What is the Best Search Engine for Chemists?

And then there were two.

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In last year's CCCE Newsletter column I lamented the fact that the long expected conflict between Microsoft and Google for technical supremacy in search engines had failed to materialize. Aside from real time search, which seemed to have little professional interest for chemists, there were few technical developments to report. Since then, there have been plenty of developments, perhaps the most significant of which was the deal allowing Microsoft to fold the Yahoo search engine into Bing, the newest Microsoft engine. As of this writing it is reported that Yahoo and Microsoft have completed the integration of their search engines in the U.S. and Canada, including Yahoo's Internet, image, and video search on both desktop and mobiles computers and mobile phones. According to a story this month, Bing has now gained a larger fraction of the search market than Yahoo and Yahoo has no plans to keep its engine up to date; therefore, Yahoo will no longer be evaluated as a separate engine in this column.

Technical Developments

Recently, the New York Times ran an article entitled, "A Race for Smarter Search." The subtitle was a pretty good summary of the tone of the article, "Bing Innovates and Google Plays a Little Catch-Up." According to the New York Times, Bing has made a number of changes, such as putting the navigation tools on the left-hand side of the page and adding a colorful background picture. In addition, Bing has used a combination of in-house developments and purchase of smaller companies with special expertise to provide improved results in some special areas, such as travel. Microsoft has also agreed to pay consumers and search partners who are willing to make Bing their preferred search engine. The Times calls these changes a "renaissance in search." As a result, Bing has increased their share of web searches from 8% to 12.7% as of June, while Google's share fell to 62.6%.

While Microsoft has been working on the user interface, Google has been working to develop a next-generation architecture, called Caffeine, that is intended to make major changes in the way that the engine crawls, indexes, and ranks the WWW. According to Google, the biggest change is that Google now analyzes the web in small sections and adds the results to the index immediately, rather than waiting until the results are available for large chunks of the Web. This means that your search results will be much more current than in the past. Probably the most authoritative description is from the Official Google Blog, which says that "Caffeine provides 50 percent fresher results for web searches than our last index, and it's the largest collection of web content we've offered." Google claims that Caffeine processes hundreds of thousands of pages in parallel every second, and is designed to cope with the ever expanding size of the Web to make Google an even faster and more comprehensive search engine in the future. David Cosper writes in a blog post entitled, "New SEO Practices for a Google Caffeine World, that Caffeine is already live for many types of search, and the biggest change may be that it will identify and

remove sites that "game" the search process to get higher positions in the Search Engine Results Pages. If the early comments are accurate, this represents a significant step forward for Google, even though the results may not be obvious to the typical user.

An article in the New York Times reports another new feature for Google search, Google Instant. Instant predicts the most probable results and displays them on the screen as the user types each letter into the search box. It is the default setting for Google Search, so many readers have probably already begun to see this feature. Experts predict that this will change now people search. For sophisticated searchers, who plan to use several word search phrases to focus the search more precisely, the initial reaction may be that this is merely a distraction, but for the average searcher, who often uses only single word search terms, the results that are displayed will allow him or her to adjust the search on the fly. It is claimed that by showing results before a user has completed typing the query, Google says that Instant may save three to five seconds on each query. Is that really enough to make a difference to the average chemist user?

My initial impression is that this is not as significant a change as Caffeine. Speed is a big focus on the Web, but it remains to be seen if this will be enough to give Google a real advantage. On the other hand, it is probably too early to fully appreciate the impact of Instant on the search process; it may take a while for users to adjust their habits to take advantage of this new capability. Perhaps the biggest immediate change is that Instant represents a real headache for people who have optimized their sites to show up most often on Google for the least money. For example, it is more expensive to insert an advertisement into the "Paris hotels" results than into the "Paris hotels in the Marais" results. With Instant search, the user may never get far enough in the phrase for the latter ad to appear.

Several months ago, Google introduced a new feature called Wonder Wheel. This feature breaks down some search topics into subcategories, creating something that is similar to a concept map. Insert a query into normal search, and then activate Wonder Wheel to produce a circle with the subcategories spun off as spokes. It is then possible to click on any of the subcategories and break it down into further subcategories. This is an innovative way to drill down into a search term and narrow the search. Bill Ferriter points out in his blog that this feature does not work with Instant; as long as Instant is turned on it is not possible to access Wonder Wheel. To try out Wonder Wheel, click on the words "instant is on" just to the right of the search box and change it to "instant is off." Now scroll down on the left hand sidebar and click on Wonder Wheel. Warning, this doesn't work for all search terms, so try it first with a term like "chemistry" (because I know this one works). I'm not yet sure how useful it may be, but it certainly looks cool. By the way, users can follow new features that Google introduces at the Google New site, where there is a short description of each new feature that Google has introduced.

Much as I hesitate to disagree with the New York Times, it would appear to this writer that while Bing is adjusting the appearance of the search process, Google is working on making a better engine. Travel results and a glitzier page for the search box may be important to someone who is searching for a hotel in Minneapolis or Brittney Spears' latest sexploits, but I don't think that these features will be sufficient to change the minds of serious searchers.

Comparing the engines

The basic question for chemists remains, "Which engine will do the best job of finding chemical terms." This is not going to be determined by pretty home pages. As was noted in previous columns in *this Newsletter*, there are three main criteria that should be used to evaluate search engines: currency, relevance, and comprehensiveness. Currency measures how often the search engine revisits sites to add any changes into the index. Relevance is a measure of whether the most useful sites not just included but listed early in the search results. This factor is probably the most difficult to evaluate quantitatively. Google's Caffeine and Instant would seem to give it an increased edge in these categories. The final criterion is Comprehensiveness, which measures what fraction of the accessible sites on the World Wide Web the search engine actually includes in its index. This is particularly important for chemists, who are more likely to be looking for specialized information that may not be included in the index of a less comprehensive engine.

Comprehensiveness is probably the easiest to measure quantitatively. Both Google and Bing report the total number of hits, but this can be deceptive. Multiple word searches tend to give unreliable counts, since the engine algorithm may rapidly begin to include related terms, despite the best efforts to focus the search using Boolean algebra or quotes around the phrase. Another problem is that engines may stop a search when it appears that the number of hits appears adequate. The difference between 20,000 hits and 40,000 hits may be connected more to the search load on the server farm at the time rather than the size of the index. The way to avoid this problem is to use single word search terms that deliver as few hits as possible, since these numbers are more likely to be meaningful.

As in the past, the engines were compared using unusual chemical terms to minimize the possibility that the search process would time out before the search was complete, and single word searches to make sure the counts were more accurate. The results are shown in Figure 1 below. As was observed last year, Bing seems to have a smaller index since it gives significantly fewer hits on every term. Thus, Google continues to be a better choice for chemists. Caffeine was still being deployed as these searches were being done, so it is not apparent that it had any impact on the results. Hopefully, next year's results will find a way to take these new capabilities into consideration.

Figure 1: Comparing number of hits on different engines (Aug. 9, 2010)

Search term	Bing	Google
polyphosphazine	57	2860
perfluorophenyl	4090	11,000
dynemicin	2040	15,900
Discodermolide	6390	35,600
chlorocatecholborane	32	918
Radiosumin	18	1800
"PCST buffer"	3	4

Since more and more people are searching for images, it seemed appropriate to do a similar search for some chemical images. In this case, some multiple word searches were included, but this seemed to make little difference, Google was still far better for chemists than Bing. The

results are shown in Figure 2 below. Google has recently changed its image search results page to show thumbnails of a larger number of results, making it faster to check through and find the best image. Personally, I also prefer Google images because this preview function in Google allows me to get to an image I want to see with only one click, while Bing requires two clicks. It sounds like a trivial difference, but it seems to make a difference to me.

Figure 2: Comparing image hits on different engines (Aug. 9, 2010)				
ferrocene	3,530	11,700		
adamantane	506	7,520		
nanotube	36,700	69,200		
spectrophotometer	37,700	267,000		
"reflux apparatus"	68	529		
"soxhlet extractor"	168	2,250		
"beer's law"	508	4510		

What is Coming Next for Search

Perhaps the most surprising development being discussed in the search engine world is the possibility that Facebook might become a search engine. In the middle of the summer, Eli Goodman pointed out that there were about 600 million searches per month performed on Facebook, and although the total was still far less than the billions of searches done on Google, it still suggested that Facebook might be competitive as a search engine. Most of the Facebook searches are for people, but the number of product searches is steadily increasing. A recent (July 25, 2010) post on the Search Engine Watch blog suggests that searches on Facebook now link directly to third-party websites. People are increasingly sharing interesting content on social network sites, and with over 400 million members, Facebook is in an ideal position to leverage their opinions to evaluate sites. The addition of the "Like" button to Facebook offers a powerful tool for making the Web more connected. It is not clear how this might be helpful to chemists, even those who are on Facebook.

According to Mashable, Google has given notice that it may challenge social sites, like Facebook, by acquiring Ångströ and hiring its founder. Ångströ is a service designed to search a person's professional network. This suggests that Google is trying once again to create a legitimate competitor to Facebook; however, a different article in Mashable (a great place to troll for rumors) reports that Google plans to soon launch Google Me, which will be an integration of social information in the existing results page rather than a full-scale challenge to Facebook. Even Google has finite resources, and so one might ask if moving in this direction will impact the old-fashioned search that is the basic need for chemists. These developments will surely bear watching although they may not directly impact chemists.

This has been an unusually active year in the area of web search, and in most cases it is still too early to predict what the ultimate effect will be on chemists searching the Web. The only prediction that is totally safe is that the coming years seem to be primed for major changes in the world of search engines. There should be plenty of material for me to discuss.

Addendum

Just as I was doing the final editing of this article, I checked on Delicious and found a headline from BBC that read, "Microsoft launch (sic) Internet Explorer 9 web Browser." Microsoft has released a beta version of Internet Explorer (IE9). In 2003, the Microsoft Internet Explorer browser had 97% of the market, but since then Microsoft's market share has dropped to 60%. This change has been caused by a combination of the perception that Mozilla's Firefox and Google's Chrome were technically more advanced and the decision by the European Commission to force Microsoft to offer other browsers rather than just giving IE as a default. According to the BBC, Microsoft's new browser uses technology that allows it to go directly to the computer's graphics chip rather than to the processor. This should make web pages perform faster and more like applications. The new browser will also support the new web standards, such as HTML5. The down side is that the new browser will not run on Windows XP, and apparently Microsoft has no intention of producing a version of IE9 that will. As I said previously, there will surely be plenty to write about in next year's Newsletter.

