have. Everything a student needs is at his or her finger tips: a "pop-up" calculator, periodic table, and help screens. The special use of keys is

explained quite well. In addition, the logic and flow is exactly the same in all of Weyh's tutorials, making them all easy to use once the basics are learned.

Another highly regarded chemistry software series is "Introduction to General Chemistry", produced by Dr Stanley G. Smith's group at the University of Illinois (8,9). The series includes more than fifty instructional programs and must be regarded as the most comprehensive series currently available. As with Weyh's software, Smith's series has very consistent operating instructions from program to program. Many of the programs make excellent use of color for illustrating chemical reactions. As with many other tutorials, the Smith tutorials are slow. Slowness is an advantage to a student who needs the extra time in the learning process, but a nuisance to a student who simply needs extra practice.

Tutorials or *review* are but one use of computers in chemistry. In many instances, however, it seems as though a student would be much better off if he or she simply used the time spent on tutorials to work homework problems from their textbook! But these tutorials can provide a tireless, patient mechanism for teaching students fundamental chemical principles. In that regard, the proper integration of tutorials into a chemistry curriculum can help to fill many gaps. But for the chemistry laboratory, the *investigative* role of the computer is a more valuable role than that of review.

Investigative

The *investigative* role of the computer in the laboratory can provide the main assistance in exploring the experimental aspects of chemistry. The first use of computers in the investigative role was for providing computational support for experimental data and theoretical calculations, certainly pre-dating computerized tutorials. As early as 1959, Swinnerton and Miller discussed using digital computers to solve complex chemical equilibrium problems (10). By the mid 1960's, computational methods for acid-base chemistry, equilibrium, and kinetics became more common

(see, for example, references 11, 12, and 13). Physical chemistry was also an early beneficiary of these computational techniques, with molecular orbital calculations becoming a common topic (14,15). In fact, physical chemistry has been one of the most progressive areas of chemistry in terms of using the computer. Entire physical chemistry courses have recently been built around the use of microcomputers to individualize instruction (16). Error analysis and least-squares programs were also early favorites in applying computers to instructional chemistry (17,18).

On the basis of sheer volume of literature, the maturation of computers in chemistry instruction seems to have begun in the early 1970's, coinciding with greater accessibility to mainframe computers and the birth of minicomputers. It should also be noted that during the 1970's the hand-held, programmable pocket calculator also made a significant contribution toward "personalizing" computer use in chemistry. References 19-21 are just a few examples of using programmable calculators in chemistry. It was the 1980's, however, which brought computers into the adulthood of chemistry instruction with the wide-spread introduction of the micro, or personal, computer. Since this thesis involves the use of personal computers in the laboratory, I will focus primarily on post-1980 computer advances.

The introduction of the microcomputer to chemistry has spawned two major development areas within the traditional chemistry laboratory. These areas are *computer simulated experiments* and the *microcomputer-based laboratory*, or *MBL*. (Note: The term microcomputer-based laboratory, MBL, has been borrowed from several sources, including references 22 and 23.)

Computer Simulated Experiments. It can be fairly stated that computer simulated experiments provide the "extreme" alternative to the traditional laboratory. Equipment and chemicals are replaced with the computer and software. Computer simulations create the "no chemicals/no glassware" laboratory. All of the processes involved in laboratory -- the mixing of chemicals, heating and cooling, and control of

apparatus -- are accomplished via the simulation program. Dr. Donald L. Pavia, a leader in the design of computer simulations for chemistry, points out that simulations have two great advantages. First, simulations can focus time, allowing more situations to be covered during a given time period. Secondly, simulations "can relieve students of dependence on their technical and manual skills," which translates into more time to think abstractly about what they are doing (24). As Jones et.al. add, simulations allow students to perform or view reactions "too hazardous, too expensive, or too time-consuming for them to perform in the laboratory" (25). From the literature, 1984 seems to mark the beginning of well-designed simulation programs. The well-designed simulations are highly-interactive, flexible, easy to use, and non-threatening. Computer simulations fall into three categories: *simulated experiments*, *instrumentation emulators*, and *interactive video.*

With *simulated experiments*, the only hardware required is a personal computer or a terminal tied into a mini- or mainframe computer. Because of the relatively straight-forward calculations involved, acid-base titration curves were among the first simulated experiments in chemistry (26). More recent advances in simulation have emphasized decision making skills. Weyh has developed a simulated inorganic qualitative analysis program which duplicates the thinking skills and powers of observation required in a traditional qualitative analysis laboratory (7). All of the thinking is still left to the students; poor choices can give contradictory results and tests can fail. The simulation does not interpret the results. Similarly, Pavia has developed a simulated organic qualitative analysis program which includes spectroscopic data (24). David Whisnant's simulation, BCTC, provides a scenario in which a hypothetical toxic substance has been released into a river (27). The student must do a simulated analysis of the water to identify the substance and also make economic decisions regarding the control and clean up of the pollutant. These simulations provide color, activity, and help to degrees that will make even the computerphobe smile!

