Overview of a Project in Quantum Modeling: Research Design, Systemic Issues, and Technical Issues

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The Quantum Science Across Disciplines (QSAD) project is a National Science Foundation research project (REC-9554198) to study how to introduce high school students and undergraduates to the basic concepts of quantum science. The physical principles of quantum mechanics evidence themselves in any attempt to provide a modern microscopic explanation of chemical or physical behavior. Moreover, with the growing interdependence of the disciplines, we now explain much of modern biology from a microscopic perspective and again invoke quantum principles. All of the sciences rely heavily upon modern spectroscopic means ranging from optical spectroscopy to atomic force microscopy to study local and far environments. These observational techniques and their derivatives rely upon quantum principles.

For these reasons, the QSAD Project has been investigating how to teach quantum principles in the classroom without imposing an overwhelming overhead of mathematics. Our objectives have been to:

(1) determine the feasibility of developing interactive computer software which provides students with a visually descriptive approach to models of quantum behavior;

(2) study student alternative conceptions about atomic and molecular behavior and mechanisms to support student adoption of the quantum model;

(3) study teacher understanding of quantum principles as well as issues related to teachers' adoption of explanations based on quantum behavior; and,

(4) study teachers' use of software in the classroom to discover the roles of teachers' beliefs and pedagogical content knowledge in their decisions about software implementation.

To accomplish these objectives, the members of the QSAD research team were drawn from the communities of science, science education research, teaching, and software design. The team members brought to the joint research effort their individual deep content knowledge, extensive classroom and curriculum development experience, extensive prior science education research experience, and accumulated knowledge of software design for education.

Underlying the software design and development work are the theoretical ideas about learning articulated by the National Research Council (1999a). Our objective in the software design was to provide students with the opportunity for constructing knowledge by in-depth explorations of the underlying quantum model for the electronic structure of atoms and molecules.

Our study of teachers has been grounded in prior work on how teachers extend their pedagogical content knowledge and the effects of teachers' beliefs on their instructional strategies. As discussed by Robblee et al (paper this session), we have investigated teachers' responses to our materials through observations and interviews during their participation in a summer workshop intended to familiarize them with our materials, through classroom observations, and by interviews. Student learning has been assessed through clinical interviews of a small number of subjects, and analysis of concept maps from a larger cohort. The concept mapping and interviews were conducted both before and after use of our materials. Some of the results of this work are discussed by Hurwitz et al (paper this session).

The greatest significance of our research is in providing a steppingstone for understanding how to teach an admittedly difficult subject using modern technology. This challenge will arise with greater frequency over the coming decades since computers are now both a principal tool for scientific research and the primary medium for making intelligible the consequences of scientific models. Computers have redefined our means of understanding natural laws and the way that science is conducted. For these reasons, we must learn how to use them in an analogous manner in the classroom.

What follows is divided into three sections. The first is an introduction to the materials produced by the QSAD project. This is intended to provide a context for the three papers which follow. The second section is a history and discussion of the role of the teachers who have collaborated on the project. The final section is a discussion of the relationship between the QSAD objectives and capabilities and the national standards.

Introduction to the Quantum Explorers

Description of the Software

We have developed five programs which we call the Quantum Explorers. These are:

1. the Bond Explorer for investigation of the sharing of a single electron between two orbitals located on different centers (Figure 1);
2. the Atomic Explorer for investigation of the electronic structure of atoms (Figure 2);
3. the Diatomic Explorer for investigating the bonding between two atoms as function of distance (Figure 3);
4. the Polyatomic Explorer for investigating the electronic structure of molecules with more than two atoms (Figure 4); and,
5. the Spectrum Explorer to investigate blackbody spectra as a function of temperature and to investigate the emission spectrum of hydrogen (Figure 5).

The Atomic, Bond, and Diatomic Molecule Explorers share a common style of interface. Each of them is available over the internet to run as an applet. In addition, they can be downloaded to be run locally as applications. The Polyatomic Explorer and the Spectrum Explorer are currently only available as applications.