Yahoo is not dead! Having sold the cow, it is now trying to sell improved milk that it buys from another dairy. I recently found an article describing the new initiatives that Yahoo is taking to provide "more 'visually compelling' search results intended to make it easier to find news and entertainment topics (remember that the actual search process is now controlled by Microsoft). None of this seems likely to impact chemists (except for those fixated on Britney Spears - you know who you are) so, as noted above, this column will no longer pay much attention to Yahoo. ***end*** Return to Fall 2010 CCCE Newsletter

Introduction of the WWW-based Teaching and Learning Material for Organic Chemistry in the University

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Introduction

In these days, computers and networks are used in the university classes as if they had been used for decades. The blackboard has been substituted by a large screen for projecting images from our liquid crystalline displayed (LCD) projectors. Many textbooks or lecture notes are available electronically on the Internet instead of purchasing from bookstores or print services. Most announcements to students are delivered not on the traditional bulletin boards but on the www-based portal systems.

I have been teaching organic chemistry at Soka University for twenty years as a one-year sixty-hour course. Facing the changes depicted above, I have tried to introduce a new technology for assisting and improving the class teaching and learning. This article describes my experiences in this aspect for more than ten years.

1. Construction of the Home Page for the Organic Chemistry Class
The first prototype of the home page for my organic chemistry class was constructed gradually for five years in the following manner.

1.1 Assignment Tasks and their Solutions
The first item I disseminated on the www-based system in 1998 was the assignment tasks for reviewing the class contents. Since the www was not so popular in Japanese universities in those days, this activity also aimed at directing students familiar with the use of www. Since there was no www-based class-assisting system available, I prepared the www page and the www server by myself. After the students' task reports were submitted, my teaching assistant checked the students' answers and returned the reports to the students, while I disseminated the solutions to the tasks for further reviewing.

1.2 Q&A Page
Generally speaking, Japanese students were hesitant in raising questions in class, but rather eager in raising questions when they were encouraged to do so as part of the assignment. This often resulted in the repetition of answering the same questions again and again both to one student and another and in one year and the next. This repetition was difficult and frustrating for the teachers.

In 1998, I encouraged the students to raise questions as part of their assignments, and disseminated commonly and repeatedly asked questions accompanied by the answers on the

above www page. The next year, the collected sets of Q&A's were disseminated on the newly prepared Q&A web page, which was included in the prototype of the class home page. After two years of encouragement, more than one hundred of the Q&A sets were collected, which were categorized not only as organic but also as other fields of fundamental chemistry, such as physical, inorganic, and other fields of chemistry (Scheme 1).

This was quite successful. The number of questions submitted with the task reports was much less, suggesting that students first came to seek for answers on the Q&A page. In addition, most of the questions were new and did not have answers posted on the page. The page is updated with new sets of Q&A's and revisions every year (Figure 1)[1]).

Organic Class-related (11)
- General (15)
- Nomenclature (10)
- Bonding and Structure (18)
- Electronic State (4)
- Conjugate System and Delocalization (12)
- Structure--Property Relationship (4)
- Stereochemistry (17)
- Electronic Effects (10)
- Acids and Bases (3)
- Organic Reactions-General (6)
- Nucleophilic Substitution (4)
- Elimination (2)
- Addition (4)
- Aromatic Substitutions (4)
- Reactions of Carbonyl Compounds (2)
- Oxidation and reduction (2)

Others
- General and Fundamental (12)
- Historial (2)
- Physical (13)
- Inorganic (4)
- Miscellaneous (2)

Scheme 1 Categories and number of questions (in 2010) in the Q&A page (Corresponding to Figure 1)

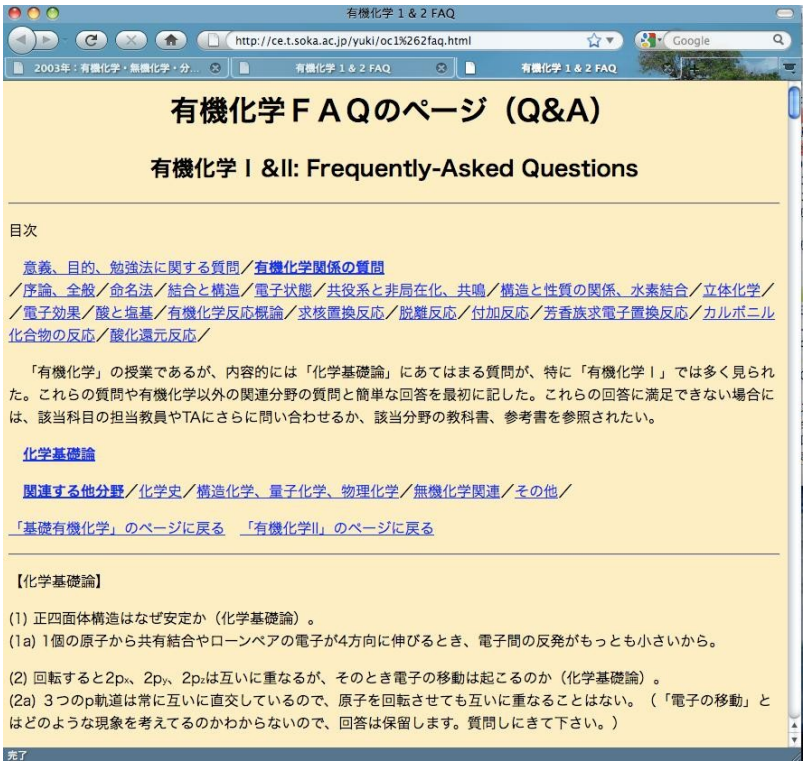
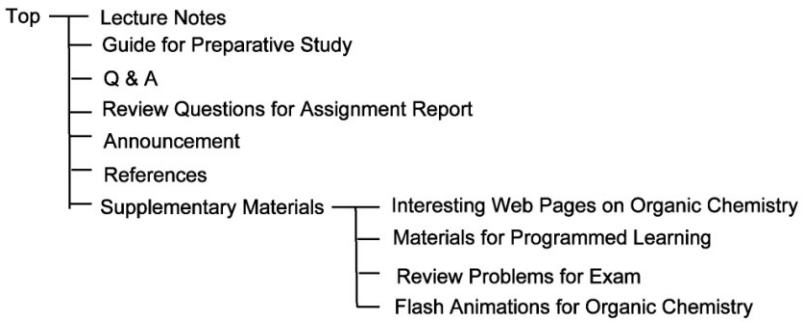


Figure 1 Cover page of the Organic Chemistry Q&A page1) (see Scheme 1)

Figure 2 Top page of the Organic Chemistry home page for the class3) (see Scheme 2)

1.3 Distribution of the Lecture Notes

Since 1994, I have provided students in my organic chemistry classes with handouts of the lecture notes that were prepared with Chem Draw, instead of drawing them on the blackboard. Every year, this caused a surplus of undelivered sheets of paper undelivered, because several students were absent or would not take the handouts. In 2003, with the popularization of the pdf readers such as Acrobat Reader and pdf files on www, I decided to deliver the lecture notes electronically on the www page for the class2). With this, the basic structure of my home page for the organic chemistry class has been constructed, which remains with revisions and modifications (Figure 2)[3]).



Scheme 2 Structure of the home page for the organic chemistry class (Corresponding to Figure 2)

1.4 Home Page for the Organic Chemistry Class

The structural outline of this page is shown in Scheme 2. There are a few additional contents in this page. "Guide for Preparative Study" shows the day-to-day contents taught in the class, in relation to the chapters and sections in the electronic handout of "Lecture Notes". Students find the contents taught in the next class and may prepare for it. From the "Supplementary Materials" page, students can get the information of other web pages both inside and outside the university that are useful for their autonomous learning. "Review Problems for Exam" page collects the problems for past term-end examinations of this subject, which are reorganized to the corresponding chapters in the "Lecture Notes". With these problems, students recognize the expected achievement at the end of the semester and may make practice so as to prepare for the term end exam.

In summary, the contents in this home page for the organic chemistry class are so designed as to help the class students' learning in various stages. Note, however, that all of these materials could be manuall distributed and parts of them were actually done in the traditional classroom settings. The development of computers and the Internet has just made it much easier for teachers to disseminate and for students to make use of them. They are not considered as "new" trends in education that were developed in this age of information and communication technologies (ICT).

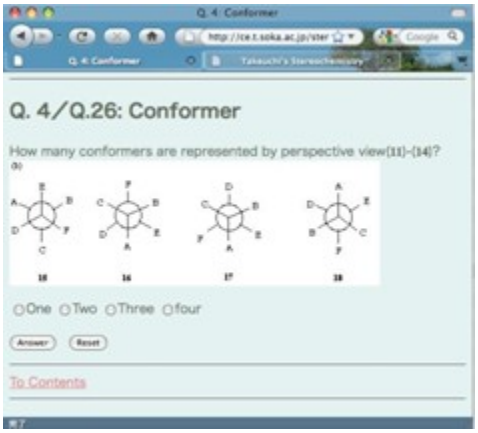
2. New Approach in Chemical Education using the WWW-based ICT

In 1999, I joined the project "Virtual Chemical Education (VCE)"[4]), which was headed by Professor Yoshito Takeuchi, a project of the IUPAC Committee on Teaching of Chemistry (CTC). This project aimed at using the Internet to make new educational tools. Among the various new functions of the Internet, we focused on its visual (animation), interactive (by-directional), and world-wide (beyond the restriction of distance in space and time) characteristics.

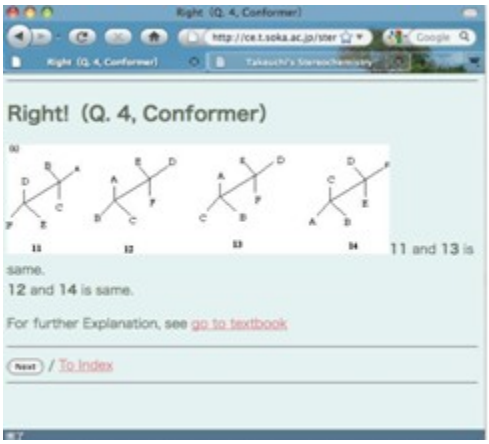
2.1 WWW-based Programmed Learning System

One idea we explored was to apply the programmed learning system to the Internet. Programmed learning has long been known as an effective method of self-learning and was often used as a supplement to traditional class learning. It is possible for students to learn the content of their choice anywhere at any time with the textbook of well designed programmed learning materials. The learning extends beyond the restriction of space and time. Introduction of this system to the Internet would enhance interactive characteristics and enable far broader accessibility beyond the restriction of space and time to it.