Sophisticated *instrumentation emulators* for personal computers have also been developed. Manual spectrophotometers were perhaps the first instruments to be emulated (29), with development continuing because of these instruments' popularity in general chemistry (30). Not only can instrumentation emulators simulate an actual experiment, but they can also provide valuable, non-threatening experience before ever touching the actual instrumentation. The mainstay tools for organic chemistry -- nuclear magnetic resonance (NMR) spectroscopy, mass spectroscopy, and infrared spectroscopy -- have all been emulated at least to the extent of being valuable training tools for undergraduate chemists. Because of the high costs of such instrumentation, the use of emulators solves time constraint and economic problems, as aircraft operators have realized for decades! Paul Schatz at the University of Wisconsin has developed an outstanding emulator for a Varian EM360 60 MHz NMR (31), while Howard and DuBois have developed a similar emulator for the Varian T-60 NMR (32). Robert Rittenhouse at Eastern Michigan has developed an emulator for High Performance Liquid Chromatography (HPLC) (27). Calculational techniques have also been developed to synthesize mass spectral isotopic abundances, in which simulated spectra are produced (33). In addition, our research group has made initial attempts to use the MSU laboratory interface software to simulate infrared and mass spectra. Instrumentation emulators hold much promise for developing better trained students using modern, complex chemical instrumentation.

Perhaps the most unique approach to computer simulations has been in the area of *interactive video.* Interactive video, primarily with videodiscs, has made it possible to incorporate recorded television images and audio into a computer program. This allows the programmer to combine and overlay computer texts and graphics on the same screen. This technique requires specific and expensive computer and videodisc hardware, described in reference 25. The unquestioned leaders in this technology as applied to chemistry is the group headed by Smith and Jones at the University of Illinois (25). Their group has developed numerous chemical experiment simulations

using interactive videodiscs, including the topics of the physical properties of elements, chemical reactions, and chemical kinetics (34). The interactive videodisc has the advantage of allowing the student to see videos of actual chemical reactions taking place, not computer-generated images which lack realism. This allows students to see chemical reactions not normally performed due to cost or safety issues. In many interactive scenarios, the student can choose what reactants and how much of each reactant to use. The University of California at Los Angeles and the University of Nebraska have also been extremely active in developing videodisc technology for chemistry, developing programs for acid-base titrations and classroom demonstrations (35,36). It is clear that the interactive videodisc is rapidly becoming a usable tool for the chemistry laboratory.

As innovative and useful as computer simulated experiments are becoming, they are still not a direct substitute for laboratory work (25). As Pavia notes, "it is still necessary for the chemistry student to master certain manual laboratory techniques", with the computer simulation enhancing the learning experience (24). MacKenzie points out that simulations "suffer by their abstract presentation of real world phenomena" (22). Students can simply develop a false sense of reality from the simulation of complex phenomena where the possibility of error becomes minimized or non-existent. Computer simulations, then, do not provide the ultimate solution to the implementation of computers into the chemistry laboratory. Treading the water between the traditional laboratory and the simulated laboratory is the microcomputer-based laboratory, or MBL.

The Microcomputer-Based Laboratory. The MBL can be thought of as an intermediate between the simulation at one extreme (abstract, little human involvement), and the traditional experiment at the other (inaccurate, of limited scope, labor intensive) (22). The MBL, also known as laboratory interfacing, uses a computer connected to an experiment to detect and control what is occurring in that experiment.

(I will use MBL and computer interfacing interchangeably throughout this thesis.) A very simplified block diagram of the MBL concept is shown in Figure 1.

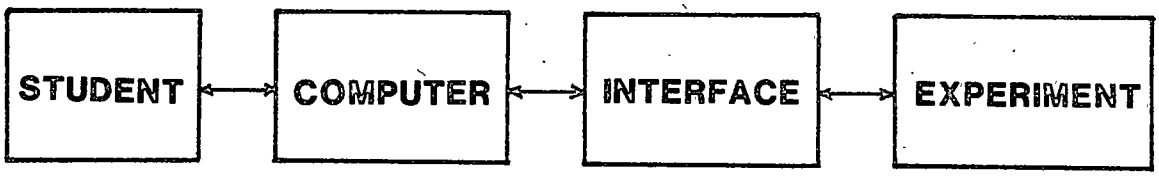

FIGURE 1. The Microcomputer-based Laboratory (MBL): Laboratory Interfacing.

