Proceedings of the Nova Scotian Institute of Science (2025)
Volume 54, Part 1, pp. 23-35

CHEMISTRY AND COMPUTERS – A PERSONAL RECOLLECTION

JOHN C.O'C. YOUNG*

Department of Chemistry, Saint Mary's University
Halifax, NS B3H 3C3

PREAMBLE

Employment as a senior chemical research engineer with a US oil company led me to a two year loan assignment to its refinery in Dartmouth, Nova Scotia, in 1967-69. During this period, I came to like living in Nova Scotia, so in January, 1970, I resigned and became a computerization advisor to then President of Saint Mary's University (SMU), Dr. Henry Labelle, S.J. Subsequently in 1972, I was offered the position at SMU as an associate professor of physical chemistry with a particular research interest in computerization of analytical chemistry procedures.

EARLY COMPUTERIZATION (1970-72)

My first task in 1970 was to upgrade the University's computerized registration and timetable system. At that time, computerization at SMU consisted of a single small mainframe unit, an IBM Model 1130 (Fig 1). It sat in air conditioned splendor in its own room and probably had no more computing capacity than a modern day laptop. The IBM 1130 Computing System was introduced in 1965 aimed at price sensitive, educational and engineering technical markets.

Data input to this computer was by key punching Hollerith cards that were then optically scanned by a reading machine (Fig 2).

I vividly remember the twin evils of punched Hollerith card data input and batch processing. After hours and hours sitting at a card punching machine, I would submit my humble offering of a box or two full of these punched cards to the tender mercies of the attendants of the computer who looked after "batch processing." I would return the next day, often to find one of my boxes sitting on a shelf with one card turned on its side pointing upwards from its fellows indicating

* Author to whom correspondence should be addressed: john.young@smu.ca

Fig 1 The IBM 1130 computer and system layout.

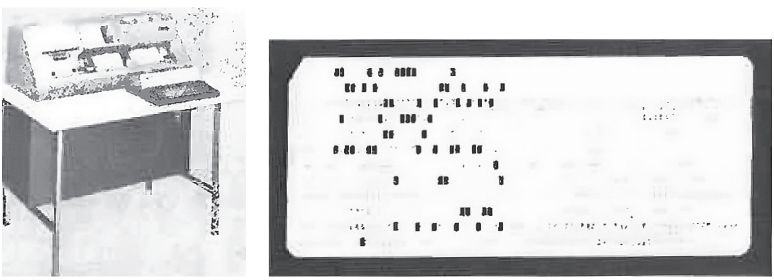


Fig 2 Card punching machine and punched card.

that, after key punching numerous entries in several hundred cards correctly, I had made an error of entering a colon instead of a semi-colon in that one card. This would cause the computer to imperiously reject my offering. I then had to re-punch this card, resubmit my card boxes and return once again the following day to collect the results.

With luck, all would be well with the handed in cards but after a card deck had been submitted and read a few times, the card reader had a tendency to chew up cards. Another problem was that the card punch would get slightly out of line and not place slots in exactly the right places for the optical card reader to find them.

The eventual replacement of this technology by direct entry of data from a keyboard into computer memory came as a merciful relief.

COMPUTERIZED INFORMATION ACCESS (1972-77)

I introduced undergraduate courses at SMU in "Environmental Chemistry" (CHE 371.0) in 1972 and "Marine Chemistry" (CHE 372.0) in 1974. As part of the laboratory components of these courses, I required my students to make supporting, mainframe-based computerized, background studies.

In 1977, we upgraded our exploration of information data bases and their search engines when, in collaboration with a Research and Reference Librarian, Douglas Vaisey, we began computerized information searching on the mainframe computer using the WATDOC data base of the of Department of Fisheries and Environment, Canada. Somewhat later, we switched to the more sophisticated DIALOG and CAN/OLE systems.

THE APPLE II MICROCOMPUTER (1976-1980)

Steve Wozniak designed the original Apple computer and formed Apple Computer Inc. with Steve Jobs in 1976. The Apple II microcomputer was introduced by the two Steves in 1977 and was followed in 1979 by the amazingly capable and very successful upgraded Apple II Plus version (Fig 3).

This microcomputer eventually sold over five million units mostly for educational purposes. Shown in Fig 4, it featured data input from and data storage on floppy disks and a pair of "game paddles" to manipulate screen images, precursors of the computer mouse. Student members of my group and I played many happy primitive computer games of "Pong" and "Little Brick Out" on this setup. We also connected sensors of temperature, pressure and pH to the computer's game port to monitor the progress of analytical experiments.

