Research on Computers in Chemistry Education: Reflections and Predictions March 29, 1993

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Chemists have been accustomed to the use of technology since the alchemy stage of the discipline, and incorporation of technology into the teaching laboratory has been a natural occurrence. Thus, it should not be surprising that chemists were some of the first people to include computers in the educational setting, such as Lykos at Illinois Institute of Technology at Chicago in 1959 (*1*). As computers became more powerful and less expensive, chemists found different ways of using them for educational purposes.

It is interesting to note that usual progression of chemistry enterprise has been from research to development. That is, research into the nature of a chemical concept precedes the development of chemical applications. This progression, however, has not been evidenced in the history of chemistry educational computing. From 1966 to 1981, 5% of the journal articles that concerned computers and chemistry were educational research reports. This figure actually decreased 1% in the next 10 years (1982–1992).

The purpose of this paper is to present a short overview of the significant milestones in the history of chemistry educational computing, a discussion of educational computing research techniques, and suggestions about the implementation of chemical educational computing research. I also will present a short discussion of new and forthcoming technologies that hold promise for the advancement of computers in the chemistry classroom. I hope that this paper will cause discussion and encourage chemical educators to expand chemical educational computing research. However, before we discuss where we should go, it would be a good idea to look at where we've been.

A Brief Overview of the History of Chemistry Educational Computing

Lykos' IIT chemistry educational computing project was the first to receive extensive funding from the National Science Foundation ($3.9 million) (*2*). The students in this project used the computer to find Chemical Abstracts Condensates references for two topics. They also searched manually through CAC and were asked to evaluate the benefits and problems associated with the computer searches. Later in the project, Lykos emphasized student programming activities (*3*).

The first record of chemistry educational computing research was published by J. J. Lagowski in 1970 (*4*). This project was implemented at the University of Texas–Austin in 1969 and the researchers investigated the effects of a lab simulation that was supposed to help the students build decision-making skills. Lagowski and his team used a randomized, treatment-control, quasi-experimental research design that used student performance and questionnaire data. The results indicated that the treatment group scored significantly higher on computer-related material, while no or little difference was noticed in their scores on other chemistry material that was not included in the computer simulations.

Perhaps the best known landmark in the development of chemical educational computing is the proposal and NSF funding of Project Seraphim in 1983 (SERAPHIM, by the way, stands for Systems Engineering Respecting Acquisition and Propagation of Heuristic Instructional Materials) (*5*). This project was proposed soon after the advent of small personal computers and was designed to provide an avenue for the distribution of educational software for chemists and summer training programs for chemists who wished to design educational software (*6*). Project Seraphim still serves as the major conduit of chemical educational software, though NSF funding has elapsed. The chemical educational computing community has been served well by individuals such as John and Elizabeth Moore, who continue the Project Seraphim mission.

During the years since the first implementation of computers in chemical education, the equipment has changed a great deal. The first computer used was a huge mainframe that would occupy a large room. By the time that Project Seraphim started, the educational computer had become equipment that could be placed easily on a small desk. But while the smaller computers of the early 1980's offered good calculation capability, their relative (to today's personal computers) lack of speed and computational power limited their use in the classroom. The personal educational software of the early 1980's primarily tended to be drill and practice software (in which the user paged through the computer screen at the press of the space bar or enter key), simple games (one of my favorites at the time was a chemistry trivia game), and some simulations. These computers were good information displays and instrument controllers, but their use in the classroom was soon discovered to be limited to those educational uses that involved limited user interaction.

An exception to this was the freshman chemistry development project at University of Illinois at Champagne–Urbana (*7*). This university was a pioneer in many areas of general computing and was one of the earliest schools to incorporate computers extensively in the general curriculum. The installation of the PLATO system, a computer that allowed students to check their grades, take tests, and receive messages (among other things), demonstrated an early commitment to educational computing (see previous discussion). This commitment was extended by Stanley Smith and Loretta Jones by their development of computer-controlled interactive videodisc chemistry laboratory experiments (*8*). Note that UI hired the first person in a chemistry department whose formal doctoral training had a major instructional development component for the expressed purpose to expand and bring innovation to their freshman chemistry program (the significance of this will be explained later in this paper). Jones and Smith developed computer-based titration experiments that pushed the frontiers of computer-based instruction. One of the most important features of their software was that the program displayed different pictures of the titration in response to the previous user actions. As the user made errors in the preparation of standards and samples, the computer "tracked" these and the subsequent titration data reflected these variations. Thus, the titration pictures appeared exactly as a "wet" titration would, even to the point that the shade of the endpoint color differed by the amount that the student undertitrated or overtitrated!