When run as applications with a Windows 95/98/NT operating system, all of the programs except the Spectrum Explorer provide three-dimensional views of isosurfaces of orbital density or amplitude. For lack of appropriate compiled plug-ins we cannot support three-dimensional views with the Apple OS.

In addition to these core programs for high school use, the QSAD project has also developed an applet for finding bound-state solutions of Schrodinger’s equation for a number of classic potentials. This program (The Shooter) is being used for undergraduate instruction.

The Atomic Explorer affords the student views of the atomic orbitals of the first fifty-four elements (through xenon). An electronic structure window displays the energy levels while the spatial distributions are shown in the orbital window. The student can select to display the atomic size of the atom (that is the covalent radius) or the expected radius for an electron in the selected orbital. With the exception of hydrogen, only occupied states can be viewed. For hydrogen all orbitals can be viewed. Students can investigate the periodic trends of atom size and ionization energy; discover the Aufbau principle; learn to distinguish core and valence electrons by energy levels; and have their first introduction to the shapes of atomic orbitals which ultimately determine the shapes of molecules.

The Bond Explorer provides the student with the opportunity to investigate the bond creation process as an atomic orbital centered on one “nucleus” overlaps an atomic orbital centered on a second “nucleus”. The resulting molecular orbital is occupied by one shared electron. Parameters that the student can control include the distance between the nuclei, the symmetry of the atomic orbitals on each of the nuclei, and the energy of each of the orbitals. The Bond Explorer provides a tool for inquiry into the fundamental meaning of electronegativity, polarity, covalent and ionic bonds, the difference between bonding and antibonding orbitals, and the role of atomic orbital overlap in determining the formation of bonding orbitals.

The Diatomic Explorer allows the student to investigate molecular bonding between two atoms selected from the Periodic Table (currently through argon). The distance between the atoms can be varied. As it is, on an accompanying energy meter the student can watch the competition between the energy gained by the sharing of the electrons, and the energy cost of trying to bring two positively charged nuclei together.

The Polyatomic Explorer is the Diatomic Explorer but for molecules with multiple atoms. The three-dimensional display can be zoomed and rotated with CosmoPlayer. The molecule is constructed based upon a PDB formatted file. The student can then manipulate atoms within the molecule and measure distances, angles, make atomic substitutions, and observe the variation of the energy of the molecule as a result of these alterations.

The Spectrum Explorer is currently in two pieces. One provides a study of the blackbody spectrum as a function of temperature. The other allows the student to construct an emission spectrum by interactively exciting electrons and watching the result of their decay.

Discussion

There are several professional packages available for chemists to study molecules. Our programs are not meant to be merely quantum chemistry software packages with easy interfaces for high school students. However, as discussed in the next section, in order to satisfy the concerns of our collaborating teachers we found ourselves toeing a line closer than we expected to traditional chemistry software.

As part of the compromise with the objectives of the teachers, the computational scheme we adopted (the extended Huckel molecular orbital scheme) runs fast in Java on a Windows platform, gives answers that qualitatively agree with the trends of the Periodic Table and is usually reasonably quantitatively in agreement with experiment. However, there are parameter ranges where the model does not work (large nuclear separation), or the trends are OK but the numerical values are substantially different from experimental ones (e.g., the dipole moment). Neither in workshops, nor later in class, has any teacher expressed a qualm about using the program because of these inaccuracies.

All five applications can be used for inquiry-based instruction. The Atomic, Bond, and Diatomic Explorers have been extensively used for such instruction by two of our cooperating teachers. The PI has used them and the Spectrum Explorer for such instruction with pre-service teachers in an integrated sciences course.

The controls and menus for the user interface are standard. Perhaps for this reason students and teachers alike use the applications without apparent difficulty. When seeming problems arise (intensity too dim, orbital does not appear on the screen) it is usually a function of the nature of the object to be viewed (e.g., large principal quantum number so the orbital is diffuse). From a learning experience perspective, such problems are can sometimes be classified as features rather than GUI problems. Nevertheless, we have worked to control learning experiences of this nature.