In laboratory interfacing, real world experimental variables are measured or controlled with a variety of sensors. The signals from these sensors (of light, temperature, etc.) are monitored by the interface electronics. The computer provides the data acquisition and control. Unlike simulations, laboratory interfacing is a part of the laboratory environment, not an extension of that environment. In the MBL, computers are *in* the laboratory, not outside of it.

Of all of the uses for computers in the chemistry curriculum, laboratory interfacing is unquestionably the least developed. Although computer manufacturing variety (non-standardization) and other hardware factors have contributed to underdevelopment, the most probable reason is economic. In the past, the cost of competent microcomputers and complexity of interfacing made it economically impractical on a large scale. Within the last 5 years, however, inexpensive and powerful microcomputers have made the MBL an economically attractive alternative in laboratory modernization. As will be developed in this thesis, the MBL is attractive from a pedagogical standpoint as well.

The MBL has many advantages over the traditional laboratory and computer simulations. First of all, *computers in the laboratory expose students to the way science is really done in the 1990's!* Nearly every research effort in chemistry and physics

involves the use of computers for data acquisition, analysis, instrument control, or information retrieval. It is the disadvantaged student indeed who happens to drudge through graduate school in the sciences today without computer experience! Why shouldn't we use computers for the same functions in our undergraduate laboratories?

Secondly, *computers can gather large amounts of data rapidly and accurately.* This advantage creates the opportunity to design experiments and study chemical concepts which would normally not be possible in the traditional laboratory. More complicated and challenging experiments can be developed. The computer allows the student to manipulate these massive amounts of data in meaningful ways.

The third main advantage of the MBL provides much of the impetus for this thesis work. The MBL can *help teach students to think independently in the laboratory and to participate in the process of science.* As Marcus Mendenhall puts it, one of the most important skills to learn in the laboratory is "to think about the limits to an experiment or, more generally, the limits to anything with which one might interact in the real world" (37). Simply put, *the MBL allows the student greater control of a laboratory experiment.* As this thesis will develop, the MBL can foster creativity in the laboratory for even the non-scientist. The computer can remove barriers to experimentation while teaching new skills, thus promoting creativity. With time, the computer can become as natural and as important a tool in the laboratory as beakers and chemicals. In addition, the MBL makes it easy to incorporate nearly all of the aspects of computerized chemistry instruction previously described.

The remainder of this thesis will detail the application of computer interfacing in introductory chemistry laboratories. This INTRODUCTION chapter will conclude with sections describing the basics of a MBL, including basic interfacing concepts and data analysis. The remaining chapters of this thesis will detail the application of the MSU lab interface system at Montana State University.

Basic Interfacing

The purpose of this section of the INTRODUCTION is to provide the reader with some background information about different types of computer interfacing. This section will contain very little detailed electronics specifications, though many of the references cited contain this type of information. The text will focus on describing basic interfacing concepts and some of the approaches to computer interfacing found in the literature. The details of the interface used in this research, the Montana State University (MSU) laboratory interface system, will be discussed in Chapter 4.

What is meant by the term *computer interfacing*? In a general sense, computer interfacing means the integration of the computer into the laboratory as a scientific instrument; the microcomputer-based laboratory (MBL). In a specific sense, computer interfacing means connecting a computer to laboratory instruments for data acquisition and control. Certainly, data analysis should be considered a part of computer interfacing. But because of its strictly software nature, I will discuss data analysis separately in the last section of the INTRODUCTION.

The fundamental goal of basic computer interfacing is quite simple: to develop hardware devices which act as sensors in the experimental environment and software which can access these sensors (38). Sensors include devices to measure time, temperature, light, current, voltage, humidity, pH, radiation, or whatever is needed in the experiment. Dr Michael H. Powers, one of the nation's leaders in developing and promoting do-it-yourself interfacing, divides computer interfacing into two categories: connection via the *computer gameport* and via *external circuitry* (38).

