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Developing and Implementing Web-based Computer Simulations for In-Class, Individual, and Small Group Work

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Abstract

Should introductory chemistry be "taught" by a mode of instruction other than lecture? How can the web alter the way chemistry is learned? These questions are on the mind of many chemical educators. The answers to these questions will undoubtedly be influenced by the needs of each institution, individual instructors, and (most importantly) students. The web provides a "universally accessible" platform for the delivery of educational resources. The medium is relatively easy to develop materials for and provides a level of interaction that cannot be provided in a textbook. This interactive nature can be used to deliver simulations of chemical and physical processes (animations of phenomena) or interactive simulations of experiments that may (or may not) be done in the laboratory portions of a general chemistry course. This paper will discuss a variety of the interactive materials that have been tested in the first semester of the author's general chemistry course. Presently the simulations involve material from approximately three quarters of the course. The topics addressed through the use of interactive simulations include density, mass laws, combustion analysis, stoichiometry, gas laws, calorimetry, the first law of thermodynamics, and some aspects of bonding. Additional guided discovery activities (without on-line simulations) are also used and include periodic properties, the atomic mass scale and the mole, atomic structure, and aspects of the "intermolecular" forces involved in condensed states of matter. The use of interactive web based activities as the starting point for small group classroom discussion and assignments will also be discussed. It is important to make the use of simulations an integral part of the course, provide a motivation for individual students to perform the simulations, and to provide a setting in which the students can exchange ideas and insights. The author's attempts (both successful and not so successful) to implement these course materials in small groups will be described. The positive aspects of, and technical requirements for, the learning tools discussed in the paper will be highlighted. However, the web cannot solve all of the challenges of teaching chemistry. Therefore, brief discussion of the difficulties (technological and pedagogical) encountered in creating and using web based simulations will also be discussed.

Outline

Introduction

Why develop simulations for use in teaching chemistry? When deciding upon making changes to any course, there are several questions that instructors typically consider. First, "What works in the present course and are there 'problems' that need to be addressed?" Second, "Who are the students in the course?" and "What is the nature of the institution?". The answer to these questions will suggest what ought to be changed and help the instructor decide what changes best fit the needs of the students and the institution. A final question that is key to the success of any changes in the course is "Who is the instructor and what role are they comfortable with in the classroom?".

The following conditions apply at the author's institution. The Pennsylvania State University is large and geographically dispersed. Some campus locations serve primarily non-traditional commuter students while other locations serve primarily traditional students with large campus residential populations. General chemistry is offered in several formats. However, all freshmen are tested and their mathematics and chemistry test scores are used to determine their placement in the chemistry curriculum. Some students place out of the first semester of college chemistry. However, for students that are not well prepared, there is an "Introductory Chemistry" course designed to prepare them for the "regular" college chemistry course. Students that are somewhat better prepared may take either (a) the three credit "Principles of Chemistry" (general chemistry) course plus one credit of a "Problem Solving in Chemistry" course or (b) at some locations a five credit "Introductory and General Chemistry" course. Finally, the "well" prepared students take only the three credit "Principles of Chemistry" (general chemistry) course. At the author's campus, the "Principles of Chemistry" (general chemistry) course plus one credit of a "Problem Solving in Chemistry" option is not presently offered.

The author's course is the three credit "Principles of Chemistry" course (offered in the fall semester). The students enrolled in this course are nearly all traditional age students, over 70% are first semester freshman, and are nearly all required to take the course as part of their major. A majority are pursuing a bachelor degree in engineering or science (but few are chemistry majors) and a fraction are in associate degree programs. Over the last four years the class size has ranged from 75 to nearly 100. A final note worth mentioning is that all majors that require the three credit "Principles of Chemistry" course do not require the associated one credit lab or the second semester (lecture and/or lab) of the first year chemistry sequence. Therefore, some students in the three credit "Principles of Chemistry" course take the lab concurrently, some take the lab after completing the lecture, and some students never take the lab. The two problems the author wanted address were: (a) students were not spending adequate time engaging the course material and (b) some students in the course had no high school chemistry lab experience and/or were not required to take a lab course concurrently with the instructor's lecture course.