Research Design with Teachers Enlisted as Consultants and Subjects

The structuring of our research project followed our perception of the science education community's view of how best to enlist teachers as consultants and materials developers. For us, this perception was in-part validated by the reviews we have received in recent years on proposals submitted to the National Science Foundation, as well as the research literature.

Our interpretation of how to engage teachers in our project development was that science teachers should be brought in early in the software design and development process so as to ensure their early feedback on the nature of the software, the curriculum which the software was to address, and the affordances supplied by the graphical user interface. The need for such teacher inclusion is nearly self-evident. Teachers are the gatekeepers of classroom, and without their inclusion there can be no meaningful access to students.

There was an inherent tension in this collaboration with teachers. The QSAD team members were content experts with years of experience in software and curriculum design, and possessed an expert vision of what could be accomplished using the computer as a visualization tool. The scientist members of the team could invoke in each other's minds visual images which were unavailable to the teacher consultants. In effect, the senior members of the development team stood in relation to the teachers as the teachers stood in relation to their students. Nevertheless, the content and developer experts of the research team put aside their predilections for instructional methods and practice and listened to how the teachers wanted to modify and use our materials.

The rationale for this process lies in the complex dynamics of national priorities, national standards, accountability, and dissemination. As a result, the project was born with a legacy of checks and balances implicitly and explicitly woven into its contract. The teachers represented such a checkpoint. How we regarded them and worked with them unarguably shaped the output of our project.

Here we describe our experience in enlisting, working with, and accommodating the teachers who served as our consultants and subjects. The names adopted to refer to teachers and communities are all consistent with those in the paper by Robblee et al (this session).

History

Year One

For the first summer of our project (between the first and second year), we recruited three teachers to work with us. Each had the credentials to be considered a potential master teacher. In accord with the scope of our project, one teacher taught chemistry, a second biology, and the third taught both physics and chemistry. The latter was science department chair, and the chemistry teacher had served as department chair at her school. The physics and biology teachers had significant prior experience in the integration of computers into the classroom. The biology teacher had just spent a sabbatic year consulting on a computer based science education project. The chemistry teacher came highly recommended based on her collaborations with university colleagues.

The workshops were designed to introduce the teachers to quantum phenomena. Our objectives were: (1) to ensure that the teachers understood the content material; (2) to inquire how they saw our materials fitting into their classroom activities; and, (3) to provide the teachers with an opportunity to create curriculum with the software.

We attended carefully to the responses of these teachers to our first materials. We found and were advised the following:

1) Despite the years of teaching experience these teachers had in their fields, they had only a rudimentary understanding of quantum phenomena and molecular bonding. This was despite the fact that the textbooks they used, and the assignments they gave to students, referred to these subjects. The vocabulary was familiar to them, but their interpretation of the vocabulary fitted the vague usage in their texts.

2) When the approximation we used in our program provided results which did not agree with textbook, the teachers implied strongly that they would be unable to use such a program in their classroom. As discussed further below, this was an early turning point for the project. Without much difficulty we were able to incorporate a different numerical scheme which modeled the electronic interactions better. The PI recalls this decision vividly. At the time it seemed transparent that the program had to agree with the textbook.

3) We were urged by the teachers to provide three-dimensional representations of molecular bonds. Our early software showed only two-dimensional slices through the electronic distributions. The chemistry teacher explained that she found it difficult to visualize three-dimensional objects and that a manipulable computer representation would help her, and her students, greatly.

We recruited one more chemistry teacher. He had had significant prior experience working with us on other projects, and had the opportunity to learn the quantum concepts with us during the school year. Teaching in the well-heeled community of Easthaven, Matt became one of the master teachers for this project.