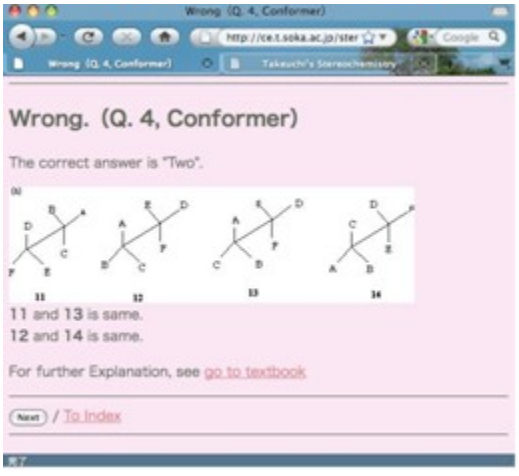
We already have a well-designed textbook of programmed learning on organic stereochemistry, a best seller written by Professor Takeuchi[5]). Thus, we reconstructed the problems so as to fit the web-based programmed-learning system that was designed and prepared by Moriya[6]) with cgi and disseminated its Japanese version in the class home page in 1999 (see also Scheme 2)[7]). Later, their contents were translated into English and internationally available in 2005[7]).



(a)



(b)



(c)

Figure 3 A typical set of question and response pages in the programmed learning system[7]). (a) The question page, (b) the page displayed when students choose a correct answer, and (c) the page displayed when students choose wrong answers.

Figure 3 shows an example of the question-response set in the system. Students read the question page (a) and choose one of the branches. If the choice is correct, then the page (b) is displayed and students can proceed to the next question. If the choice is wrong, then page (c) is displayed with the correct answer and a brief explanation. Then the student may either proceed to the next question or visit the relevant online textbook. Thus, depending on the understanding of the students, the system may guide them in an appropriate direction.

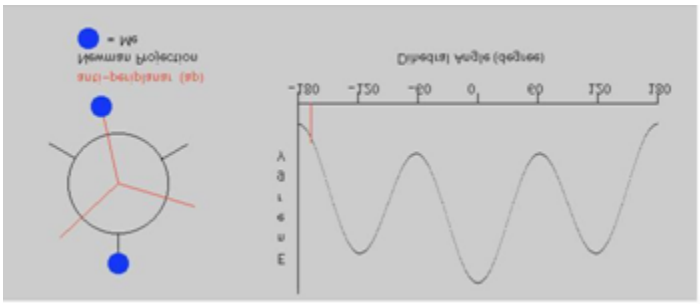


Figure 4 Java Animation for Conformation of Butane[8])

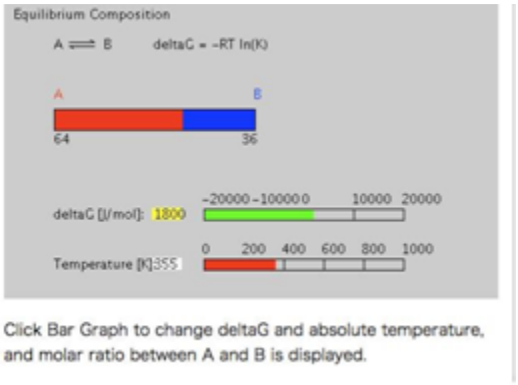


Figure 5 An Interactive Java Applet Showing Relationship of Isomer Ratio with G and Temperature[9])

2.2 Animations as an Aid for Learning Stereo and Dynamic Phenomena

As part of the effort on the VCE project, I developed two java applets, which were aimed at understanding of fundamental issue in stereochemistry, with the technical supervision of Dr. Yoshida. One was related to the conformers of butane (Figure 4)[8]). This animation displayed the relationship among the torsion angle, steric energy (right), and the name of the conformer (left, in red letters). The other was an interactive tool showing the dependence of the molar ratio of isomers in equilibrium (A <-> B) on their free energy difference (delta G) and temperature (Figure 5)[9]). Students could change the delta G and temperature in the equilibrium by a clicking on the respective bars to see how the molar ratio changed with them in an interactive manner.

More recently, Flash animations became increasingly popular, due to its feasibility and wide applicability. A few students helped me with the preparation of a few samples of Flash animations for learning Organic Chemistry (Figure 6)[10]). Its contents are as follows:

1. Drawing resonance structures
2. Newman projection and conformation (ethane and butane)
3. Fischer's stereo formula and the three-dimensional structure
4. Ring inversion of cyclohexane
5. Nucleophilic substitution (SN1 and SN2)
6. Elimination reaction (E1)

Figure 6 WWW page for the sample Flash animations for learning organic chemistry

The stereoscopic manner in the structure of organic molecules and dynamic manner of organic reactions are not easy to comprehend if taught only with the textbooks or on the blackboard. Animations is expected to serve as a good aid for students by raising their imagination and understanding of many other fundamental concepts and phenomena in organic chemistry. The animations complement learning with textbooks and in the class.

3. Impact

Among the teaching and learning contents shown above, the Q&A and Programmed Learning cgi seem to have been most successful, as is depicted in the access report of the ce.t.soka.ac.jp

www server11). Figures 7 and 8 indicate the monthly number of accesses to the Q&A and cgi files. Every year since 2003, more than six thousand students have visited the Q&A site (Figure 7), which corresponds to sixteen visits per day. Although the number of accesses to the programmed learning cgi exceeds forty thousands hits every year since 2003, more careful evaluation of the numbers is needed. Each visit to any query is counted as one access to the quest.qa file. Supposing that one student has accessed to twenty queries (approximate number of queries in one chapter) in one visit, the forty thousand corresponds to the two thousand visits per year and five to six accesses per day.

Organic Chemistry FAQ (/yuki/oc1&2faq.html)

year	Jan.	Feb.	Mar.	Apr.	May	Jun.	Jul.	Aug.	Sep.	Oct.	Nov.	Dec.	Total
2000							66			244			310
2001	150	125	50	161	244	260	270	21	99	177	209	346	2112
2002	502	333	124		450	649	566	232	335	506	546	401	4644
2003	513	362	187	318	720	685	771	280	347	607	805	695	6290
2004	740	614	341	578	983	1490	1477	604	427	863	904	740	9761
2005	1031	837	440	339	543	624	628	246	369	492	531	398	6478
2006	526	471	249	463	924	891	1122	380	470	839	914	804	8053
2007	808	586	411	547	1003	1227	1219	553	563	837	1014	878	9646
2008	1178	925	479	701	1296	1285	1403	793	683	1009	975	611	11338
2009	685	540	378	442	706	679	735	313	347	586	543	513	6467
2010	629	539	277	294	418	385	475	324	273				

Figure 7 Monthly Number of Accesses to the Q&A Page[11])

Programmed Learning, Problems (/quest.qa)

year	Jan.	Feb.	Mar.	Apr.	May	Jun.	Jul.	Aug.	Sep.	Oct.	Nov.	Dec.	Total
2000	698			203			1839			498			3238
2001	273	328	39	395	530	931	910	662	941	1521	1440	931	8901
2002	2112	921	529		1260	1473	2108	1452	1253	2180	2557	2883	18728
2003	5871	3506	1938	2788	4521	4551	7573	2872	2370	2275	3743	2234	44242
2004	5187	3384	1316	3749	6200	5043	5936	3118	2215	3011	3342	3016	45517
2005	6157	3579	2148	2661	4022	3968	6188	1624	2623	3856	2688	1775	41289
2006	3725	2621	1274	2868	5341	6927	9060	2890	2518	4349	3837	3039	48449
2007	7618	4617	1660	4064	6234	5341	8359	3953	1879	3682	3729	3596	54732
2008	4583	2967	2011	2383	4996	5069	7482	2798	2143	2809	3423	3824	44488
2009	5199	3318	3181	3149	3444	3437	6488	1777	1775	1614	2620	2270	38272
2010	3386	4849	1483	2022	2971	4648	6472	5149	2612				

Figure 8 Monthly Number of Accesses to the Queries at the Page for Programmed Learning[11])

Most of the work described here was done more than five years ago. Considering that the site is open outside the university, the number of accesses to the pages is not very large. Nevertheless, they helped a relatively large number of students who were learning organic chemistry every year, not only in Soka University but also in Japan, and will continue to do so in the future. I will be happy if my experience serves as a clue for younger more technologically savvy teachers, to develop new teaching strategies in organic and other fields of chemistry in many countries.

I give my hearty gratitude to Professor Yoshito Takeuchi and Dr. Hiroshi Yosida for their inspiring and encouraging me with these works. I also thank Mr. Takashi Moriya (Programmed Learning cgi), Dr. Naoki Yamamoto (the first Flash animation), and all other students whose names appear in the web pages in References.

References

1) "Organic Chemistry : Frequently-Asked Questions" (in Japanese), url = http://ce.t.soka.ac.jp/yuki/oc1and2faq.html.
2) "Organic Chemistry Class Materials" (in Japanese), url = http://ce.t.soka.ac.jp/yuki/shiryo.html
3) "Organic Chemistry" (in Japanese), url = http://ce.t.soka.ac.jp/yuki/.
4) Y. Takeuchi, H. Hosoya, H. Yosihda, and M. M. Ito, Pure Appl. Chem., 71, 825-834 (1999).
5) Y. Takeuchi, "Introduction to Stereochemistry-A Programmed Study" (in Japanese), Kodansha, Tokyo (1980).
6) T. Moriya, M. M. Ito, Y. Takeuchi, and H. Yoshida, 16th International Conference on Chemical Education (16th ICCE) Book of Abstracts, 308 (2000).
7) "Professor Takeuchi's Stereochemistry-A Programmed Study", url = http://ce.t.soka.ac.jp/stereo/index-j.html.
8) "Conformers and their Nomenclature", url = http://ce.t.soka.ac.jp/stereo/Ch2/icce.html.
9) "Free Energy Difference to Molar Ratio against Temperature", url = http://ce.t.soka.ac.jp/stereo/Ch2/stereo2.html.
10) "Flash Animations for Learning Organic Chemistry", url = http://ce.t.soka.ac.jp/flash/; M. M. Ito, 2005 International Chemical Congress of Pacific Basin Societies (Pacifichem 2005), COMM 84 (2005).
11) "CE Web Server: Access Report", url = http://ce.t.soka.ac.jp/report/.