Aside from the adjustments to the "normal" structure of their lives that traditional age freshman must make when they enter college, there are a number of factors that make the first year college chemistry course challenging:

1. the quantity of the material covered
2. the variety of material covered
3. the requirement to perform calculations (especially solving "word problems")
4. the requirement to relate the abstract to the concrete
5. the misconceptions, alternate conceptions,(1) from prior courses or life experience

Furthermore, traditional lecture and recitation sections do not capture the interest of students. The difficulties with traditional lecture include: (a) little time to do remediation of basic skills (students who start behind fall further behind), (b) ineffective for different learning styles, (c) students cannot control time, place, or pace, and (d) interaction with the instructor is avoided (especially in medium to large classes). As a result of these difficulties, students do not engage the course material actively nor do they develop the depth of knowledge that is desirable. For many students, interest in the course is low and student learning and grades suffer. The results of recent study indicate that a general chemophobia may also contribute to lower achievement in chemistry.(2)

Some of the difficulties described above can be addressed by using modes of instruction other than traditional lecture. As many instructors know, a major key to improving student learning is getting the students to spend time engaging the course material. It is in this area that the web can be useful as a way to "teach" chemistry. The web provides a "universally accessible" platform for the delivery of interactive educational resources. The medium is "relatively easy" to develop materials for and provides a level of interaction that cannot be provided in a textbook. Additionally, students can control (to some extent) the place, time , and pace of interaction with the material. The interactive nature can be used to deliver simulations of chemical and physical processes (animations of phenomena) or interactive simulations of experiments that may (or may not) be done in the laboratory portions of a general chemistry course. A variety of interactive materials have been developed and tested in the first semester of the author's general chemistry course. The author's attempts (both successful and not so successful) to implement web-based course materials, especially the use of simulations, will be described.

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Interactive Web Based Simulations

The author has developed a series of interactive simulations for use in the first semester of a first year college chemistry course. All of these activities (see list below)can be found at the author's web site. Through the use of the simulations, students are exposed to activities that require their involved participation. The activities require students to "perform experiments", collect and analyze data, and arrive at conclusions about the behavior of matter. This is more consistent with the practice of science than the traditional lecture mode of teaching. This allows the students to:

1. become involved in the process of learning,
2. develop a sense for the process of doing science (chemistry is not just a series of facts previously discovered by others),
3. and learn to think more independently relying less on a textbook for answers and more on their own ability to understand and correlate data.

The simulations address areas of content typically found in the first year college curriculum:

1. density of solids and liquids- provides the opportunity to perform density determinations on liquids and solids (including some that cannot be done safely in a teaching lab)
2. mass laws - provides the opportunity to investigate mass changes in reactions to "discover" (a) mass conservation, (b) law of definite proportions, and (c) law of multiple proportions
3. compound stoichiometry - simulation of combustion analysis allows students to determine empirical formulas
4. reaction stoichiometry - provides the opportunity to investigate mass changes in reactions to "discover" (a) limiting reactant and (b) theoretical yield
5. ideal gases - provides the opportunity to investigate relationships between pressure, volume, temperature, and number of moles of an ideal gas in order to discover (a) simple gas laws and (b) the ideal gas law
6. investigations of bonding - students examine the effect of electronegativity difference on bond strength as an introduction to the differences between polar and nonpolar bonds.
7. calorimetry - a comprehensive site allowing students to perform simulated experiments using both a bomb calorimeter (to determine heats of combustion) and/or a coffee cup calorimeter (to determine heats of solutions of ionic compounds in water and/or determine the specific heat capacities of a number of metals

8. heat and work - provides the opportunity to investigate relationships between heat and work in both a constant pressure and a constant volume system in order to "discover" (a) energy is conserved and (b) energy can be converted into work

These interactive web based activities can serve as the starting point for small group discussions.

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Small Group Work

Small group work was employed as a result of research that has shown that cognitive learning has an important social aspect.(3) Small group use of the interactive web-based activities has been attempted in two ways in the author's course. In the first and second year of use, students were clustered into groups of three to five students and given an "experiment" to complete using a simulation. The group completed the experiment using a worksheet to help guide them. They had to analyze the data collected and determine the significance of the results. Based upon their interpretation of the data, the group developed a lesson to deliver to the rest of the class. Prior to teaching these lessons, groups met with the instructor as a quality control check for the lesson plan. Students received an individual and a group grade for their efforts.