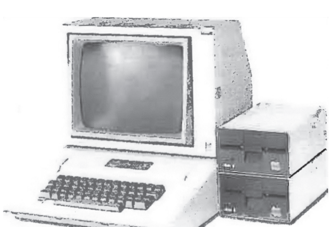


Fig 3 The Apple II Plus microcomputer.

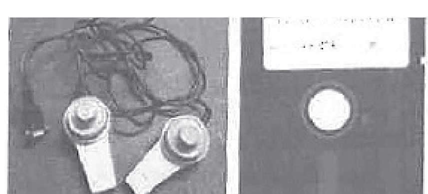


Fig 4 A pair of game paddles and a floppy disk.

DEVELOPMENTS (1981-1990)

In 1981, physics teachers, David and Christine Vernier, started Vernier Software & Technology, a US company to produce and market software for analyzing and presenting experimental data from the Apple II Plus microcomputer, an event of major later importance for us at SMU.

At around the same time, John Moore founded “Project Seraphim” to collect, evaluate and distribute chemistry-related computer software as part of a U.S. National Science Foundation funded initiative to bring active learning methods to the chemistry curriculum. This initiative produced a substantial library of chemistry and physics experiments that was made available on 5 1/4 inch floppy disks for Apple Il Plus and PC microcomputers through the U.S. Journal of Chemical Education’s “JCE Software” program.

In the late 80s, we took our first faltering steps into real-time computerized data logging. Using a combination of an Apple II Plus microcomputer, Vernier’s Voltage Input (A/D) Unit, and a thermistor temperature probe run by Vernier’s Unit Plotter software program, we monitored the temperature of my research laboratory. Based on these early experiences, I introduced courses on “Scientific Uses of Microcomputers” in 1989 and 1990 (CSC 387.1 and 388.2).

THE ARRIVAL OF THE MACINTOSH (1984-1990)

Somewhat earlier, back at Apple Computer Inc. in Cupertino, the two Steves were busy introducing the first of their line of Macintosh computers in 1984. This model had a measly 128 K of RAM and a fragile power supply that delighted in frying itself. Apple rapidly replaced this original version with a 512 K Model and then got it right in 1986 when the Company introduced the Apple Mac Plus with a luxurious 1 meg of RAM and a decent fan to cool its power supply.

The Mac Plus (Fig 5) was the first commercially successful microcomputer to feature a mouse accessible, graphical user interface (GUI) (Fig 6).

I and fellow SMU faculty members, Vic Catano and David Swingler, purchased Mac Plus microcomputers from the first batch of forty of these machines imported into Canada, whereupon I abandoned our venerable Apple II Plus microcomputers. My original Mac was eventually stolen!

Fig 5 The Apple Mac Plus microcomputer.

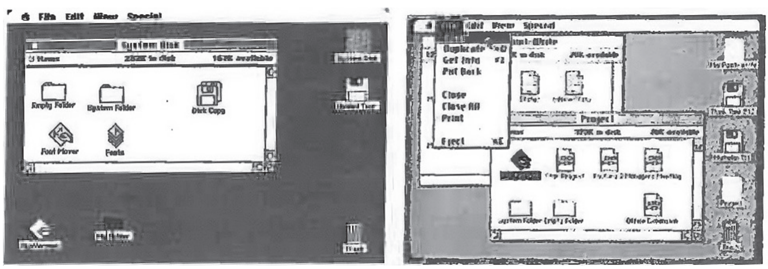


Fig 6 The Mac Plus desktop layout.

In the early 1990s, Vernier introduced its Serial Box Interface, the simple but very capable, two channel 12-bit A/D converter (Fig 7) in which the analog signals from sensors of physical properties such as temperature and pressure were digitized and delivered to Vernier's Data Logger program for analysis. With all the essential features of a modern data logging, analysis and presentation system, this was the combination we had been waiting for.

The outcome of a Boyle's Law validation experiment obtained with this data logging and analysis system is shown in Fig 8.

In July 1996, I retired from the university, the last year of mandatory retirement. However as a professor emeritus, the university provided me with modest office and laboratory facilities and, with a generous annual operating grant from the Federal Department of Energy, Mines and Resources, my research group of undergraduate students continued its studies of computerized analytical chemistry procedures.

Fig 7 The Serial Box Interface.