Computer Gameport

Historically, the early proliferation of Apple, Commodore, and Atari computers made gameports a popular hardware target for interfacing. This is due to the easy access to input and output signals (39). Gameports are normally attached to a joystick or game paddle for use with video games. A joystick is simply a set of four switches, whereas a game paddle is a potentiometer connected as a variable resistor. Depending on the model of computer, the gameport is either an internal 16-pin input/output (I/O) connector socket inside the computer, or an external 9-pin "D" connector. Each pin has a particular assignment (data flow, ground, +5 volts, etc.) and are discussed in detail in references 40 and 41.

DeJong and Layman have led the way in the development of do-it-yourself gameport interfacing for science teaching (primarily in physics), beginning in the early 1980's (41-43). Their applications, primarily with Apple II computers, include using thermistors, phototransistors, and timers. It should be noted that DeJong and Layman's do-it-yourself approach requires significant skill in electronics and programming in either assembly language or BASIC. However, much of the driving software is readily available and inexpensive. Many others have developed data collection devices and experiments for Apple II computer gameports with a variety of transducers and instruments, with temperature being the most commonly measured quantity (44-53). Similar gameport interfacing projects have been developed for the Commodore VIC-20 and C-64, which include experiments with thermistors, cadmium sulfide light cells, radiation detectors, and colorimeters (54-56). Again, these efforts require considerable programming and electronics skills. Several gameport enthusiasts cite the removal of tedious data collection as a primary reason for developing computer interfaced experiments. In other words, an important reason for interfacing is to save time, allowing students to focus on the analysis and interpretation of their results.

The main advantage of these homemade gameport interface experiments is that they are usually very inexpensive, with basic tranducers and connectors costing less than $10. The main disadvantages, already pointed out, are that considerable programming and electronics skills are often required. In addition, gameport devices tend to be slow. These disadvantages severely limit the flexibility of gameport interfacing. Greater flexibility is offered through *external circuitry.*

External Circuitry

Using external circuitry involves using electronics packages outside of the computer. An external circuit, then, is an *interface* between the computer and the sensing device. The interface conditions signals, translates signals, and essentially allows for communication between the computer and sensing devices. Of course, no communication is actually possible unless there is software which can translate between the interface and the computer. External circuitry devices will normally allow faster sampling rates and higher resolution than gameport devices. In addition, external circuitry devices will generally allow multiple sensors, a variety of different sensors, and protection of the internal computer circuitry (38). These devices range from the very simple to the very complex.

A very simple device can be an integrated circuit, along with a few electrical components, wired to a breadboard. More complicated interfaces are prepackaged (like the MSU lab interface) and involve many more components. It should be pointed out that most modern chemical instrumentation, like a nuclear magnetic resonance spectrometer, incorporates very specific interface devices (complete with software) which allow the operator to completely control the instrument.

The fact that Apple and IBM-type microcomputers are bus-based make them ideal candidates for interfacing by external circuitry. A bus is simply a bundle of wires which can pass commands from one part of the computer system to another.

These computers contain a motherboard which houses the computer bus. The system can be expanded for computer interfacing by plugging in boards into the bus (57). The bus-based system makes communication with the computer a reasonably straightforward, though not simple, task.

External circuitry devices can communicate with the computer in a number of ways. These include serial communications (also known as the RS-232 standard link) and parallel communications. The GPIB (general-purpose interface bus), often referred to as the IEEE 488 parallel transmission system, is a popular option for instrumentation control. Annino and Driver provide an excellent discussion of standard computer communication interfaces in Reference 57. Communications can be accomplished via ports already built into the computer, or via specially designed cards which are installed into the computer.

There are many instances in the literature of application- or instrument-specific interfaces designed and built by researchers. References 39 and 58-60 provide a few examples. Some are simple, some are very complex. Commercial vendors, such as Vernier Software (38), HRM Software (38), Champ (61), IBM (23), and Tel-Atomic (62,63) provide completely assembled interface packages over a range of prices. All vendors seem to take a different approach to hardware design and communication methods. Some require the user to program the interface unit using BASIC. Others have prepackaged software designed to take specific measurements, offering little flexibility to the user. From a general sense, key design considerations for data acquisition external circuitry include signal conditioning, transmission cabling, filtering, sampling rates, digital input/output (I/O), and analog I/O (57).