As an example, the "Ideal Gases" simulation was used by four groups to investigate simple gas laws as shown in Table 1. The students worked as a group to collect and analyze the data. They were not told the name of the gas law they were to investigate prior to the meeting with the instructor. Each group had to collect several sets of the requested data. Each data set was collected using different values for the constant variables. For example, in the Boyle's Law case, P vs. V data would be collected with one set of n and T values, then again with a new set of n and T values, and finally a third time with one more set of n and T values. The worksheet prompted the students graph the data to determine whether the relationship between the two variables was direct or indirect (inverse). If the relationship was inverse the group then had to graph one variable vs. the inverse of the other (Boyle's Law case). The students are asked to represent the relationship for their data as a proportionality. This allows students to then solve initial state/final state problems using the simple gas law they have "discovered". Students also are prompted to calculate $^{PV}/_{nT}$ for every data point collected.

The four groups would present their finding in class on the same day. The instructor would then use this as a starting point for discussion of the combined gas law and the ideal gas law. After covering these relationships, the class concluded with a discussion of the significance of the slopes of the lines in the graphs of the simple gas laws.

Table 1. Assignments for "Ideal Gases" Simulation

Group	Gas Law Assigned	General Directions
1	Boyle's Law	Vary V and measure P while holding n and T constant.
2	Charles' Law	Vary T and measure V while holding n and P constant.
3	Amonton's Law	Vary T and measure P while holding n and V constant.
4	Avogadro's Law	Vary n and measure V while holding P and T constant.

The success of this method was more limited than the author had hoped. The students in the small groups learned the material well: they did the assignment, developed a lesson plan, met with the instructor, taught the material, and fielded questions. Not too surprisingly, this process increased the group members' success with the material. However, students who were not assigned the material did not respond well to peer teaching: they did not use the web pages themselves, they "turned off" in the classroom during peer teaching, they did not engage the material, nor did they develop good questions for the presenters. Additionally, this method of using the simulations with small group and peer teaching was time consuming for the instructor. In addition to developing and coordinating the assignments for all of the groups (approximately 20), each group required a minimum of one half-hour meeting to review the lesson plan developed for the class. Some groups needed a follow-up meeting.

With the idea that time is needed to work out the kinks in any new method, this same method was attempted a second year. The author hoped to increase the involvement of the "non-presenters" with the material during the peer teaching. However, participation points were rejected as one method due to the logistics involved (spreading questions among all the students who were not presenting seemed to be an impossible task). Instead, questions based on the presentations were included on quizzes and exams, however, student reaction to peer teaching was still poor. Perhaps this method of peer teaching could be adopted successfully by other instructors. However, the author opted for a different approach.

In the most recent semester (Fall 1999), the author committed to getting **all** students involved in **every** activity. The class was divided into large groups (one scheme had three groups while another had four). Each of these groups was given a different investigation to perform with the simulation. In the case of the "Ideal Gases" example discussed above, the four group scheme was employed and the assignments were the same as those listed in Table 1. Each student was required to complete his or her group's assignment. Therefore, every student now had to access the web pages and use the simulation. On the assigned day, all students were required to bring the results of their investigations (compiled data/completed worksheets) to class. The students then split into small groups, each comprised of one member of each larger group (in the "Ideal Gases" example each small group would have members from groups 1, 2, 3, and 4). The students then shared what they had learned. Since each of the large groups had a different assignment, each student could make a unique contribution to the discussion. Additionally, since each student had completed a worksheet and graph for the assignment, it was easier for them to process the data presented by other students.

In order to provide external motivation to complete the assignments, the instructor randomly collected three assignments (completed data/worksheets) from each student. Students did not know in advance which assignment would be collected from them. Make-up assignments were not given (except in exceptional cases with documented excuses) but only the best two assignments counted toward a student's final grade. This method proved to be successful in increasing student involvement with the assignments. The logistics were somewhat simplified since the meetings with individual groups were eliminated. However, there were additional written assignments to grade, and some students either handed in poorly completed worksheets or none at all.