After training these teachers and benefiting from their feedback, it had been our hope to follow the use of our materials in the classrooms of these teachers during the second year of the project. As luck had it, the physics/chemistry teacher retired and the biology teacher was assigned lower level life science courses in which he could find no place for our materials. We were able to continue with Matt in Easthaven and with the chemistry teacher, Nancy, who taught in the professional community of Thomsonville. However, even here we faced two obstacles. The first was the discovery that her teaching style produced an inherent resistance to using computers for instruction. She provided us with access to her students and frequent conversations, but she had no clear sense of how to incorporate the new materials into her teaching. The second obstacle was a technology barrier of putting our programs on older style Macintosh computers which could not support the full range of the program.

The experience of this first summer cemented for us the logic of beginning our development work with materials appropriate for chemistry instruction. Such materials seemed to be the common denominator for biology and physics. In addition, we decided that our software needed to be in close enough agreement with experimental data that we would not quantitatively contradict trends presented in chemistry textbooks.

Year Two

In year two we ran a second summer workshop for which we recruited biology, chemistry and physics teachers. We further chose to broaden our base to a high school with a diverse student body in a working class community. The community of Bridgeton is suburban, however the percentage of college graduates in Bridgeton was 24% as compared to 52% in Easthaven, and 60% in Thomsonville and Cary, the towns from which our other teachers were recruited. Our workshop lasted a month. During that time we had three teachers (two from Cary, one from Bridgeton) for a month, and two other teachers for two weeks each (one from Bridgeton and a physics teacher not followed further for this study).

Despite the disparity in communities, we had high hopes for the teachers from Bridgeton. First, we had recruited a chemistry teacher and a biology/chemistry teacher to work with us. Second, these two teachers were already team-teaching the chemistry course using computer software. The chemistry teachers at Bridgeton had written their own curriculum for this course and had incorporated extensive use of chemistry software on computers present in the classroom. We thought that we had an ideal setting: the teachers from different disciplines were working together and were experienced in teaching using software. As we were to subsequently discover (Robblee’s paper this session), the facility with incorporating computers into their curriculum was at best illusory.

Again we listened carefully to our teachers. As with the first year’s cohort, we discovered that we had to teach the teachers the rudiments of quantum behavior. Despite their education in the sciences, and despite the fact that the chemistry teachers covered bonding and orbitals in their classes, the teachers immediately acknowledged that what we were showing them was new for them.

This session we pushed hard to find common ground between the chemistry and biology teachers. Towards the end of the session we had an illuminating discussion about photosynthesis and metabolism. During this conversation it became apparent that the biology teachers (two of them) and the chemists (two of them) could not even agree on the definition of an oxidation-reduction reaction! The teachers in the different disciplines had different understandings of the chemistry of metabolic processes.

It was at this point that it became very clear to us that without extensive collaborative work between our chemistry and biology teachers, use of the materials we were poised to develop could not occur. Based on our discussions with the biology teacher from Cary, to discuss biological processes from an electronic perspective, she would require coordination of her curriculum with the chemistry teacher’s. While in this instance this could be arranged, one of the participating chemistry teachers was her colleague, generally it was not practical for other schools. Generally, the threshold for use of our materials appeared too high for biology teachers to use on an independent basis.

Entering our third year we were poised to pursue research in high schools in the upscale communities of Cary, Thomsonville, and Easthaven, as well as in Bridgeton. Again, as fortune would have it for our small cohort of teachers, the biology teacher in Cary took a leave from school to have twins, and the biology teacher in Bridgeton was assigned elementary biology classes in which he could not reasonably use our materials.

Year Three

At the beginning of Year Three we had to make decisions on what to emphasize for development and research. Lacking a bridgehead in biology, we decided to focus closely on how our chemistry teachers used our materials, and how their students responded. We chose not to follow the one remaining physics teacher in our group despite his continued use of our materials.

The two graduate students on the project, Dr. Karen Robblee and Mr. Charles Hurwitz, gathered most of the data for their doctoral theses during this year. Following their own inclinations, the two students conveniently decided to respectively focus their research on teacher use of the QSAD materials and how students responded to these materials (see their papers this session).