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A Fully Assignable Electronic Textbook

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I. Introduction

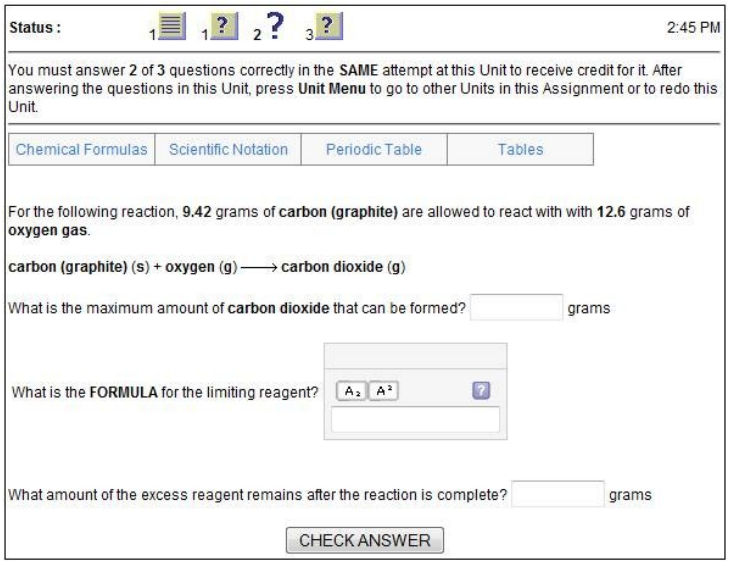
Electronic homework systems are now approaching, or exceeding, twenty years in use. They have evolved from simple multiple choice question banks to the use of randomly selected "question pools" to the use of both numerically and chemically randomized parameters. More recently, stepwise tutorials and interactive simulations, animations, and videos have been included as part of homework assignments. We have worked on integrating these assignment types in the general chemistry OWL (Online Web-Based Learning) system for the last 15 years or so. They system now contains thousands of randomized homework assignments, each with extensive randomization and feedback. This note highlights our current work creating an integrated hybrid textbook that contains a hardcopy version and an online version that fully immerses assignable content throughout the text narrative.

II. A Review of Interactive Homework Modules

The OWL system contains the following types of modules:

A. Core OWL Mastery Assignments

These modules most often offer the student a set of three questions and ask them to solve two of them correctly to gain mastery credit. However, each of the three "questions" might well require multiple correct responses. An example problem (on limiting reactants) is shown below. This problem counts for one of the two they need to complete.



When the student enters an answer, they receive feedback on whether they are correct, as well as a full solution to the problem.

Feedback:

1. Write a balanced chemical equation for the above reaction:

$C\,(s) + O_2\,(g) \longrightarrow CO_2\,(g)$

2A. Determine the number of grams of **carbon dioxide** that can be formed from the available **9.42** g of **carbon (graphite)**:

$$9.42\text{ g C} \times \frac{1\text{ mol C}}{12.01\text{ g C}} \times \frac{1\text{ mol } CO_2}{1\text{ mol C}} \times \frac{44.01\text{ g } CO_2}{1\text{ mol } CO_2} = 34.5\text{ g } CO_2$$

2B. Determine the number of grams of **carbon dioxide** that can be formed from the available **12.6** g of **oxygen gas**:

$$12.6\text{ g } O_2 \times \frac{1\text{ mol } O_2}{32.00\text{ g } O_2} \times \frac{1\text{ mol } CO_2}{1\text{ mol } O_2} \times \frac{44.01\text{ g } CO_2}{1\text{ mol } CO_2} = 17.3\text{ g } CO_2$$

---

3. It is possible to form **34.5** grams of **carbon dioxide** from the available **carbon (graphite)**, but only **17.3** grams of **carbon dioxide** can be formed from the available **oxygen gas**.

The limiting reagent is O_2. All **12.6** g of O_2 will be used and **17.3** grams of CO_2 will be formed.

---

4. Calculate the amount of **carbon (graphite)** that is used by reation with the **12.6** g of **oxygen gas**.
Keep an extra significant figure here and round after step 5.

$$12.6\text{ g } O_2 \times \frac{1\text{ mol } O_2}{32.00\text{ g } O_2} \times \frac{1\text{ mol C}}{1\text{ mol } O_2} \times \frac{12.01\text{ g C}}{1\text{ mol C}} = 4.729\text{ g C}$$

---

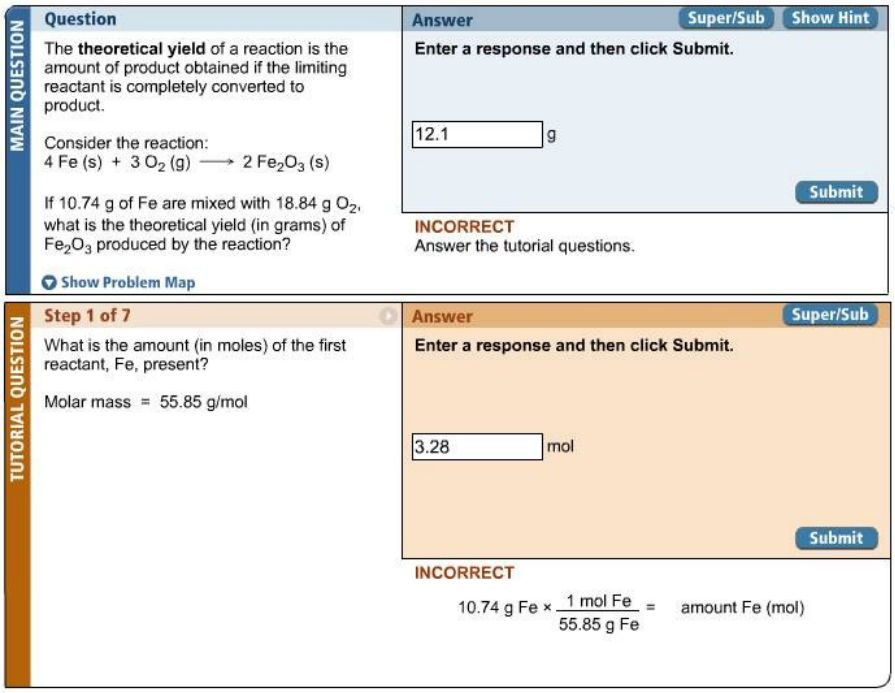
5. Calculate the amount of **C** that remains in excess.

9.42 g C originally present - **4.729** g C used = **4.69** g C in excess

If the student does not answer correctly, a new version of the question is offered that has different numbers, different chemical systems, and, often, different wording.

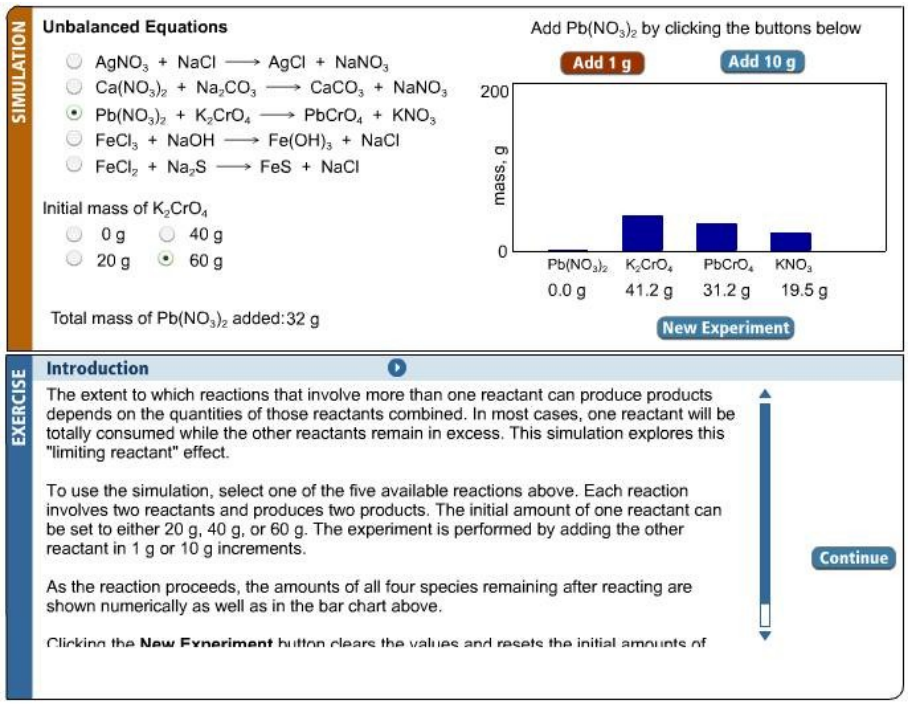
B. Tutorials

Each major problem type includes a step-by-step tutorial. These modules ask a typical question, and should the student answer incorrectly, the module asks a series of simpler questions to lead them through the solution to the problem. The example below shows the first tutorial step for a similar limiting reactant question. This example is linked here.



C. Interactive Conceptual Simulations

Each major concept is supported by one or more simulation, video, or animation-based exercises. These exercises typically give the student a panel with which they explore a chemical system as well as a guided-inquiry panel that asks questions that lead them through the exploration. These modules are also given to the instructor without the leading questions so they can be used during class. This module is linked here.



III. Traditional Linking of Texts to Online Homework

To date, electronic homework systems have been used in conjunction with traditional textbooks by two-directional annotations. In the text, each particular area that has a supporting homework module notes the presence of the module and directs the student to go work on it. In the homework, each module notes where to find in the textbook the information to help understand and solve the problem at hand.

IV. The Integrated Approach

The genesis of this project comes from the following questions: Why are the homework and the text separate? Can they be an integrated, single, assignable unit? The purpose of the project is to create a single, integrated system where traditional items within a text become assignable modules in the homework system, but not in a separate way. The goal is to make a system where reading the textbook is working the textbook, and working the textbook is doing your homework.