There were two aspects of the UI software that mark a turning point in the nature of chemical educational software. Their programs contained artificial intelligence programming and included computers as an integral part of educational media. Educational media (at the time that Jones and Smith started their work) primarily consisted of slide shows, overhead projectors, and films, and computers were not used as a part of common classroom media. Smith and Jones also programmed the computer-based training so that the computer kept track of the users input and adjusted what the user experienced accordingly. This type of programming is part of what has been called educational artificial intelligence (AI). Artificial intelligence programming is best thought of as an attempt by a computer programmer to make the computer "behave" as a person (*9*). Adaptive programming such as that in the UI software is a fundamental feature of educational artificial intelligence (educational AI will be discussed in more detail later in this paper).

So here we are in the 1990's and computers seem almost human at times. A small portion of the USA population may say that they have no interaction with computers, but the average citizen in our country experiences computers in some form every day. The majority of our students are comfortable with computers and technology. But how does the chemical educator know that the computers are a positive influence in her/his classroom? Educational computing research will provide some basis for selecting, evaluating and implementing this technology in the chemistry classroom.

Educational Computing Research

Educational computing research could be thought of as the application of educational research activities to the use of a specific technology. As stated before, chemists are quite comfortable with the idea of research, but often traditional chemistry research investigates ideas and theories. So the proposal to research a technology may seem strange to our colleagues. When chemical educators say that they are researching computers in the classroom, the notion is that while anyone can set up a computer in a classroom and have students use it, there are aspects of how it is implemented that influence its effectiveness. Perhaps, we should think of an analytical chemist who is seeking the optimal conditions for the use of a separatory column to resolve a specific analyte from a difficult matrix. The chemist carefully considers the chemical characteristics of the analyte and selects a column that is known to separate related compounds efficiently from similar matrices. If the column fails to perform adequately, then she changes the temperature, solvent, carrier flow, or finally, the column length and packing to improve resolution.

This example captures the essence of what the chemical education researchers are trying to do when they research the use of computers in the classroom. It is important that the chemical educators who have a commitment to use computer technology know something about the learning characteristics of the students in their classrooms. This information helps in the selection of the type of computer-assisted instructional materials to use. No piece of software is ultimately successful with all users, and the teacher needs to consider and modify the environmental factors that influence the success of the educational activity. If the environmental changes do not improve the student's success, then a new educational program may be selected. Now that we have established the purpose of chemical educational computing research, we should discuss the major influences on general educational computer research.

Theoretical Influences on Educational Computing Research

Perhaps the discipline with the greatest impact on educational computing research is Instructional Development. This relatively new academic enterprise is an outgrowth of what was once known as educational technology. Before the late 1970's, educational technologists primarily developed new ways of using photographic and print media in the classroom and the emphasis was on the production of materials, with little formal thought about underlying cognitive psychological notions. Journals of this era emphasized techniques and little theory or research. With the establishment of professional organizations such as the Association for Educational Communications and Technology and the American Society of Training Developers, individuals within educational technology began to search for unifying principles that produced successful technology-based educational programs. From these roots, several universities formed formal departments of instructional development or educational technology to support research to establish a theoretical basis for the design of educational programs.

The purpose of instructional development (ID) theory is to provide a coherent basis for the planning and implementation of educational programs. While there are at least five specific theoretical perspectives within ID (*10*), there are two that seem to have the greatest prospect for educational computing research. John Keller's theory of motivational ID and Charles Reigeluth's elaboration theory describe two important aspects of educational computing.

Charles Reigeluth has suggested that the most effective educational programs take a particular concept and elaborate its details within the context of the individual learner's prior knowledge and learning abilities (*10*). He writes of the need for the educator to provide an example (epitome) that provides a guide to the learner concerning the relationships within the components of the concept being presented. This provides a framework of understanding for the learner and the goal of the teacher becomes the provision of epitomes that meet the individual student's learning characteristics. Note the similarity between this theory and the constructivist notion of knowledge and education as presented by writers such as Herron and Bodner (*11, 12*). Keeping a store of epitomes is quite a job for educators and determining the aspects of the students' prior notions that effect the successful integration of the new information can seem to be an impossible task. But this is exactly what is necessary for the student to have a successful and motivating learning experience.