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Assessment of Effectiveness of Web-based Activities

Student surveys, and the author's personal assessment, have been used to assess the use of simulations and other on-line materials. Student surveys assessed:

1. reaction to the use of simulations (there are also questions about the other on-line materials)
2. interest in and/or attitude toward learning science/chemistry
3. attitude toward science/chemistry as a process (vs. a set of facts and equations)
4. student self-assessment of their level of ability to carry out scientific data collection and analysis

The results of these surveys indicate a positive assessment of the simulations and other web-based materials (for example, on-line course notes). After completing the course with the simulations student self-evaluation also indicated improvement in the other three areas. However, data from a control group (a section of the course taught without the simulations) were not complete at the time this paper was submitted.

The author has also examined other means of assessing the new course materials. An interesting trend was observed in official student course evaluations (Student Ratings of Teaching Effectiveness, SRTEs). The students' overall evaluation of both the course and the instructor declined for the first two years that on-line course materials and simulations were employed (fall semesters 1997 and 1998). Several colleagues (in a number of different disciplines) at the author's campus have also noticed a decrease in course evaluation upon adoption of "nontraditional components" to their courses. The most recent semester (fall 1999) showed a reversal of this trend with evaluations climbing back to the level from the fall of 1997. Course retention rates have been evaluated from late drop data and have been compared to data from previous years of the author's course (1996 to present). Retention rates in the author's course have been declining steadily when referenced to his first year at PSU, 1996. The number of late drops rose again in the fall of 1996. Class grade point average has also declined during the same period. Exams comparable to previous years were given and student averages on each quiz and exam have been compared to the same quiz or exam in the previous years. Not surprisingly, the average grade on individual quizzes has also experienced a decline. However, these comparisons do not account for differences from one semester to another in other variables linked to student success rates (average preparation level, motivation level, and other class demographics). The reasons for these trends may be related to the teaching methods used in this course, or they may reflect trends at the national or institutional level. In order to place the trends observed in the author's course into context more data is needed (for example, the average math and chemistry placement scores could be tabulated and compared for each class).

Improved performance of the "learning" taking place in the course is much trickier to assess. The author has anecdotal experiences that indicate use of the simulations and small groups can help students overcome misconceptions, better *understand* concepts and phenomena, and better *learn* "problem solving" skills (vs. using rote algorithmic methods to solve problems). For example, many students have deeply rooted misconceptions about density, displacement, and buoyancy. The density determination simulations serve as a good starting point to discuss phenomena related to density (for example Archimedes Principle). The simulation of solid density simulation relies on displacement for the volume determination. During the in-class discussions, the instructor carefully reviews the requirements for a solvent that can be used to determine the volume of a water reactive low density solid (like sodium, Na). The discussions invariably turn to other "real world examples" of displacement and buoyancy (for example the class has discussed ice cubes floating in liquid water and hot-air balloons). Students completing the simulated density experiments and the small group work appear to have a better understanding of the phenomena of displacement.

A second example involves mass conservation and the concept of limiting reactants. When performing mass conservation simulations some students (even some that have had two years of high school chemistry) are surprised to observe that reactant remains after a reaction goes to 100 percent completion. Class discussion time is then spent in careful examination of atomic theory to see how it can explain the Law of Conservation of Mass, the Law of Constant Composition, and the Law of Multiple Proportions. However, even after this effort, some students are still confused when the concept of limiting reactant is introduced in the following chapter in the context of mole calculations. The simulations are employed again, but this time students are expected to work in moles instead of in mass. Although the average quiz score on this chapter has not improved, the author has noticed an increase in the number of students employing mass conservation concepts (although sometimes incorrectly), mass ratios of elements in compounds, and other "interesting options" when solving stoichiometry problems. Although these methods are not always employed properly, it seems that some students are doing more than simple algorithmic problem solving on these questions; that is they seem to be thinking. The use of the simulations along wit the small group work allows students to: (a) engage the material actively, (b) develop ideas/relationships, (c) test them, and (c) learn on their own and from other students. In-class examples and instructor led discussion are used to supplement the group work as needed.

One final difficulty with the assignments is the vast range of prior knowledge and skill level of the students present in the course. The "best" students found some of the assignments trivial, while other students found some other assignments (or perhaps just the instructions) confusing. It is clear from this work, and from other studies (ref. 4 and references within), that computer-based assignments can improve student performance and attitude toward chemistry. However, it is important that the level of the student and the assignment be well matched. It is also important to recognize that improved student performance on exams may not reflect increased *understanding*(1). Also, gains on exam scores may not be attributable to the type of assignment or the mode of delivery. A recent study of a web-based system of homework and testing showed a strong positive effect on exams scores. (5) One finding was that scores on practice exams increased with the number of times they were attempted. This may simply be a function of the time spent engaging the material. This would not invalidate the positive aspects of the computer-based assignments; yet similar gains might be achieved by other assignments that produce similar gains in "time on task".