One of the promising aspects of computer interfacing may also be the Achilles' Heel for widespread application: there are *so many ways* to do computer interfacing! A laboratory interface may be very simple, requiring only a few electronic components. Or, the interface may be very complex, requiring intricately designed circuit boards. It is the variety of interfaces, the complexity of the electronics, and

the lack of standardization which has hampered the widespread application of computer interfacing into instructional laboratories (22). Equally important is the lack of versatile, easy-to-use software. It is important to note that we view the MSU laboratory interface as an effort to establish an integrated approach to laboratory interfacing. *This integrated approach requires not only hardware development, but integrated software, experiment, and curriculum development as well.*

Data Analysis

The ability to use a computer to perform rapid data analysis must be viewed as an integral part of the microcomputer-based laboratory. The hardware and software to accomplish data acquisition is the high visibility aspect of the MBL. But it is the software that can analyze, graph, and display the data which is often the most important to the user. Being able to organize data and draw conclusions from that data is an important part of the process of doing science. A data analysis package can make it much easier to see what experimental data *really* means, removing boring and tedious activities such as repetative calculations.

It should not be surprising that there are many examples in the literature of using commercial spreadsheets for data analysis. Commercial, multi-purpose spreadsheets such as Lotus 1-2-3 and Quattro are highly developed, well polished products. These spreadsheets offer a wide range of calculational and graphing capabilities. Levkov gives a good discussion of the uses and capabilities of Lotus 1-2-3 for the science lab (64). Joshsi offers a similar, more detailed discussion of Lotus 1-2-3 specifically for physical chemistry (65). Kari and Dubreuil have used SUPERCALC 3A for an Apple IIe computer in their chemistry laboratories (66). Powers details the use of the Vernier Software voltage input unit and pH electrode to obtain pH titration data for sodium carbonate and HCl (67). The data file is then analyzed and/or graphed using the Vernier Software Voltage Plotter III, AppleWorks,

PROSTAT, and Sigma-Plot spreadsheet packages. IBM has attempted to integrate a data analysis package into their Personal Science Laboratory MBL concept, with mixed results (68).

For the most part, commercial spreadsheets are *not* easy to learn how to use. The quality which makes these spreadsheets so popular is also their biggest drawback for widespread laboratory use. This quality is versatility. Versatility implies many options and capabilities. This can lead to confusion for the user who simply wants to do data analysis and graphing of his or her experimental data. We felt it was necessary, then, to develop a data analysis capability tailor-made to the capabilities of the MSU lab interface hardware and to the abilities of our students. An integrated, easy-to-use spreadsheet should be an important part of any MBL effort.

Although many bits and pieces exist, an integrated approach to using computers in the chemistry laboratory simply does not exist outside of MSU. It is the purpose of this research project to establish a laboratory program and develop experiments around the laboratory interface concepts designed and built at MSU. I will discuss the objectives of my research project (or, a statement of the problem to be solved) in the next chapter.

CHAPTER 2

STATEMENT OF THE PROBLEM TO BE SOLVED

The Objective of the Research Project

As discussed in Chapter 1, there have been many, varied efforts to employ the personal computer into instructional chemistry. However, it is apparent from the literature that the personal computer has not yet been well integrated into the instructional laboratory, especially at the introductory level. Certainly, no researcher has come close to applying computer interfacing to the general chemistry laboratory in a broad, effective manner. In some areas, it almost seems that the computer has been a solution waiting for a problem. In some instances, the computer has been used without really thinking about what it is that needs to be accomplished. The previous statement is in no way meant to diminish the many fine efforts already made in developing the computer as an instructional tool in chemistry. On the contrary, it is meant to underscore the need for careful development of computer usage in instructional chemistry, especially as a laboratory tool. One of the greatest potential uses for the computer as an instructional tool lies in the introductory laboratory. *The objective of this research project is to develop an introductory chemistry program which uses computers in the laboratory for experiment design, data acquisition, and data analysis.*

The Goals of the Research Project

The MSU laboratory interface system gives us the chance to make this opportunity a reality. As will be discussed in subsequent chapters of this thesis, computers offer us a chance to teach laboratory science in the manner in which it is

actually done. This requires developing new curriculum materials which take advantage of computers in the labs. It also requires the "rethinking" of the types of labs we do, taking advantage of the new areas of experimentation which computer-laboratory interfacing-- the microcomputer-based laboratory-- can open up to us. The following goals were developed to meet the objective previously described:

(1) Develop a model which explains how computers in the laboratory can improve a student's overall understanding of chemistry and laboratories.

(2) Develop a laboratory program which successfully teaches students how to use the MSU laboratory interface system to design their own experiments.

(3) Develop, test, and evaluate experiments designed to utilize the capabilities of the MSU lab interface system.