John Keller proposed a theory of motivational ID that categorizes learner motivational needs into four areas, Attention, Relevance, Confidence, and Satisfaction (ARCS) (*13*). It is hard for the traditional educator to hold the student's attention, make all of the subject content relevant to the student, provide activities that build the student's learning confidence and at the same time satisfy the educational needs that the student perceives. Today's students have become accustomed to movies and videos that provide scene changes as often as every 18 seconds. Is it any wonder that the same students become bored and inattentive when the teacher is lecturing for 20- to 30-minute intervals? Chemical educators try to teach content that is important for future scientists, but how do we make information relevant to every student, given the diverse cultural and educational backgrounds that they have? Confidence is a function of the student's own perception of her/his learning abilities. As you can imagine, these perceptions will vary constantly, and it is apparent that the classroom teacher would become busy when constantly trying to track one student's confidence, and when we think of trying to do this with 25–30 students, mental overload sets in. Finally, satisfaction is a function of immediate educational gratification (which builds confidence). Can we immediately provide feedback to each student concerning his or her own educational success? Teachers will have greater opportunity to meet these learner needs when they use adaptive educational computer applications. AI researchers try to produce these types of programs and their research has implications for educational computing research.

Artificial intelligence is an area within computer science that seeks to investigate the simulation of human thinking processes through computer algorithms. We encounter the results of AI research every day, because the major credit card companies use such programs to make credit approval decisions. Within the general AI community, there are researchers that investigate the application of AI to educational settings. The primary focus of such researchers is the development of "smart" programs that determine the user's educational needs ("student modeling") and change what the user sees on the screen in response to this diagnosis ("teaching model") (*14*). Student modeling may involve the administration of tests prior to the use of the computer program and/or the recording of the user's computer actions. The computer builds a user profile from this data and may change the order of topic presentation, difficulty of content, or even the appearance of the computer program. The general intent of educational AI research is to find ways to use the computer to provide individualized instruction and to make computers more effective educational tools. One of the factors that influences the accuracy of the student model built by the computer program is the nature of the way that the user perceives and uses the computer. Human interface and factors research examines these factors.

Human Factors or Interface research (I will use HI to refer to both of these related areas) is an outgrowth of research sponsored by the Department of Defense that investigates the design of technology that improves or eases the ways that people use machines and tools. The earliest example of this type of research involved cockpit layout design for the US Air Force (*15*). Early cockpit designs were identified as a source of problems for pilots in the middle of tense situations, and the layout and appearance of various controls was changed to help eliminate pilot errors. These investigations have developed into research into biomechanics and other areas of engineering. But the newest focus of this type of research is the investigation of the physical and programming appearance of computers. Xerox's Palo Alto Research Center (PARC) focused on this type of research and some commonly found aspects of modern computing that are a result of this center's work are the computer mouse and graphical user interface (such as the Apple Macintosh operating system or Microsoft Windows) (*15*). These characteristics of computers are designed to make computer use more natural and reflect human characteristics. The theory is that if the computer is easy or natural to use, then the user can focus on the computational work task. Research in this area continues and has extended to investigations of how the computer can present simulations with such realism that the computer user doesn't notice that they are participating in an artificial experience. This last area is known as virtual reality research, which will be discussed in more detail later in this paper.

Each of these areas influences general and educational computing and has implications for chemical educational computing researchers. At this point, I have presented information about the historical use of computers in chemistry and several influences in educational computing. But, you may ask, how do we determine whether the design and implementation of instructional computing programs are effective? There are two major types of educational research (qualitative and quantitative) that can provide answers to this question.

The Implications of Educational Research

Methods for Chemical Educational Computing Research

Qualitative and quantitative research have been common occurrences in chemical research. We have traditionally tried to identify what a chemical substance is, how it is formed and then measure the precise effects of chemical factors on its characteristics and production. Chemical education researchers model the historical development of chemical research when they apply both qualitative and quantitative research methods in the chemistry classroom.

The central purpose of qualitative research is to determine "what is there". In other words, the qualitative researcher attempts to characterize the realities of the educational situation (*16*). Amy Phelps has presented a good discussion of qualitative methods for chemical education research (*17*). The strength of this type of research is that it gives the educator a good sense of what actually goes on in the chemistry classroom, from an outsider's perspective.

This type of research is valuable for chemical educational computing research for several reasons. Determining whether the computer program interface or another educational computing factor is affecting student performance is difficult. Qualitative research methods such as videotaping computer users at the computers can provide information that is useful for making this distinction. Videotapes capture user comments that often indicate student attitudes. These individual perceptions can provide key information that is useful for identifying cultural factors that influence learning and, therefore, should influence computer program design.