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Individual Use

The simulations need not be employed solely as a means for developing small group activities. The author has used the simulations to provide practice problems for individual students. They have been used to develop problems during office hours and have also been assigned to students needing extra practice in problem solving. The stoichiometry pages can be used to develop a large number of limiting reactant/theoretical yield problems. The gas law page can be used to practice a large number of simple gas law or ideal gas law problems. Students can attempt the problems and then check their answers against the simulation's result. The author plans to add more "drill and practice" types of exercises to the course site during the summer. The exercises are intended for students in need of skill development or remedial work. In particular, the author plans to provide a number of exercises involving SI unit conversions, significant figures, and other simple conversion calculations (mass to moles, moles to mass, molarity to moles, dilution calculations, etc.). Hopefully, these additions will help to address the increasing number of students who use their calculators poorly.

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In-Class Use of Simulations

The author has also used the simulations as a classroom presentation tool. As the small groups meet and hold discussions in class, the instructor can circulate around the room to evaluate problem areas or listen for misunderstandings. When the group discussion time has ended, the instructor can use the simulation to correct an obvious misunderstanding or simply to drive home a concept that did not seem to be well understood. Additionally, the simulations can be used to explore interpretation of experimental data.

An example of this kind of application involved using the "Mass Laws" simulation of the following reaction:

$$2\ Na_{(s)} + Cl_{2(g)} \text{ ---> } 2\ NaCl_{(s)}$$

Near the end of a class period the following experiment is explained to the students. A fixed quantity of the first reactant (Na) was combined with increasing quantities of the second reactant ($Cl_{2(g)}$). Then the mass of the product (NaCl) was graphed against the mass ratio of the second reactant to the first (see Figure 1). The interpretation of the graph is discussed with emphasis on the relationship of the region of zero slope to the concept of limiting reactant. Particular attention is also paid to the significance of the mass ratio at the point where the slope becomes equal to zero. When this mass ratio is converted to a mole ratio, its significance becomes immediately apparent.