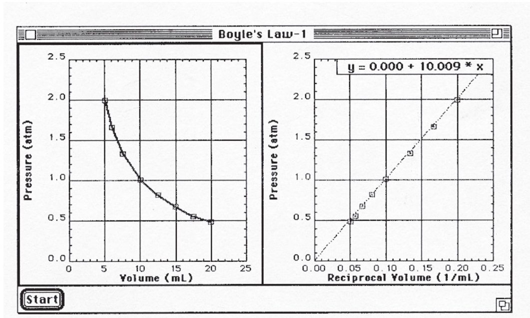


Fig 8 Boyle's Law relationship investigation.

In the Spring of 1996, I became the chairperson of the Nova Scotia – Gambia Association, a Halifax based NGO that carried out health education programs for high school students in The Gambia. It also provided on-site administration of a university course extension program there for SMU, that small African country not having its own university at the time. Under this extension program, faculty members from Maritime universities were recruited by SMU to teach undergraduate program courses in a compressed, five full day a week, six to eight week format, the students only taking one course at a time.

In November 1996, the notice (Fig 9) appeared on information boards around the Chemistry Department announcing my talk on "Computerization of the Introduction Chemistry Laboratory."

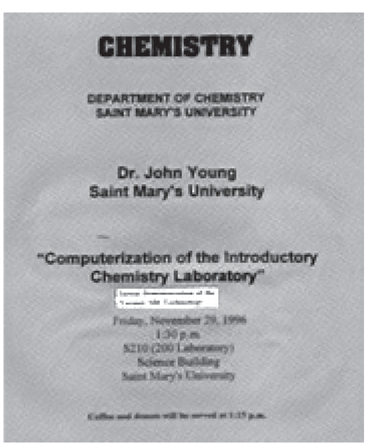


Fig 9 A chemistry meeting notice.

Despite free coffee and cookies, my talk failed to convince my colleagues to introduce the Data Logger and SBI computerized data collection and analysis system as part of the Department's first year general chemistry course. However, having anticpated this outcome, I had planned ahead.

OFF TO THE GAMBIA

Earlier in the summer of 1996, I began my plan to deliver our regular first year chemistry course in The Gambia, coupled with my computerized version of the associated laboratory course beginning in January, 1997. I purchased glassware and chemicals with a contribution from the Canadian High Commission in Dakar, Senegal, scrounged a dozen used Macs "from somewhere", and shipped these laboratory requirements off to Vernier in the United States. The company there combined these items with its contribution of Data Logger program disks and sets of pH electrodes, conductivity probes, pressure sensors, temperature probes and colorimeters sensors, and shipped everything off in a container to the port city of Banjul, the capital of The Gambia.

After a short flight from Halifax to Newfoundland, I was one of a few passengers as we took off again from St. John's for Heathrow at close to midnight on December 31st 1996. Air Canada gave me a celebratory New Year offering of warm champagne in a paper cup!

I was on my way to the first of three very enjoyable visits to The Gambia in 1997 and 1999 to teach my computerized chemistry course, and in 2000 as a member of team sent there to advise its government on how to establish a university which it did subsequently.

Somewhat to my surprise, upon my arrival in The Gambia, I found that my various boxes of supplies and equipment had all arrived, were intact, had been cleared through local Customs, and were waiting for me at the Gambia Technical Training Institute (GTTI) where I was to deliver the course with the help of my able Gambian assistant, Momodou Jain.

Over my first weekend in The Gambia, Momodou and I set up a dozen laboratory stations with glassware, solutions and of course the Macintosh microcomputers with their Serial Box Interfaces and Data Logger operating program (Fig 10).

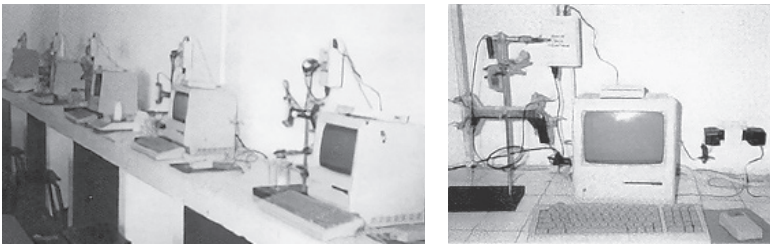


Fig 10 Computerized chemistry at the Gambia Technical Training Institute (GTTI).

I began the lecture component of the course the following Monday morning. Momodou and I delivered an introduction to the laboratory component in the afternoon.