Quantitative educational researchers attempt to numerically evaluate and describe the educational setting, with the intent to provide a statistical basis for educational decisions. Robinson, Nurrenburn, and Pribyl have given a more detailed discussion of these types of methods and their application to education research (*18, 19*). Quantitative data analysis helps the chemical educational computing researcher determine whether a computer program is effective and test the qualitative factors' relative impacts on learning.

Now that I have presented a brief overview of theory and methods that impact chemical educational computing, the big questions in your mind are probably, "So why is all this important and where is chemical educational computing research going?"

The Importance and Future of Chemical Educational Computing Research

One of chemical educators' hopes for computers and other advanced technologies has been providing more effective and efficient provision of educational activities for the learner. For the most part, these have not been realized to date. In fact, I would suggest that the implementation of computers in most classrooms has added to the complexity of the educational situation. While there are some examples of chemistry computer programs that relieve teachers from performing repetitive educational activities, most simply are traditional chemistry activities that have been "transported" to a computer delivery medium. While this is meritorious in some respects, there is a general lack of identification of what is unique about the computational environment that can enhance our ability to provide better educational activities and in some cases important characteristics of chemistry activities have been lost in the transfer.

The consideration of theoretical notions when the chemical computer educator begins to design and implement a program is important. Why, you may ask? I propose that there are three issues that can be addressed if greater consideration of theory is done; credibility among traditional chemists, which and how new technologies be implemented, and cost effectiveness. The first is the issue of credibility among traditional chemists.

When I first arrived at MTSU, one of my colleagues (that had just finished his PhD in analytical chemistry) asked me, "What is a degree in chemical education?" His notion was that if you teach chemistry, then you are a chemical educator. I have noticed that his confusion is shared by a great number of the chemists with whom I interact and the report of the Task Force on Chemical Education Research of the ACS Division of Chemical Education addresses this issue (*20*). I believe that one way for computational chemical education researchers to build a sense (among their traditional chemist peers) of validity in what they do is to have a theoretical basis developed *before* the program production begins. The areas of theory that I have quite briefly described offer a starting point for this.

The second reason that I propose that building a theoretical basis for chemical educational computing through research is the advent of new computer technologies. The newest wave of computing environments seems to be predominated by the development of inexpensive computerized multimedia. Jones and Smith were early pioneers who recognized the utility of this environment for chemical education, at a time when producing videodiscs was a very expensive activity. Today, however, the same information that used to be stored on large videodiscs is put on CD–ROMs at a tenth of the cost. Digitizing video has become so inexpensive that most word processing software allows the user to imbed digitized "movies" within the document. Thus, the ease of production has allowed general users to produce programs that only trained professionals were able to do five years ago. Desktop video has replaced desktop publishing as the "hottest" computer activity. But just as early novice desktop publishing was characterized by hard to read collections of pictures and fonts, it is most likely that general desktop video will exhibit similar confusing characteristics. Development that is driven by tested theory will avoid this problem.

The other technology that I believe to hold great promise for chemical education is known as virtual reality. When I first read about this new medium six years ago, my thoughts were, "This has potential for use in chemical education." Virtual reality (VR) is a computing environment where the user is "engaged" in a simulation of experience that he or she begins to believe is real. In 1987, the equipment to do this was quite crude and realism had little to do with the experience. But advances in display miniaturization and increased computational density have allowed VR to provide realistic experiences for the user. Some of the most exciting applications for VR have been in organic synthesis where researchers "grab" molecules and attempt to place them in positions along a complex molecular chain. The computer calculates repulsive and attractive forces and translates these into electronic signals that are felt by the user as pressure exerted by a computer-controlled glove on the user's hand. According to early reports, this has led to discovery of new bonding sites on chains and has allowed the acceleration of identification of new synthetic mechanisms. This same technology could be a great benefit during first time exposure to general chemical bonding principles and organic mechanisms. The student actually would "experience" chemical bonding at the atomic level! Imagine a trip as an electron in a weak acid–base system, becoming an atom being "passed" around in an equilibrium, "wandering" among the atoms in a crystal as you are hooked to a scanning tunneling electron (or for that matter X-ray) microscope (this very thing is happening with the so-called "nanomanipulator" at the University of North Carolina–Chapel Hill), or "running" among the atoms in a protein while connected to a magnetic resonance imagining system. These can be exhilarating experiences, but the educational value can be enhanced if the design of the computer program reflects a theoretical basis that is supported by educational research.