Textbooks have a particular structure for a reason- certain concepts and skills naturally precede other concepts and skills. Because of this, we have fully retained the traditional textbook structure:

- Chapter 1
  - Section 1.1
    - Subsection 1.1a
    - Subsection 1.1b
    - Section 1.1 Summary Assignment
  - Section 1.2
    - Subsection 1.2a
    - Subsection 1.2b
    - Subsection 1.2b
    - Section 1.2 Summary Assignment
  - Section 1.3
    - Subsection 1.3a
    - Section 1.3 Summary Assignment
  - Chapter 1 Summary Assignment
    - Challenge Problems
    - Chemistry and You Problems
- Chapter 2…

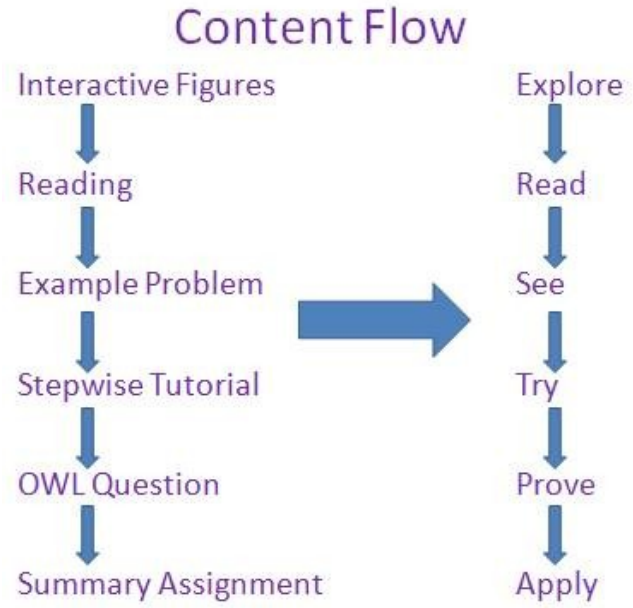
Each Section begins with an "Opening Exploration" that, while relatively easy, gives the students a flavor for what concepts will be introduced and what purpose they serve. An example is linked here. The core content then resides in Subsection pages. These typically have a number of elements:

- Text
- Interactive Figure (assignable)
- Text
- QuickCheck Question (assignable)
- Example Problem Suite
  - Static Example Problem with hidden, expandable solution
  - Video Solution, narrated whiteboard walkthrough of the static solution
  - Stepwise Tutorial (assignable)
  - Mastery Question (assignable)
- Text …

Interactive Figures are assignable versions of problems that turn photos into videos, charts into simulations, and graphic art into animations. These have a series of questions that lead the student to pay attention to the aspects of the figure that are important to note. Examples are linked here and here. QuickCheck questions are simple reading comprehension questions and are there- frankly- just as an incentive to get the student to pay attention to the reading.

Throughout the text, the difficulty of assignments is "ramped up" from concepts to practice problems to mastery assignments to challenge problems. Modules that introduce concepts (interactive figures and tables) are generally supported by fairly easy questions- the idea is to get the student to pay attention to what is being covered. Example problems begin with a stepwise tutorial that is generally fairly easy to work through because of the detailed, step-by-step help. Mastery questions are more difficult because the student must start over with a new version of the question if they get it wrong. Section summary assignments are more difficult yet because they require students to answer multiple questions in a single setting, and the questions are less defined. Finally, the chapter summary assignment is most difficult because the questions are not categorized for the student, and the most challenging questions are asked in that section. This progression starts at exploration and moves through mastery of the material and finally the ability to apply it.

This pedagogical flow through the assignable content is summarized in the figure below.



V. Other Features and Plans

Through testing and interviews with students and instructors, we recognize the necessity of a physical hard copy text. The plan is to provide a text that includes all the narrative, figures and example problems, but not the summary assignments. Those assignments are intended for online work. The text will therefore be relatively brief compared with more traditional texts. The online

version will include the kinds of tools one expects: bookmarking and note taking, instructor insertion of notes and links, tools for student-student and instructor-student communication.

Creation of the assignable text involves creation of the text, and of the assignments. The pieces are then built into the electronic book system and into a physical text. This process is nearing its completion and we have performed tests on sample classes using mostly but not fully functional test systems. In general, students find the integrated approach useful and we find an average of 4-5 hours of student work to move through a chapter. Further limited-scale testing is planned for Spring 2011 semester and use by a wider group of larger classes is planned for the Fall 2011 semester.

The completed assignable text will be published and distributed by Cengage Learning, who has licensed and distributed the OWL system for the last decade.

Anecdotal Uses of Facebook, Google Calendar, and Cell Phones in a High School Classroom

Lauri McCormick McDonald, Chemistry Teacher, Highland Park High School

As a high school educator, one of the biggest priorities (after covering the required standards tested on state assessments) is finding a way to engage students and "meet them where they are." In a world of fast-paced and flashy media, sometimes school classrooms can feel like a time warp for students. While working to find a way to create a rigorous Pre-AP Chemistry course, I have determined that utilizing some new technologies has been successful without sacrificing course content. Over the past few years, I have incorporated Facebook, Google Calendar, and cell phones into my curriculum with favorable results.

In a world of digital communication, students, unlike many professional adults, do not feel the pressing demand or necessity to check their email daily; in fact, a number of my students have confessed to checking their email once a month or less. In an effort to find a more effective way to contact students other than calling or texting, I decided to create a Facebook account and group for my chemistry classes. The majority of my students spent much after-school time on their Facebook accounts, and I soon found that communication with them became quick and effective through my chemistry group.

After setting up an invitation-only Facebook group, most of my students joined and participated, though involvement was not required. By sending out group reminders or posting important events on my Facebook group "wall," I watched my homework completion rate and class preparedness spike. My Pre-AP chemistry students, who were already highly motivated but mostly over-scheduled, no longer forgot to wear correct lab attire or to turn in major assignments. I also found an increased level of communication, as many students felt more comfortable addressing me through Facebook rather than in a face-to-face class discussion.

Since the Facebook group was optional and not accessible to all students, I also posted all information on my school website. But, I found that the information on Facebook reached more students. Even the most motivated of students did not go to the school website on a regular basis or "hang out" there for fun, yet free time spent on Facebook's site was a norm for even the "nerdiest" of high-schoolers. At first a few students thought it odd to have an overlap between their social life and school life, but most saw that the benefits overshadowed any issues created. In a survey, one of my students commented that Facebook, for her, had become "a common thoroughfare, a one-stop school and extracurricular info spot."

Fresh off the success of Facebook, I felt the need to organize the daily calendar for my classes. Our campus instructional technologist introduced me to the fabulous organizational tool Google calendar, which has proved invaluable in my classes. After creating a public calendar for my chemistry classes, my students were able to subscribe to it for free and immediately populate

their own Google calendar with information on upcoming events in my chemistry class. Users with a google account (also free to create) could sign up for email reminders and/or texts from their Google calendars. The daily posting of a calendar entry detailing the minutiae covered in class, including specific homework, was now available to every student from the comfort of their own home or anywhere with internet access. I no longer had to worry about an inflexible, print-out syllabus that could easily and quickly become outdated, especially in the high-school world of last-minute assemblies, pep rallies, and other class interruptions. Absent students no longer had to seek me out to find out their makeup work, as they could check the calendar from home and get caught up on their own. (For a high school teacher, putting this responsibility in the hands of the students was a wonderful help and relief!)

Another perk to using Google calendar was the ability to embed it on all websites. So, instead of populating 3 different calendars from 3 different website programs, I was able to put my class calendar, which was now always accurate and current, on all websites and programs used for my class, and it was automatically updated. Consequently, I have found my course content is more organized, which has been a help to both my students and me.

After the incorporation of Facebook and Google calendar into my classes, I felt ready to take a big step and work on conquering many classroom teachers' and professors' biggest fear: the cell phone! I had heard the facts: one of the most widely unused tools in American classrooms is the cell phone; with computing power beyond that of the first mainframes, a handheld cell phone has many powers that we have been wont to embrace in our halls of learning; and one of the most common quotes in classrooms today is "Please put your phones away." But, after listening to an innovative teacher present on different means to tap the powers of the cell phone, I decided to give it a try.

I learned about Poll Anywhere, a website that allows the user to create a free account and then create free polls with limited options. In lieu of clickers, I created polls eliciting student responses via text, web, tweets, or smartphone voting. These polls worked in the same manner as voting for a favorite on American Idol or Dancing with the Stars, so students were familiar with the format and immediately understood the process. Poll Anywhere also provided a link that kept a live update as student responses were entered, and I was able to post the live poll on a website or Powerpoint presentation shown at the start of class. I used the polls as a way to grab student interest for the topic of class that day. Of course, there were expanded options with a paid monthly fee, such as matching responses to specific students, moderation of open-ended comments, or polling of an audience of more than 30 at a time, but, for the general purposes of providing a "hook" to grab a student's interest, the free membership worked well in my high school classroom.

I am fortunate to teach at a school where I have an administration that is supportive in the incorporation of new technologies and where over 90% (and probably closer to 100%) of students own cell phones, many of which are smart phones. So, the utilization of these technologies into my classroom did not create some of the hurdles that many teachers have experienced. However, I would encourage chemistry educators to find means to embrace new methods of communicating and interfacing with their students. Globalization and progress points to the fact that we as educators are preparing our students to perform in a society in which job

skills and technologies are still undeveloped today. So we must teach our students to be adaptable, and we must adapt ourselves, to an ever-expanding technological culture. While that may sound overwhelming, it is easy to start with implementation of simple, user-friendly ideas like Facebook groups, Google calendar, and cell phone polls.

Websites:
Facebook. <*http://www.facebook.com*>
Google Calendar. <*http://calendar.google.com*>
Poll Anywhere. <*http://www.pollanywhere.com*>

References:
Alexander, Bryan. 2004. Going Nomadic: Mobile Learning in Higher Education. *EDUCAUSE Review* 39(5): 28-35. <http://net.educause.edu/ir/library/pdf/ERM0451.pdf> (Accessed October 20, 2010).
Drive Belonging and Engagement in the Classroom. <http://org.elon.edu/catl/conference/documents/FacebookEducation.pdf> (Accessed October 23, 2010).
Johnson, L., A. Levine, et al. 2010. *The Horizon Report: 2010 Edition*. Austin, Texas, The New Media Consortium. <http://www.nmc.org/pdf/2010-Horizon-Report.pdf> (Accessed September 3, 2010).
Pence, Harry E. *Reference Librarian*, in press.

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Resources and Strategies for Creating Molecular Animations

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Why create molecular animations?

Molecular animations have been used extensively in undergraduate science courses to teach concepts that are difficult or impossible to represent with static diagrams. Animations can assist learning by providing multiple perspectives of complex structures, or they can be useful in depicting changes in a system over time.