The organization of the remainder of this thesis will follow the presentation of these goals. In Chapter 3, I will discuss a *model* for using computers in the chemistry laboratory. Chapter 4 will follow with a description of the *MSU lab interface hardware and software* and how it compliments the model described in Chapter 3. The *laboratory program* will be discussed in Chapter 5, with a description of *experiments* following in Chapter 6. I will *summarize the results* of this thesis work in Chapter 7.

CHAPTER 3

A MODEL FOR USING COMPUTERS IN THE LABORATORY

One learns science by doing science. A simple statement, but it provides the underlying reason for teaching chemistry laboratories in the first place. It will also provide the rationale for using computers in the laboratory. From this "doing" perspective, science is very similar to art and sports. One becomes good at science by doing science, not just by being a passive observer. Chemistry is very much a "doing" science, a laboratory science.

But how does one *do* science? Most scientists would agree that one does science using the *scientific method* or the *process of science.* Others consider the scientific method as the ground rules within which the game of science is played, not a prescription for carrying out scientific research (69). Nonetheless, the *process of science* provides a framework for a systematic approach to scientific research (70). *The process of science will provide the basis of our model for using computers in the chemistry laboratory.*

The Model: Duplicating the Process of Science

Our main goal in involving computers in our general and introductory chemistry labs is to teach science the way science is actually done. In the process of science, also known as the scientific method, the following iterative process is prescribed (71,72):

(1) Look for unexplained behavior in nature (Identify Problem).

(2) Design experiments which will yield information concerning this behavior (Design Experiment).

(3) Collect this information (Collect Data).

(4) Organize this information to look for cause and effect relationships (Organize Data, Draw Conclusions).

A graphical representation of this process is shown below in Figure 2. The circle and quadrants were chosen to represent the process because the scientific method is a dynamic, interactive process. In reality, science is seldom done in a rigid, step-by-step process. Indeed, it is far more common that one group of scientists propose an important problem to study, with others designing and performing the experiments. Still others may propose theories to account for the results, while other groups design experiments to distinguish between competing theories (69).

PROBLEM –> EXPERIMENT –> DATA —> GENERALIZATION

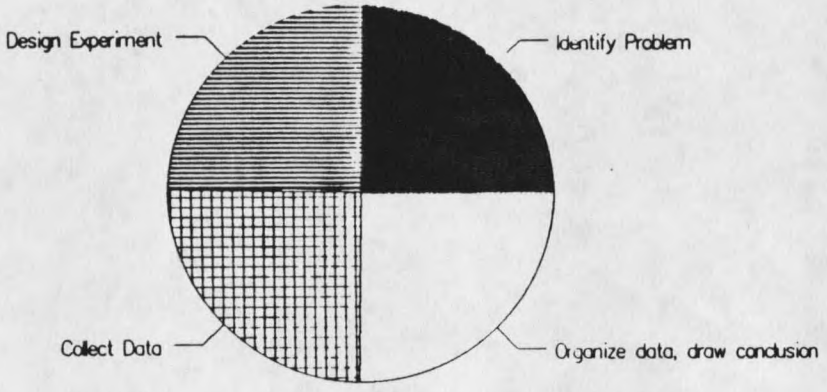

FIGURE 2. The Process of Science.

The process of science is a creative process. As J.V. Mallow states, "Science is not simply a series of cookbook recipes. In fact, as any creative chef knows, neither is cooking simply a series of recipes" (69)! It takes creativity to know what to look for in nature. It takes creativity to design experiments which yield information about behavior in nature. It certainly takes creativity to develop meaning and theories from experimental data. The process of science does not provide the answers; it provides a method for *finding* the answers.

Learning science involves the learning of basic skills. As Chang notes, the study of chemistry involves three basic steps: observation, representation, and interpretation (70). *Observation* skills are learned in the laboratory by seeing chemical reactions and observing the results of chemical and physical phenomena. Important clues to a chemist will likely mean nothing to the average student unless observation skills are developed. A chemist *represents* what he or she observes through the use of chemical equations, mathematical formulas, graphs, and tables. These methods of representing observations communicates the information to others. Therefore to learn chemistry, a student must also learn the methods by which chemists communicate. Finally, chemists *interpret* chemical concepts by proposing theories involving atoms and molecules which they cannot see, but account for their observations. As one can see, using the scientific method involves not only understanding the process, but having the skills to apply it. Figure 3 is a different representation of the process of science shown in Figure 2, emphasizing some of the skills involved in the process. Again, the process of science is an iterative and dynamic one. The steps in solving laboratory problems shown in Figure 3 hold true regardless of whether it is a research lab or a student lab. The only difference is the degree of difficulty and the point at which the student may enter the picture.