The contents of this laboratory program were as follows:

The Gambia Laboratory Program, January – March 1997

EXP01: Boyle's Law: Pressure-Volume Relationship in Gases
Pressure Sensor/Event Mode (*Calculation of R*)

EXP02: Charles' Law: Pressure-Temperature Relationship
P and T Sensors/Event Mode (*Absolute zero of temperature*)

EXP03: Vapor Pressure of Liquids: Clapeyron-Clausius
P and T Sensors/Time Mode (*Two liquids,* D*Hvap*)

EXP04: MW Determination by Freezing Point Depression
Temperature Sensor/Time Mode (*Kf determination*)

EXP05: Heat of Reaction, Hess's Law of Heat Summation
Temperature Sensor/Time Mode (*Plastic cup calorimeter*)

EXP06: Heat of Combustion of Magnesium
Temperature Sensor/ Time Mode (*Three step reaction*)

EXP07 : Chemical Equilibrium Constant Determination
Colorimeter Sensor/Event Mode (*Beer's Law calibration*)

EXP08: Acid and Base Titration
pH Sensor/Event Mode (*End point from second derivative*)
EXP09: Diprotic Acid Titration
pH Sensor/Event Mode (*Buffering, pK determination*)

EXP10: Solubility Product by Conductometric Titration
Conductivity Sensor/Event Mode .(*BaCl2, H2SO4*)

EXP11: Weak Acid Dissociation Constant Determination
pH Electrode/Event Mode (*Acetic acid)*

EXP12: Crystal Violet Decolorization Kinetics
Colorimeter Sensor/Time Mode (*Orders of CV+ and OH-*)

The first year chemistry course is one of the most difficult that students face and Momodou and I were determined that no student would fail our version in The Gambia. We worked the students hard during the week, injecting enough humour to keep the stress level low, and Momodou's boot camp review sessions on Saturday and Sunday mornings ensured that not one of our twenty students finished with a grade level lower than C and there were a number of As. Some years later, Momodou obtained a doctoral degree in chemistry from the Norwegian University of Bergen, then became the first Registrar of the fledgling University of The Gambia.

Our chemistry lecture and laboratory program garnered a considerable amount of favorable local publicity in The Gambia and a long and interesting visit to the lab by Dr. Federico Mayor. Dr. Mayor, a chemist and then the Director General of the United Nations Educational Scientific and Cultural Organization (UNESCO), was in Banjul to determine whether the GTTI should receive financial support from UNESCO. I made sure that news of these events leaked back to Halifax.

RETURNING FROM THE GAMBIA

When I returned from The Gambia in April, 1997, the Chemistry Department Chairperson, Michael Zaworotko, asked me to set up the "Gambia Laboratory System" and implement it in September, 1997, as the laboratory component of the Fall offering of the Department's first year general chemistry course.

In the summer of 1997, student Andrew Corbett and I set up twenty four computerized laboratory stations in the first year teaching laboratory. As shown in Fig 11, so as not to occupy laboratory surface space, we constructed a dozen stands on which we installed the computers in pairs above the laboratory sinks. Each pair of Mac Plus computers shared a printer and each computer system was fitted with the Data Logger program, a serial box interface, a set of sensors, a mouse and a stirrer-heater unit. The set of sensors included a thermistor, a pressure

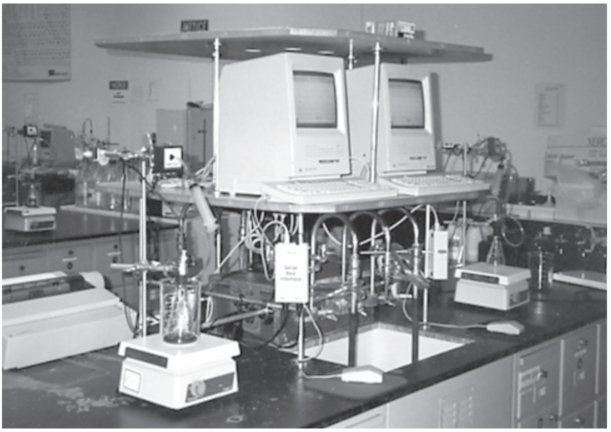


Fig 11 A pair of 1997 laboratory workstations.

sensor, a pH electrode, and even a personal spectrophotometer for each pair of students.