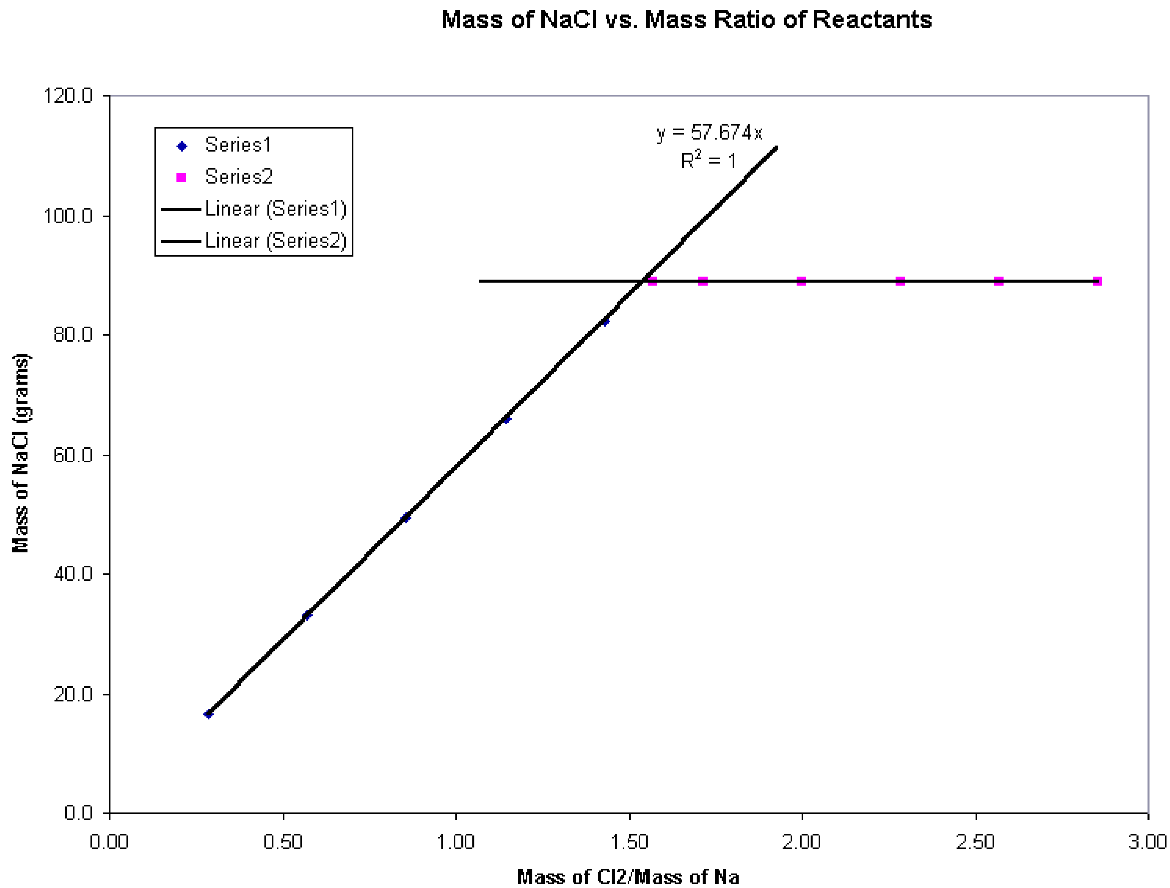

Figure 1. Mass of NaCl vs. mass ratio of Cl_2/Na.

Students are then requested to develop a similar graph for the following reaction by the beginning of the next class period. There is a simulation of this reaction that can be used to perform the "experiment".

$$P_{4(s)} + 6\ Cl_{2(g)} \text{ ---> } 4\ PCl_{3(l)}$$

The students have been capable of completing data collection and graphing required by the assignment. Their results are reviewed at the start of the next class period. Typically they do a good job and are able to convert the mass ratio to a mole ratio (some convert to a mole ratio for the compound while others find a mole ratio of the reacting species).

The instructor then presents the following (unbalanced) reaction with two possible products.

$$C_{(s)} + O_{2(g)} \text{ ---> } CO_{(g)} + CO_{2(g)}$$

After a brief description of performing the same type of experiment as performed above, the students are presented with the data in graphical form (see Figure 2) . Note that the amount of each product present in the graph is controlled solely by the relative quantity of reactants present and not any of the reaction conditions. Most students are able to interpret the graph with some success, however, few are able to see the full significance of all the data. Some time is spent discussing the fact that oxygen is the limiting reaction when only CO is formed and that carbon is the limiting reactant when only CO_2 is formed. However, the intermediate region seems to create some confusion for the students. The author is working on some exercises that will minimize this confusion. Exercises like these require that students evaluate data in a form not usually presented in first-year college chemistry texts. In this manner an instructor can begin to assess whether students are thinking about the information they receive or merely using algorithmic problem solving (for example by using the normal rote procedure to determine theoretical yield).