While some instructors create animations for their courses, many rely on animations provided by textbook publishers, supplied on physical media (CDs or DVDs) or deployed on the web. Even though there are numerous existing animations, some instructors will want to create new animations to assist their specific aspects of their teaching. Many instructors are intimidated by the complexity of the software used to create the animations found in textbooks and on the internet, many of which were created by artists with expertise in the digital realm. But with a little persistence, it is possible for any would-be animator to create simple and reasonably effective animations to communicate key ideas for which static figures are inadequate.

Animations can take on many forms, from simple frame-by-frame 2D animations, to complex cinematic quality 3D animations. While the latter receive the most attention, there is no strong evidence that their "realism" necessarily helps students grasp complex concepts (Smallman & St. John, 2005). An individual should weigh the cost (time and effort) required to create an animation versus the learning gains that are desired.

Strategies for making molecular animations.

There are two major strategies for making animations of molecules. The simplest route, which may be the easiest, is to record images that are dynamically generated from molecular graphics programs, such as many of the research level programs such as UCSF Chimera [see tables for web links]. The recorded movies can be subsequently edited and annotated in one of many video-editing programs (such as Adobe Premiere or Apple FinalCut-both of which have simpler, cheaper prosumer versions). High quality movies can be quickly rendered using the powerful graphics engines underlying these software packages. The downside, however, is that the choreography of events is somewhat limited. Some of this can be made up by multiple "shots" and post-recording editing. Many of these programs also have a limited ability to "morph" between different molecular conformations, something that can be quite useful in depicting the conformational changes of macromolecules such as proteins. Extensions to these programs (such as the eMovie plug-in in PyMol) can be of considerable assistance in the creation of animations.

These research-level molecular graphics programs are also able to import data from programs that simulate molecular dynamics, by reading in data files that describe the trajectory of atoms or molecules over time. The advantage is that these molecular graphics programs can provide a much more elaborate rendering of the molecules in motion, since they can vary the form and shading the molecular representations, as well as spotlights, shadows, and depth cues.

UCSF Chimera http://www.cgl.ucsf.edu/chimera/	pre-installed Movie
UIUC VMD http://www.ks.uiuc.edu/Research/vmd/	pre-installed Movie extension
Schrödinger (DeLano) PyMol www.pymol.org/	pre-installed extension also: eMovie plug-in http://www.weizmann.ac.il/ISPC/eMovie.html

The more difficult path is to create these animations from scratch in a dedicated animation program. There is no royal road to geometry, and likewise is no easy path to the creation of more complex molecular animations. Most of the major applications have a formidable learning curve for creating anything beyond translation, rotation, and scaling of objects. But this is not a reason to avoid such efforts, since with a couple of weeks of hard work, the basics can be mastered, and much more complex animations can be created. Manuals can be useful, but there are also quite a number of online sources for instruction. Notably www.lynda.com or www.digitaltutors.com provides exceptional training for a reasonable fee for most of the programs described below. These online training libraries wonderfully illustrate the utility of animation, in that watching an instructor manipulate the program to achieve specific outcomes is accomplished in a way that is difficult to get from the printed page.

Good animations may not always be strictly literal. There are insights from artists, including those that created the first cartoons. A number of excellent books summarize these principles. While these insights may not be necessary in creating the simplest animations, they do have utility as the animations grow more complex.

Storyboarding is a necessity as animations grow more complex. It is best to first figure out exactly what you want to show, sketch it out via a storyboard, and only then begin the process of creating an animation. The storyboard can be a useful tool in helping the animator make critical decisions about what they should show versus what can be excluded.

Tools for creating molecular animations.

The actual mechanics of creating animations in dedicated software program requires a few things: (1) understanding how to use the basic drawing tools, (2) understanding how to use the tools that can transform the graphic objects, and (3) understanding how these transformations can be achieved over time. Most of these programs use a timeline metaphor for choreographing the changes over time. Use of this timeline requires an understanding of the concept of setting key frames, and letting the program help in the transformations of object that occur between those key frames.

The world is flat.

2D animations are intrinsically easier to create, but many of the basic principles can be extended to 3D animations. The preeminent tool for creating 2D animations is Adobe Flash, which renders animations in the SWF format that can with the use of the Adobe Flash player, be rendered in web pages. The majority of animations seen on the web have been generated in this manner. It does have the advantage that the Player is installed on the majority of personal computers, regardless of which operating system or browser is installed. This is likely to remain the default for some time, but there is rapid movement to using an open web standard, HTML5. Quite impressive animations can be achieved with HTML5, but the tools for creating these animations are still rather limited. But with the support of Apple and Microsoft, HTML5 is likely to become a major player in the next few years. At a recent developers' conference, Adobe demonstrated a Flash-to-HTML5 translation utility (reviews.cnet.com/8301-13727_7-20021213-263.html), suggesting that the adoption of this new standard will be rapid.

Adobe Flash http://www.adobe.com/products/flash/
SWISH Max http://anime.smithmicro.com/index_pro.php
Anime Studio http://anime.smithmicro.com/index_pro.php

One of the most useful additions to these programs has been the introduction of inverse kinematics, which is a way of animating jointed object with pivot points. While this might seem to be more relevant to character animation than molecular animation, these animating tools make animation of complex movements in molecules considerably easier, from changes in bond geometry to conformational changes in biological molecules, the ability to add "bones" to objects that constrain movements is a timesaver. In addition, some of these programs now have a simple physics engine that enables the simulation of some simple dynamic behaviors such as responding to collisions. The only other way to achieve this sort of physics is through programming scripts associated with the individual objects, such as ActionScript in Flash.

A bridge to the third dimension.

Some of these animation programs are able convey a limited representation of the third dimension, a sort of 2.5D perspective. Most of these programs accomplish this effect by placing 2D animations within planes that are stacked in the third dimension. Many contemporary cartoons use this strategy, and it can be effective in representing the third dimension on the cheap.

Anime Studio http://anime.smithmicro.com/index_pro.php
Toon Boom Studio and Toon Boom Animate http://www.toonboom.com/main/ http://www.toonboom.com/products/animate/

Molecular visualization programs and movie creation

Many animations strive to achieve a "realistic" three-dimensional effect, which can be accomplished as described above, but beyond simple translation, rotation, and scaling, things become much more complex or essentially impossible to do. At this point, it is necessary to make the leap to 3D modeling and animation programs. The effective use of these programs requires several distinct tasks: creating a 3D model of a molecular object, positioning it in a scene with respect to other objects, and then choreographing the relative motions of the objects, either as the individual objects change shape or orientation. or as they move relative to one another. These movements are usually orchestrated at the level of the timeline, which is fundamentally the same as in 2D animation programs, with the notable exception that many more parameters are being keyed over time.

There are many high-end 3D graphics and modeling programs that are used for this purpose. Most of these would be completely unaffordable if the software publishers did not provide huge discounts to academic users. The same software packages used by Pixar and in movies like Avatar can be purchased for less than $400, which provides a permanent license to faculty and students for non-profit uses. Many of the most sophisticated animations have been created in Autodesk's Maya program, but there are quite of number of other software packages that can yield high-quality animations. Maya, Cinema4D, and other software packages also include physics engines which can be of use in creating more physically realistic movements of molecules. Maya has been available for some time, but there are other programs that yield similar high quality "photorealistic" animations.

Another advantage that these high-end 3D graphics programs have is that they are both scriptable and extensible, and programmers have created interfaces to facilitate the creation of molecular objects and animating them. This has been especially true for Maya and Cinema4D.

There is also one open source "free" program, Blender, which has continued to evolve to gain the feature set found in the high-end 3D programs. While there may be more formal support for Maya and other commercial programs, there are excellent online resources and support forums for the Blender program. Since Blender is open source, it likely that interfaces will eventually be added via plug-ins that will enable it to directly import molecular structure data to create geometric objects.

Blender	http://www.blender.org/
Autodesk	Maya (part of a Autodesk Education Suite for Entertainment Creation) http://usa.autodesk.com/
Maxon Cinema4D	http://www.maxon.net/
Pixologic Zbrush	http://www.pixologic.com/home.php
Luxology Modo	http://www.luxology.com/
Side Effects Houdini	http://www.sidefx.com/
Cheetah3D	http://www.cheetah3d.com/
Unity3D	http://unity3d.com/

The first task in the 3D animation process is to create geometric models for specific molecular objects. This can be done by modifying primitive geometric objects, but is some cases it is possible to use molecular graphics programs to do the conversion of a structural model (such as a .pdb or .xyz data file) into a 3D modeling object format (such as .obj, .dxf, or .vrml). In this case, the converted models can then be directly imported into the 3D modeling program for further refinement and animation.

The individual molecular objects are then arranged on the "stage" within a viewing window, within the view of a specific camera that will capture and render this scene. Cameras, like the individual objects, can also be moved within the scene over time (dolly, pan, etc. as in cinematography). This is where the storyboard is essential in helping an animator make decisions of what will be shown and when. The movements of objects and cameras are choreographed via a timeline by setting keyframes and having the program generate the in-between frames of a movie. These programs have the ability to render animations in formats that can then be further edited in programs such as Adobe Photoshop or AfterEffects.

An alternative that needs more attention is to use snapshots of these animations to create a graphical narrative describing a mechanism or complex process. Given the familiarity of students and instructors with graphical narratives of all kinds (comics, graphic novels, anime), it is possible for an animator to tell a story using what could be considered a sparse form of animation. Readers understand the conventions for space and time used in these graphical narratives, and as a result, many of the actually movements can be obtained for free in the viewer's brain, since no one needs to see Superman, e.g., move in a step-by-step manner as he flies from point A to point B in Metropolis. In a sense, 3D is obtained for free.

Interactivity represents an additional level of engagement. Students are well-versed in 3D environments for gaming, and there are well-established pathways to bring 3D animations into interactive 3D environments, many of which have sophisticated physics engines that can automatically handle the dynamics of attraction, repulsion, and collisions. It is likely that there will be an increasing emphasis on deploying these sort of interactive environments on mobile devices such as Android or Apple iPhone. Some software packages are designed to facilitate this process, such as the Unity3D game development tool.

Another option for providing interactivity is through the use of sophisticated PDF (Portable Document Format) documents that incorporate interactive 3D images, with limited options for animation. These document can be created by Adobe Acrobat Pro and other programs from data created in 3D modeling programs. While this variation on the PDF document is used mostly in conjunction with CAD (computer-aided design) for engineering and architecture, there has been also some use of this interactive PDF format in journals such as Nature.