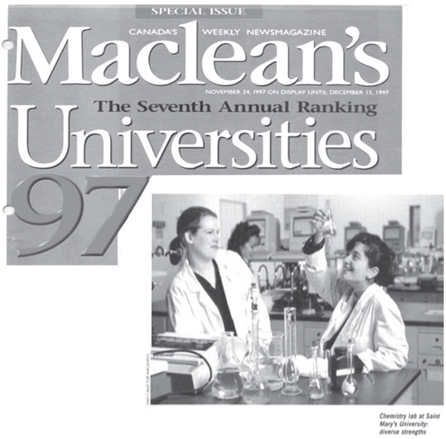
We then tested procedures for twelve experiments, wrote up a laboratory manual, and made everything ready for a September 1997 beginning. Also of note, Andrew graduated from SMU in 1997, obtained his Ph.D. degree from McGill University, and at last report was the Director of Production Chemistry for the Toronto Research Chemicals company.

Our delivery of this first year chemistry laboratory program in Fall, 1997, attracted some national attention shown in Fig 12.

SUBSEQUENT DEVELOPMENTS

In September, 2001, we switched from Macs to PCs because, aside from our laboratory and the Psychology Department, SMU was a PC shop. At that time, Vernier only offered a PC version of its new Logger Pro software to replace its venerable Data Logger program. To make this change, I scouted second-hand computer stores in Nova Scotia and New Brunswick and came up with an assortment of very used, Model 486 desktop microcomputers which we set up to run the SBI / Logger Pro system under the Windows DOS 3.1 operating system.

The first year chemistry laboratory in 2001 is shown in Fig 13 and the original desktop display of the Logger Pro program is shown in Fig 14.



Two parts chemistry, three parts ingenuity

by Peggy Berkowitz

Dr John Young works with a student in Saint Mary's chemistry laboratory.

A retired professor's insp...ion from teaching in The Gambia has gone to show, once again, that necessity ...ally is the mother of invention.

John Young, professor emeritus of ...hemistry at Saint Mary's University in ...alifax, went to The Gambia two years ...o to teach a first-year chemistry course, ...nowing that the small West African coun...y couldn't afford to buy the standard ...ieces of equipement that are found in every ...ndergraduate chemistry lab. Dr Young's ...olution to the problem was so elegant ...at Saint Mary's chemistry faculty voted ...o convert their entire first-year chemistry ...b to a model first tested in the Gambian ...apital of Banjul.

Typically, an undergraduate chemistry ...b program consists of a set of old and ...ell-tried experiments involving the use ...f a limited range of instruments (pH meters, ...pectrophotometers, conductivity bridges, ...nd the like). These instruments are generally ...uite expensive, take up scarce lab bench ...

Dr Young replaced these types of instruments with sets of compatible sensors which measure acidity/alkalinity, light absorbance, electrical conductance, temperature, pressure and various other parameters. The analog (or voltage) signals from these sensors are fed to a single interface at each work station, which digitizes this signal information and transmits it to the data processing computer. The system permits "mixing and matching" of different sensors for different experiments, as well as simple procedures for analysing relationships between the outputs of the sensors used.

The sensors, interfaces and much of the software come from Vernier Software, a U.S. company. Dr Young scrounged yard sales, among other places, for obsolescent Macintosh computers and PCs. Voilà! a flexible, low-cost system which allows students to process, analyse, graph and report the results of a wide variety of experiments in real time.

"It's the best innovation I've seen in a long time for first-year chemistry labs," says Robert Singer, a young chemistry professor at Saint Mary's, who ...

"In first-year chemistry labs, you have these traditional tried, tested and true experiments that everyone's doing across the country. They're about 20 years old and are getting pretty boring. So when Dr Young did this, I thought, Yeah! we've made it to the '90s!"

Cheaper system

In The Gambia, the main spur was price. When they weren't donated, old Macs cost from $100 to $150 each. Each Vernier sensor costs about $100 and the analog/digital interface, about $150. Some sensors aren't very sophisticated — the light absorption sensor measures only two or three wavelengths — but they're adequate for a first-year lab. For his course in The Gambia, Dr Young shipped 12 work stations worth $1,000 each plus $8,000 of chemical supplies and equipement. (The total cost of $20,000 was covered by a grant from the Canadian Embassy ...

8 UNIVERSITY AFFAIRS

Fig 12 Some national attention of SMU's chemistry laboratory program.

Fig 13 The first year chemistry laboratory in 2001.