Finally, we are very rapidly approaching the point where the costs per unit of instructional technologies such as computers are beginning to level off. It is true that the computational power per dollar has decreased, but the actual cost per unit has not significantly decreased in the past two years. It is important to demonstrate that chemical educational activities such as titrations could be reproduced in a computer environment with no lost educational value. But why move from an inexpensive technology (burets) to a technology that costs one or two orders of magnitude more per student? If it can be demonstrated through research that the computational version of the activity is more efficient, safer, and/or provides a better learning experience, then the change is justified.

Computational chemical education research can help the chemical community avoid the "rush to the current educational fad" that we have observed occurring in the precollege education community over the past 40 years. A commentator recently stated that the USA spends over $6000 per student per year on primary and secondary education, and yet we have seen a decline in student achievement as measured by standardized testing (*21*). University education has come under attack by parents and students and this has resulted in greater scrutiny of what the professor and school does in the classroom (*22*). The time has come for chemical educational computerists to provide research data to support expenditures on new computer technologies in the chemistry classroom at all levels. This will not totally eliminate the pressures that chemical educators feel, but it will at least demonstrate that as professionals, we are concerned with providing the best educational opportunities to students at all levels.

Conclusion

The society of chemical educational computing individuals (and all chemical educators, for that matter) has reason to be proud of the innovation that members of their ranks have demonstrated. Traditionally, chemists have been comfortable with the use of technology in the classroom. There are, however, research-based theories of instructional development, educational research paradigms and computer-program design research that offer the prospect of more effective educational computer programs. Educational computing research also is important because it offers the prospect for chemical educators to avoid past problems in general education at a time of general skepticism about chemical education research and increased scrutiny and economic pressure at all educational levels. Finally, there are emerging computer technologies that offer unique chemical educational opportunities. The successful development and implementation of these new technologies will be assured if we provide a research-based foundation.

Literature Cited

1. Stinson, S. *Chem. Eng. News* **1984**, *62*, 35.
2. Chem. Eng. News **1969**, *47*, 48–49.
3. Dunlap, L. W. *Chem. Eng. News* **1971**, *49*, 7–8.
4. Rodewald, L. B.; Culp, G. H.; Lagowski, J. J. *J. Chem. Educ.* **1970**, *47*, 134.
5. Worthy, W. *Chem. Eng. News* **1984**, *62*, 34–35.
6. Moore, J. W.; Moore, E. A.; Lagowski, J. J. *J. Chem. Educ.* **1984**, *61*, 1003–1008.
7. Chem. Eng. News **1969**, *47*, 52–53.
8. Smith, S. G.; Jones, L. L.; Waugh, M. L. J. *Comp.-Based Instruc.* **1986**, *13*(4), 117–121.
9. Hood, B. J. M.S. thesis, Purdue University, 1989.
10. Reigeluth, C. M., Ed. *Instructional Design Theories and Models: An Overview of their Current Status*; Lawrence–Earlbaum: Hillsdale, NJ, 1983.
11. Bodner, G. M. *J. Chem. Educ.* **1986**, *63*, 873–878.
12. Herron, J. D. *J. Chem. Educ.* **1975**, *52*, 146.
13. Keller, J. M. *J. Instruc. Devel.* **1987**, *10*(3), 2–10.
14. Lawler, R. W.; Yazdani, M.; Eds. *Artificial Intelligence and Education*, Vol. 1; Ablex: Norwood, NJ, 1987.
15. Reveaux, T. *New Media* **1993**, *3*(1), 32–41.
16. Metz, P. A *J. Chem. Educ.* **1994**, *92*, 180.
17. Phelps, A. J. *J. Chem. Educ.* **1994**, *92*, 191.
18. Nurrenburn, S.; Robinson, W. *J. Chem. Educ.* **1994**, *92*, 181.
19. Pribyl, J. *J. Chem. Educ.* **1994**, *92*, 95.
20. Bunce, D.; Gable, D.; Heikinnen, H.; Herron, J. D. Presented at the 205th National Meeting of the American Chemical Society, Denver, CO, March 29, 1993, paper CHED59.
21. Limbaugh, R. television communication.
22. D'Souxa, D. *Illiberal Education: The Politics of Race and Sex on Campus*; Free Press: New York, 1991.