Use of Materials with Undergraduates

In addition to work at the high school level, we are also piloting our materials with undergraduate students. This was done in Years Two, Three, and is underway again in Year Four. The collaborator responsible for using QSAD materials, Professor Dan Dill, Department of Chemistry, Boston University, is a co-PI of the project. Professor Dill is a strong advocate of introducing quantum mechanical ideas into the general chemistry curriculum, and began pursuing this goal before QSAD using Mathematica and other modeling tools. However, the general chemistry course at a major institution is likely to be led by more than one professor with two or three coordinated lectures running in parallel. As a result, the introduction of new materials and methods is limited in large measure by the extent to which the other course professors are willing to adopt the materials.

For the past four years Professor Dill has worked to acquaint his colleagues with the benefits of using a quantum approach to general chemistry. It is fair to say that while he has successfully used some of the programs developed by QSAD, the impact has been restricted to his section. On the other hand, he has aroused sufficient interest among the other course professors that we are now seeking additional funding for development of undergraduate curriculum with the expectation that the general chemistry course can be altered over the coming years. The conversations with chemistry faculty that Professor Dill and the PI are currently engaged in were not possible at the outset of the QSAD project.

The PI also explored the possibility of developing QSAD materials for use in the undergraduate biology curriculum at Boston University. The introductory biology program has a history of innovative instruction including collaborative efforts for integrated curriculum with the Department of Chemistry. Nevertheless, exploratory conversations initiated by the PI led to the response that there was no time in the introductory biology curriculum for interactive materials. Given the quantity of material covered, the notion that students should spend time investigating concepts interactively on a computer did not sound time effective to the professor who was contacted. This experience effectively shut the door on the project's access to undergraduate biology courses.

Analysis

Our project was deeply affected by the knowledge, skills, and availability of the teachers we enlisted as subjects and consultants. The small cohort size left us very vulnerable to teacher availability. Of the eight teachers we invited to our workshops, one took unexpected early retirement, one took an extended leave to raise her children, and two received class assignments which effectively prevented use of our software.

The teachers invited to our workshops were chosen with care. We invited teachers with whom we had collaborated in the past, and from school systems to which we could expect ready access to classrooms and students. Other teachers were selected on the basis of recommendation by teachers who were our friends or by colleagues. In Year One there was a deliberate weighting of the cohort towards teachers from communities with high quality school systems. Our goal was to pilot our software with teachers and students who did not face additional challenges.

In keeping with this approach of trying to control the variable of technology experience, almost uniformly the teachers we invited had prior experience with computer-based materials. In Year One the invited teachers were either colleagues from prior computer projects, or had prior consulting experience with computers.

In Year Two we leapt at the opportunity to include Bridgeton High School. On the one hand, it was in a working class community where teachers and students had different aspirations than in Cary, Thomsonville, or Easthaven. On the other hand, the teachers at the school had already integrated computer based materials into their chemistry course, and a flexible curriculum into which our curriculum modules could fit.

By Year Three the project was effectively limited to chemistry teachers due to fluctuations in the availability of our cohort, and because of decisions that we made based upon our experience with the teachers. Specifically, in Year Three we were following one chemistry teacher in each of Thomsonville, Easthaven, Cary, and Bridgeton.

As detailed by Karen Robblee et al (paper in this session), despite the prior integration of computers into their chemistry curriculum, despite the introduction to the materials provided in our summer and school workshops, and despite our intervention to provide written examples of curriculum, the Bridgeton teachers proved unable to support the integration of our materials into their curriculum.

Discussion

There were several significant milestones which determined the nature of the project's development. Of these milestones, the following were perhaps the most telling.

Demarcating the Project's Vision – The summer workshop of Year One led to an implicit limitation on the project's goals that were unintended at the time. Following what we considered to be the directive of the National Science Foundation to carefully attend to the advice of the teachers engaged in our project, the PI may have been overly influenced by the teachers' difficulties with the first version of the computer program for molecular bonding.