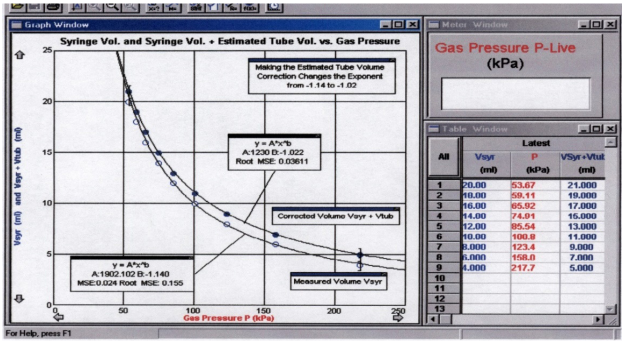


Fig 14 **The original Logger Pro desktop display.**

Fig 15 **The renovated first year chemistry laboratory at SMU.**

In 2003, we switched from Vernier's venerable Serial Box Interfaces to its more capable LabPro Interface, each of which provided four analog and two digital sensor ports in place of the two analog sensor ports of the SBI.

At about the same time, the Dean of Science, David Richardson, gave me some cash and once again I went shopping in second-hand computer stores. This time, I landed in Moncton where I picked up forty Dell Pentium III computers at $75 apiece. They had been disposed of by a government department that was upgrading.

The outcome of a major re-construction of the first year general chemistry laboratory that took place in 2007-08 is shown in Fig 15.

While many program changes have been introduced subsequently, the backbone of our chemistry laboratory is still the PC microcomputers, the LabPro interfaces, the physical property sensor sets, and the remarkable Logger Pro data logging, analysis and presentation program that puts Excel to shame. A few examples of views of activities in the lab are shown in Fig 16 and complete this overview of the evolution of chemistry and computers at SMU.

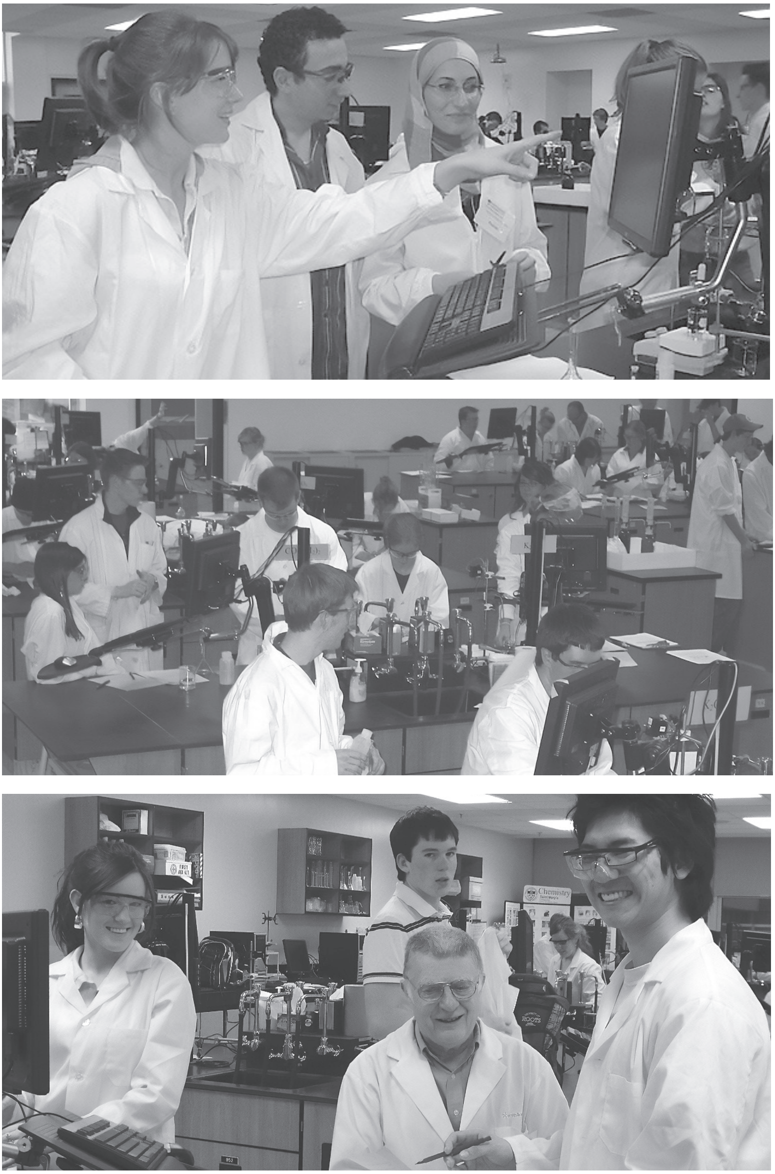


Fig 16 At work in the chemistry laboratory at SMU. The author is shown in the third photo, along with happy hard working students.