Once an animation is created, it is very important to get feedback from colleagues and students concerning its clarity and usefulness. It is typical that an animation will go through multiple rounds of revision before it is ready for use in the classroom.

How to use animations in the classroom?

Molecular animations can be used in a variety of ways in the chemistry or biology classroom. In many cases, they are used occasionally to highlight a specific point in a lecture setting that is difficult to relate with a static diagram or series of diagrams. A good example would be an animation that demonstrates a cyclic process, such as the pumping of sodium and potassium ions by the sodium-potassium ATPase in the plasma membrane of cells. Some courses and textbooks use animations extensively to teach chemical concepts, with a comprehensive set of animations that are linked to specific classroom exercises. In all cases, there should be a clear need for the animation to help students understand a concept. There are many cases in which an animation may not be necessary, and that a static diagram or written description is more effective. Animations, no matter how pretty, should support the learning objectives for the student.

There are challenges in effectively using molecular animations. First of all, to what degree do they communicate the essential point. It is quite possible to create an animation that prompts a "gee-whiz-this-is-neat" response from students without actually effecting much in the way of insight to the phenomenon that is being represented. The instructor can improve the delivery by showing the animations multiple times, with and without comments, and then followed up with questions for the students.

Another avenue for the use of animation in the science classroom is to have students create their own animations of a sort. Given that the animation programs have a steep learning curve, a simpler and accessible approach is to have the students create a visual or graphical narrative describing a complex structure or process. Creating storyboards of the type used to plan animations can be very effective in getting students to confront the essential aspects of chemical or biological processes because they are forced to explain the concept with their own words and pictures as they create a story that explains the concept to others.

Finally, assessment should have an important role in the use of animations. This can be done informally through course evaluations and review of test results, but whenever possible, there are advantages to setting up more rigorous tests of the efficacy of the animations in effecting learning. A number of studies have been carried out to look at the effectiveness of using molecular animations to teach chemical and biological concepts, but there is much more work that can be done to test various principles of design that make for a demonstrably effective learning tool.

References and Further Reading

Bromberg S, Chiu W, Ferrin TE. Workshop on molecular animation. *Structure*. 2010. 18(10):1261-5.

Iwasa JH. Animating the model figure. *Trends Cell Biol.* 2010 Sep 8. [Epub ahead of print]

McClean P, Johnson C, Rogers R, Daniels L, Reber J, Slator BM, Terpstra J, White A. Molecular and cellular biology animations: development and impact on student learning. *Cell Biol Educ.* 2005. 4(2):169-79.

McGill G. Molecular movies... coming to a lecture near you. *Cell*. 2008. 133(7):1127-32.

O'Day DH. The value of animations in biology teaching: a study of long-term memory retention. *CBE Life Sci Educ.* 2007. 6(3):217-23.

Smallman, H.S. & St. John, M., Naïve Realism: Misplaced Faith in Realistic Displays. 2005. *Ergonomics in Design* 13(3), 6-13.

Stith BJ. Use of animation in teaching cell biology. *Cell Biol Educ.* 2004. 3(3):181-8.

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OrganicPad: a freehand interactive application for the development of representational competence.

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One reason chemistry poses a challenge to both learners and teachers is that, for robust conceptual understanding, students must understand how and why molecular level structure affects reactivity and properties. Much has been written on the difficulties students have in translating between a symbolic, molecular, and macroscopic understanding of chemistry (1, 2) and most modern texts go to great lengths to provide multiple representations to students.[1] Lewis structures are probably the most important of the symbolic representations that students encounter. Students must master not only what the representations mean, but also how and why they are constructed, and what they are used (and useful) for. Unfortunately, many students have great difficulty both drawing and using Lewis structures. For example in our work we have seen that the majority of students (even in an organic chemistry course) do not appear to use structures to predict properties in a meaningful way (3). Many students (and perhaps some instructors) confuse the rules for drawing structures with the concepts that underlie bonding, resulting in students who believe that bonds form because atoms "want" or "need" an octet (4, 5). Indeed the idea that Lewis structures are symbolic representations may well be lost on many students (for example: if asked what the bond angle is in methane, when presented with a typical Lewis structure, many students will answer 90).

These problems notwithstanding, learning to draw and use Lewis structures accurately and effectively remains an integral part of most general chemistry courses, and is an especially important skill for those students planning to move on to organic chemistry. The development of these skills during general chemistry is all the more important since many organic chemistry instructors assume (erroneously as our work has shown) that students have mastered this skill before they begin the course (3).

There is a fairly large literature on "improved" ways for students to learn to draw structures, but unfortunately this is one of those tasks that requires "bootstrapping" as Taber calls it (6). For many structures, it is difficult to elucidate the connectivity between the atoms correctly unless you already know what the structure should look like. In other words, the students are caught in a kind of "Catch 22". The solution to these problems is practice and a growing familiarity with the typical types of structures that are normally encountered in introductory chemistry courses. This familiarity is often difficult to obtain if beginning students are required to draw the many exceptions to the "rules". Another common approach is to require students to draw only

structures where there is one central atom (noble gas compounds, inter-halogen ions and the like - many of which they will never meet again), which results in our distressing finding that many organic chemistry students have significant trouble drawing organic molecules with more than one carbon atom (3). Ideally, in order to master the basic skills, students need practice and immediate feedback that prompts them to think critically about what they are doing, rather than simply providing the correct answer.

Since Lewis structures are in fact rule-based representations, technological solutions are clearly appropriate, and there have been a number of systems developed that will recognize and grade input from students. While many of these systems are widely adopted and have been incorporated into publishers' course management systems, there remains the problem that the interface is typically not naturalistic, and students (who are already struggling with learning to draw structures) must also face fairly steep learning curves as they drag and drop atoms and bonds, choose items from a template, and place them in fairly limited positions on the screen.

It was in this light that we developed *OrganicPad*, (Figure 1), a freehand interactive tablet-PC based program that can recognize and respond to student input in a variety of ways and a variety of settings

Figure 1. OrganicPad with examples of some of the representations that can be drawn.

Overview

The current version of *OrganicPad* is a PC-based program designed for use on tablet PCs or for use with a Wacom slate; however, it can also be used with a mouse or trackpad. A web-based version is currently under development. This paper describes the PC-based system now in use and how we plan to extend it to the web.

OrganicPad has a number of features. Using the draw mode, the program can recognize atomic symbols, bonds, lone pairs and charges. Once a structure is drawn, it is possible to convert it to a 3D representation, as shown in Figure 2. The 3D mode allows student to convert a structure to ball and stick, space filling models and/or electrostatic potential maps. In the pen mode the screen is just like a blank sheet of paper allowing teachers and students alike to annotate the structures that they are creating. The push tool allows students to draw curved arrows when they are representing electron flow during organic chemistry mechanisms. It is important to note that in draw, pen, and push modes the students' input is recorded in a database for further analysis.

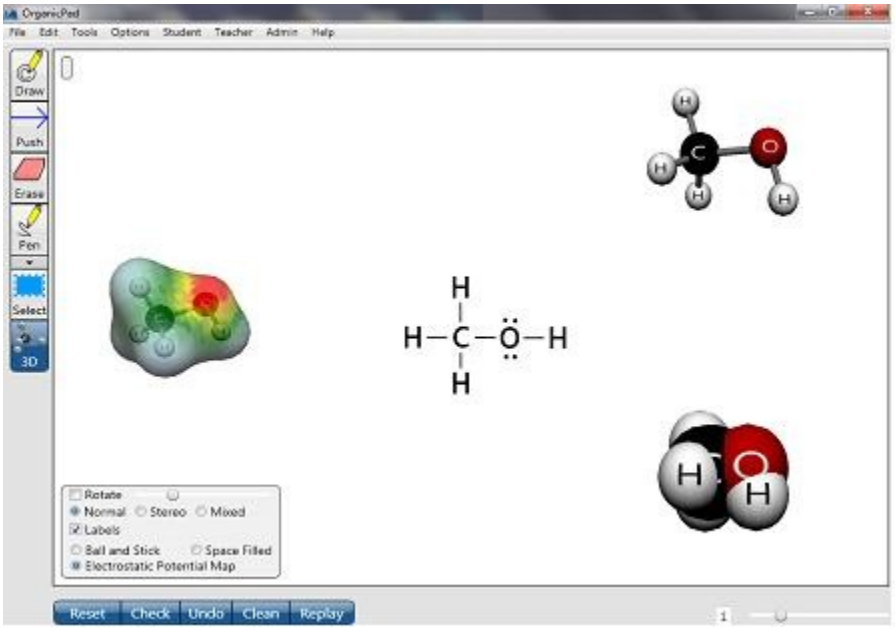

Figure 2. Types of 3D representations that can be produced with OrganicPad.

OrganicPad for teaching and learning

The simplest way to use *OrganicPad* is to draw structures as you normally would onto the tablet screen. The program can recognize the "common" atoms, that is, H, C, N, O, I, Cl, Br, F, S, P, Na, Li, Mg, Al, B. There are as few constraints as possible placed on how the student draws the structure - the system is flexible and students need not place their structure in any particular orientation or draw it in any order. When finished, the student can hit the check button, and the program will indicate whether the structure is correct, or if there are problems, where they lie as shown in Figure 3. In this example, both the hydrogen and carbon atoms have been boxed in red to indicate that the student has drawn too many bonds to both.

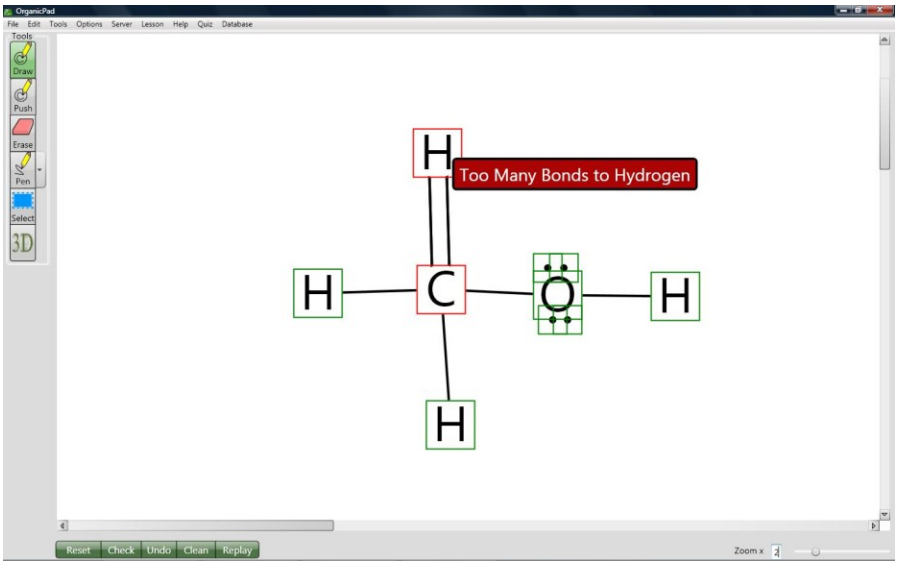

Figure 3. An example of feedback.