When the teachers objected that the program did not replicate the order of molecular orbitals quoted in their text, the discussion that followed was to the effect that the program must not contradict the text. The connotations of such a contradiction were at least two-fold. The first was that it would lead to confusion for the students. The second was that the program was not even in agreement with simple chemistry and therefore could not be relied upon to provide students and teachers with the insights necessary to develop a good intuition for chemical processes. At the time it appeared to the PI that these were legitimate objections. Moreover, the PI was very concerned that if this problem were not addressed the teachers would not have the confidence necessary to use the program in their classes.

The PI's response was further colored by the fact that he knew that resolving this problem was a straightforward matter. There were alternative computational schemes for him to draw upon which could be expected to provide better results. However, despite the fact that the apparent problem could be solved, over the course of a three year project the time investment that was necessary effectively limited options for alternative development.

This issue of program accuracy was repeatedly visited by the QSAD team in group meetings over the entire length of the project. It was always the objective of the QSAD project to emphasize modeling of scientific phenomena as opposed to obtaining accurate results. After saying that, a fine balance must always be struck with respect to what constitutes a "good enough" model for reliable classroom use.

Given our goal of emphasizing modeling to the student over accuracy, when the teachers expressed their initial doubts about the value of the program, the QSAD team could have adopted an alternative response. We could have insisted to the teachers that they should be teaching modeling and not exact computations. We could have further altered the appearance of our interface to emphasize to the student that what was being presented was not intended to strictly correspond to experimental reality. Arguably this would have been a superior approach and more in keeping with the spirit of the original proposal.

One of the programs developed by the QSAD project actually matches this description. The Bond Explorer is a model for molecular bonding which should resonate well with a physicist's or quantum chemist's understanding of bonding. In this model there is one electron, two nuclear centers, and one bound energy state for each of these nuclear centers. The distance between the nuclei can be altered as can the value of the bound energy level. With these three parameters set, the two molecular bonding states are computed and the electronic distribution computed. Most of the basic concepts of molecular bonding can be investigated with this model, but there is no correspondence to an experimentally accessible molecule.

In retrospect the products of the project might have more resembled the Bond Explorer in model abstraction if the project team had resisted the initial request of the consulting teachers to match experiment and the standard textbook.

The impact of the consulting teachers was further reflected in the project's development of three-dimensional visualizations of molecules. In each year's summer workshops, and in conversations with teachers in informal workshops we have presented, the most enthusiastic response is to the 3d capabilities of our programs, Nevertheless, in retrospect a disproportionate amount of time and money was invested into 3d visualization software. Because of the difficulty in matching across platforms, the work still remains somewhat shaky and for a short three year project it may not have been the right choice. The impact of this decision will not be resolved until the software has been hardened for nationwide dissemination through internet download.

As related in the paper by Dr. Robblee (this session), in the third year only two of the four teachers in our study used the QSAD software extensively. These two chemistry teachers were well-versed in implementing inquiry-based science experiences for their students. In addition, although we did not follow actively his use, the physics teacher who attended our second year workshop also used our software in an inquiry mode. These three teachers all pushed for more investigations into the wave nature of electronic behavior than was originally emphasized or developed under the QSAD program. Indeed, the original vision of QSAD was that it would de-emphasize the traditional wave approach to quantum phenomena. It was felt that students have sufficient difficulties already understanding constructive and destructive interference of waves. To add this as a hurdle to understanding the behavior of electrons in atoms and molecules did not appear a wise move to the PI. Nevertheless, this apparent intellectual need by these three teachers to discuss electronic structure from a wave-like perspective may reflect a legitimate need for all students of quantum electronic structure. Here again the attitudes of the teachers have changed the attitudes of the developers and researchers.

Systemic Issues and Limits – The original goal of our project was to design software that would find a place in the biology, chemistry, and physics classroom, and might ultimately support an integration of the teaching of these sciences. We did not realize this objective. In part this was because of fluctuations in the availability and teaching assignments of the biology teachers we selected.

However there was also a systemic component to our inability to penetrate high school biology. Specifically, a course sequence of in which students take chemistry before biology, and where there is coordination between the chemistry and biology teacher, appears to be necessary before the kinds of materials we were developing would sound attractive to a biology teacher.