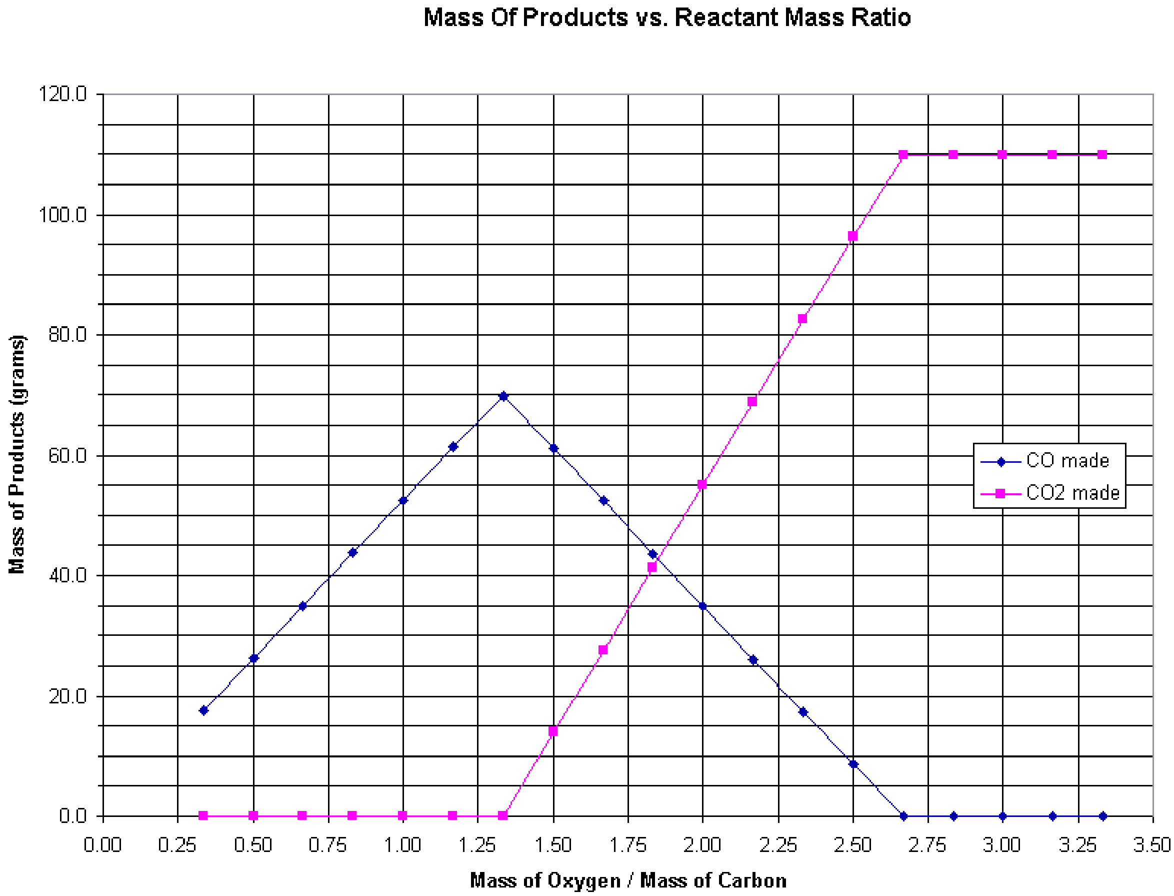

Figure 2. Mass of CO and CO_2 vs. mass ratio of O_2/C.

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Conclusion

The web is a powerful medium for developing interactive course materials. From on-line syllabi and course materials, to interactive tutorials and simulated experiments, the web provides a mechanism to alter the way that chemistry is taught. Although it is not the final solution to all of the challenges of teaching college chemistry, it does have some striking strengths.

Positive Features of Web-based Materials

1. interactive nature of activities keeps students engaged with the material
2. student has some control over the time, place, and pace of learning
3. self teaching and peer teaching can be effective (no better way to learn than to teach)
4. students can use the pages to create additional practice problems (immediate feedback - the simulation produces the correct answer, or provides "check features")

Challenges of Web-based Materials

1. web technology is still evolving (difficult to decide if/when to adopt new features)
2. the issue of browser compatibility (or more aptly incompatibility) has not yet been adequately addressed

3. there are still access issues: not all colleges have adequate computer lab space and not all students are on-line in their own/parent's home, dorm room, or apartment
4. servers do crash adding to access issues
5. some students are "computerphobes"
6. time intensive for the instructor (developing web-based materials is easier now, but still takes too much time)

Tips for Using the Web for Teaching

1. provide detailed guidelines on responsibilities and deadlines for the students
2. provide several checkpoints to make sure students are completing work
3. make the work students do meaningful and linked to the course in a tangible way

It is important to make the use of simulations an integral part of the course, to provide motivation for individual students to perform the simulations, and to provide a setting in which the students can exchange ideas and insights. If small groups are used, it is critical to take steps to minimize the difficulties created by group members that do not "do their parts". Also, students must be given time and guidance to successfully adjust to teaching and being taught by themselves and/or their peers.

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Resources

In addition to the links found on various pages of my website, I also recommend the following.

1. A nice WWW site for Harvard-Westlake Honors and A.P. Chemistry students. This site is maintained Steve Marsden. Follow the link to topics and click on a topic (for example "Gases"). There are many links to tutorials, notes, and simulations (the links are footnoted with bibliographic information).
2. A summary of some principles of using small groups. Based on notes taken at the *Workshop on Group Interactions: a Regional Instructional Development Workshop, October 22, 1997* and posted by Donald Mencer.

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