Although this conclusion reflects our experience, it is possible that with a cooperative biology teacher materials appropriate for use in the high school classroom that emphasized the microscopic quantum phenomena could be designed. If we had had engaged at least one biology teacher for an entire year materials on photosynthesis or electron transport might have been developed. Alternatively, biology teachers might now be attracted to the Polyatomic Explorer as a means to provide their students with insight into the structure and behavior of organic molecules. In short, we believe that opportunities for such connections between biology and chemistry and physics through microscopic behavior remain, but we were not able to explore them.

A second systemic problem we encountered was the difficulty our teachers faced in finding technology support in their classrooms from their inhouse staff. The teachers we worked with were either very restricted in their access to computer laboratories, or were frozen out of the machines in their classrooms. We found this to be a universal problem in Cary, Easthaven, Bridgeton, and Thomsonville. Installation of our software and access to the web was either restricted or impossible

Conclusions

The researchers comprising the QSAD team were deep in content knowledge of quantum phenomena in the sciences, deep in pedagogical methods for using the computer in the classroom, and deep in knowledge of the technology issues for bringing computer software into the classroom. For all these reasons, the team was in a position to lead the teachers to the introduction of new content and new approaches for in-depth study of the quantum basis for chemistry and physics, and the implications for biology.

At the same time, the QSAD team was aware of the gatekeeper function of teachers with respect to their classrooms, the need for teachers to teach towards standards, and the imperative from the National Science Foundation to develop materials which could appeal to a national education audience.

A three year grant is a very short time when software is being developed. If an operational final product is to be produced, decisions made during the first half of the project must be honored in the second half of the project. In an academic environment researchers can be flexible about their schedules and use no-cost grant extensions to maintain their work past the initial cut-off date. However, this is not a viable option for the production of software. A programmer is an employee who cannot be paid past the original term of the budget. Indeed, unless additional funding is secured early in the process, a programmer will frequently leave in advance of the conclusion of a project in order to secure a new job and not suffer a break in employment. This is a real life problem which a PI must consider while planning a project’s outcome.

Over its lifetime, the project has found itself subject to a confluence of systemic expectations (national standards, dissemination expectations, budgetary limitations). It is fair to say that the result of the PI’s and QSAD team’s attempts to balance these conflicting pressures was the production of software that does not match the team’s initial expectations, but nevertheless can be effectively used in the chemistry classroom. An external reviewer might respond to this by saying that this is exactly what the systemic pressures were intended to compel the investigators to do.

The question that remains for the team is whether if we had adopted a less accommodating attitude towards our teachers’ requests, would we have exercised greater creativity in our product and been truer to the original vision of the project? The outcome of our project might have been dramatically different if we had been less concerned about immediate use. Such alternate product might have in the long run been more revolutionary in the classroom and had greater impact on science teaching. This must remain forever a what-if scenario for which we have no answer.

In the end, we conclude that two factors were critical in limiting and focusing our development work. The first was the establishment of a close relationship with collaborating teachers and attending carefully to their advice and response to our initial materials. The second factor is the brevity of a three-year grant. Given the length of time necessary to develop viable software, the nature of the software to be developed must be fixed after the first year of the project. Otherwise, it will not be possible to pursue educational research with it during the project’s lifetime, and there will be no final polished software product.

The National Standards and Quantum Science as an Example of Teaching Modern Science

The National Science Education Standards (NSES) (NRC, 1996) refer in broad generalizations to the outcomes of science education. Included in these outcomes is an understanding of microscopic electronic structure. In the NSES Guide to Content Standards for grades 9 – 12 (NRC, 1996, under Structure and Properties of Matter, students are expected to learn that: (1) "The 'Periodic Table' is a consequence of the repeating pattern of outermost electrons and their permitted energies." (2) "Bonds between atoms are created when electrons are paired up by being transferred or shared. A substance composed of a single kind of atom is called an element. The atoms may be bonded together into molecules or crystalline solids. A compound is formed when two or more kinds of atoms bind together chemically." (3) "The physical properties of compounds reflect the nature of the interactions among its molecules. These interactions are determined by the structure of the molecule, including the constituent atoms and the distances and angles between them. ... Carbon atoms can bond to one another in chains, rings, and branching networks to form a variety of structures, including synthetic polymers, oils, and the large molecules essential to life", and (4) "Matter is made of minute particles called atoms, and atoms are composed of even smaller components ... The electric force between the nucleus and electrons hold the atom together" (pp. 178-179).

Discussion

Currently, the teaching of electronic structure called for by national and state standards is not being well served by textbooks and instructional methods. This situation is confirmed by our experience working with teachers, our experience as teachers, and by our interviews that show that, after normal instruction, students have difficulty in responding to questions about the connection between electronic structure and the geometry and properties of molecules (Peterson & Treagust, 1989).

Chemistry texts developed over the years present key concepts that are more specific than the broad strokes outlined by the NSES. In Table I we compare the National Standards, materials covered in typical chemistry texts, and the concepts that can be taught using the Atomic, Bond, Diatomic, Polyatomic and Spectrum Explorers.

The recent studies by the NRC (1999b) succinctly state ideas about education that we find supported by our research and the research of many others. One of the key findings of the NRC study is that "To develop competence in an area of inquiry, students must: (a) have a deep foundation of factual knowledge, (b) understand facts and ideas in the context of a conceptual framework, and (c) organize knowledge in ways that facilitate retrieval and application." (p. 12) In keeping with this, the NRC report further writes "To develop competence in an area of inquiry, students must have opportunities to learn with understanding. Deep understanding of subject matter transforms factual information into usable knowledge." (p. 12) The NRC also reports "A key finding in the learning and transfer literature is that organizing information into a conceptual framework allows for greater 'transfer'; that is, it allows the student to apply what was learned in new situations and to learn related information more quickly." (p. 13)

One of our primary goals for our work with teachers is to provide them with materials that will give their students a coherent and rich introduction to atomic and molecular structure. The NRC (1999b) finds that "Teachers must teach some subject matter in depth, providing many examples in which the same concept is at work and providing a firm foundation of factual knowledge" (p. 16). Specifically, "Superficial coverage of all topics in a subject area must be replaced with in-depth coverage of fewer topics that allows key concepts in that discipline to be understood" (p. 16).

It is our view that these observations about in-depth study of basic concepts matches our view that to understand chemistry, biology, and the physics of materials, a student must develop a model of microscopic behavior valid at the nanoscale. Moreover, to develop this model, students should engage in inquiry activities related to electronic structure at the atomic and molecular levels. It is precisely such inquiry activities (called for separately in the Inquiry Standards by the NSES) that the Quantum Explorers can provide if used skillfully.

The topics which are specifically addressed in the National Science Education Standards can be taught different ways. Consider the critical concept "Bonds between atoms are created when electrons are paired up by being transferred or shared" (pg. 179). The implications of this concept are very broad. In one brief sentence the concept of how molecules, compounds, and solids is summarized. The exegesis of this statement can fill volumes. So, how is it to be taught?

We would argue that the best means to learn about bonds between atoms is with programs such as the Quantum Explorer. Direct experimental inquiry at the nanoscale is beyond the experimental resources of almost any high school. However, with computer software students can investigate conceptually and graphically the abstract realm of atoms and molecules. Indeed it is precisely through the use of simulations that scientists practice the same form of investigation.

Summation

The QSAD project will be wrapping up its work over the next year. At this point we have a sense of incompleteness. From the outset we were very ambitious – we wanted to have an impact throughout high school science. At this point the project has produced data on how teachers respond to computer-based materials, and how students come to grips with quantum concepts. The software will be hardened over the next year (this is possible because of a no-cost extension of our grant) and archived with model curriculum on a web site. Ultimately our success may be determined by how effective the web is as a means for the dissemination of our product.

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