While this mode, in itself, can be very useful, we have developed a more sophisticated feedback system, for a limited set of structures, in which contextual responses have been developed to provide the student with increasingly directed feedback as they move through the task of structure drawing. An example of this is shown at (http://www.youtube.com/watch?v=CAqCashseYI). The feedback is based on our studies of how students often proceed as they write Lewis structures, and common errors that they make (3). We are currently conducting studies on how working with this kind of contextual feedback impacts student abilities.

OrganicPad as a classroom activity

There are a number of ways, both synchronous and asynchronous, that instructors can use *OrganicPad* in their classrooms or labs. Students can log-in to the system which then allows the instructor to send asssignments to them. The instructor can draw or choose a correct answer from the students responses and the program will grade the structures the student has drawn and send feedback to each individual. The instructor can also view what a specific student has drawn and provide further feedback to that student if necessary. If a number of students have a common error, the instructor can show an anonymous version of the structure and initiate class discussion on how it might be improved. A video of this mode is at (http://www.youtube.com/watch?v=Pbq0Dsderek) (n. b. this video shows a slightly older version of *OrganicPad*.) Quizzes or assignments can be given out of class, and graded automatically with feedback. *OrganicPad* recognizes full Lewis structures (showing all bonds and lone pairs), and line structures, depending on the circumstances. Students can draw other forms such as condensed structures (CH3CH3) with the pen, and the system will record their drawing.

OrganicPad as a research tool

We believe that one of the most important features of *OrganicPad* is the ability to record student actions, store, analyze and replay them. While there are a number of qualitative studies (7, 8) on how students construct and use representations, it may well be that the study itself could perturb what students do. Interviewing or observation of students is quite time consuming and the subsequent analyses can be difficult and complex. There is a growing understanding that studies done under controlled circumstances may not always be applicable to "real life" (9); we are interested in what students do "in the wild, and on the fly," that is, under circumstances that are as close to normal as possible. Our approach is to, combine studies using large amounts of student data (quantitative studies) with interviews (qualitative studies) to investigate how students develop representational competence. We have collected tens of thousands of exemplars of how students construct Lewis structures for many common structures. We can cluster them using Markov Modeling (10) to elicit common pathways and points where students make errors. The Markov models are based on the probability that students will move forward from one state to the next using a particular pathway. Figure 4 shows a Markov model for ammonia.

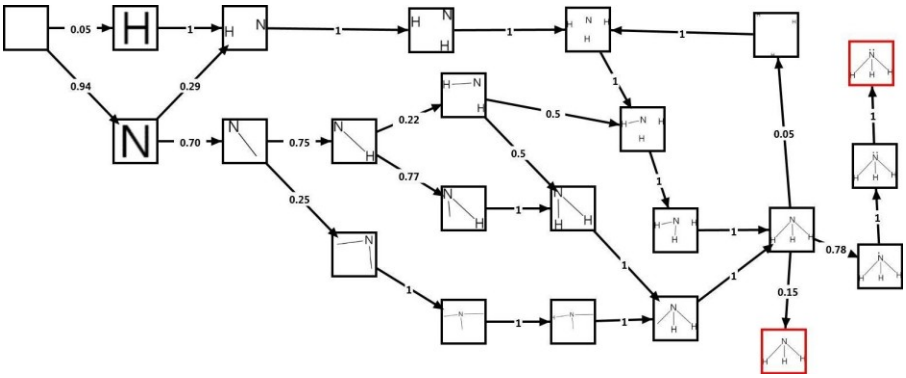

Figure 4. A Markov Model for Ammonia.

In addition to providing us with an indepth knowledge of the likely pathways students may utilize in creating their structures, the Markov models obtained through the use of OrganicPad also provide us with actionable information which we have used to create the contextual feedback system described above.

We have also used *OrganicPad* extensively to investigate how students draw mechanisms for organic reactions. Most organic chemists teach mechanistically, and assume (hope) that students will, in passing, learn to use the tools necessary for them make sense of the huge amount of material. We are currently analyzing data and preparing manuscripts on that analysis - but preliminary indications are that most students in organic chemistry do not spontaneously use mechanisms to guide their approach to predicting products of reactions. Those that do appear to be better equipped to solve far transfer tasks provided to them.

Future Directions

As previously stated, we are currently developing a web based version of *OrganicPad* that will be incorporated into a suite of tools that are currently under development. Foremost among these tools is *SocraticGraphs*, a graphical analysis tool that can recognize and respond contextually to student freehand input. We also continue to use *OrganicPad* as a robust assessment tool for a number of projects that we have initiated to help students better develop representational competence. For example: our new general chemistry curriculum development project, *Chemistry, Life, the Universe and Everything (CLUE)*, (in collaboration with Mike Klymkowsky, see http://virtuallaboratory.colorado.edu/Chemistry/index.html) is designed using research-based principles. OrganicPad will be an integral part of SocraticGraphs and, with activities based on graphical analyses, will be integral to CLUE-based instruction. OrganicPad is currently a free computer program and can be downloaded at http://www.clemson.edu/organicpad.

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Footnotes

[1]Although the efficacy of this approach is debatable and not well documented. Alex Johnstone (11) has pointed out that while experts can translate seamlessly between the different levels and representations, beginners must first learn to operate along the edges of his famous triangle. It may be that presenting students with such a profligate set of representations may only serve to overload their working memory.

References

(1) Gabel, D. Journal of Chemical Education 1999, 76, 548-554.
(2) Johnstone, A. H. J. Comp. Assist. Learn. 1991, 7, 75-81.
(3) Cooper, M. M.; Grove, N.; Underwood, S. M.; Klymkowsky, M. W. J. Chem. Educ. 2010, 87, 869-874.
(4) Taber, K. S. Int. J. Sci. Educ. 1998, 20, 597-608.
(5) Taber, K. S.; Coll, R. K. In Bonding; Gilbert, J. K., de Jong, O., Justi, R., Treagust, D. F. and van Driel, J. H., Eds.; Chemical Education: Towards Research-Based Practice; Kluwer Academic Publishers: Boston, 2002; pp 69-94.
(6) Taber, K. S. Chem. Educ. Res. Pract. Eur. 2001, 2, 123-158.
(7) Bodner, G. M.; Domin D, S. University Chemistry Education 2000, 4, 24-30.
(8) Bhattacharyya, G.; Bodner, G. M. J. Chem. Educ. 2005, 82, 1402-1407.
(9) Daniel, D. B.; Poole, D. A. Perspectives on Psychological Science 2009, 4, 91-96.
(10) Meyn, S.; Tweeds, R. L. In Markov Chains and Stochastic Stability; Cambridge Mathematical Library; Cambridge University Press: NY, NY., 2009; , pp 622.
(11) Johnstone, A. H. J. Chem. Educ. 2010, 87, 22-29.

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PhET Interactive Simulations: New tools for teaching and learning chemistry

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The Chemistry Education Research community has long recognized the power of animations and visualizations in the teaching and learning of chemistry (e.g. Jones and Smith, 1993; Burke et al., 1998; Tasker, 2005; Jones et al., 2005; Williamson and Jose, 2009; Sanger, 2009; Bishop and Kelly, 2009). Simulations also have the potential to transform the way science is taught and learned, and are increasingly becoming a focus of research. Simulations can be highly interactive and dynamic, make the invisible visible, scaffold inquiry by what is displayed and what is controlled, provide multiple representations, and allow safe (both physically and psychologically) multiple trials and rapid inquiry cycles. Perhaps most important, they make learning fun and engaging. Simulations can be readily disseminated and incorporated into today's classrooms - they are easily distributed over the web, often for free, and can be designed to allow for flexible use that addresses a variety of learning goals.

There is little doubt that simulations will be an ever-growing part of both the educational and scientific enterprise. At this point, the critical question is whether and how educational uses will be highly productive. Measurable benefits will depend on both the *quality of simulation design and how they are used*.

In this article, we introduce the PhET Interactive Simulations project at the University of Colorado, and describe our growing efforts to create and research interactive simulations for the teaching and learning of chemistry.

Introduction to the PhET Project

Since 2002, the PhET Project has been working to develop interactive simulations (sims) and provide these powerful learning tools to students and teachers worldwide. While its origins are in physics, the project has been expanding its collection into chemistry with funding from two NSF grants (NSF CCLI #0817582 and NSF DRK12 #1020362). We have now developed over 90 interactive simulations for teaching and learning science, all of which are available for free from the PhET website (http://phet.colorado.edu). Chemistry simulations like Salts and Solubility, Gas Properties, Acid-Base Solutions, and Build An Atom create animated, interactive, game-like environments in which students learn through scientist-like exploration. The sims emphasize important connections between real-life phenomena and the underlying science. They make the invisible visible by, for instance, showing electrons, photons, or molecules, and they include the key visual models that experts use to aid their thinking. These design features foster productive engagement with the simulations, which helps students build their own understanding and skills.

With a highly intuitive interface and minimal text, PhET sims are designed to give teachers control over how they are used in the classroom, enabling teachers to customize their use of sims to match their environment and learning goals. This flexibility allows PhET sims to be used in

class, in lab or as homework, and with groups or individual students. While PhET sims can be used in a variety of ways, they are specifically designed to make scientist-like, inquiry-based activities productive and fun learning experiences for students.

PhET Sim Design

The PhET project firmly grounds its simulation design in research. We draw from the existing research literature on how students learn (e.g. Bransford et al., 1999; NRC, 2005), conceptual difficulties in physics and chemistry (e.g. Nakhleh, 1992; Mulford and Robinson, 2002), and educational technology design (e.g. Clark and Meyer, 2007). Simultaneously, we make extensive use of student interviews and classroom testing to investigate usability, interpretation, and learning issues to develop and refine our simulation design principles (Adams et al., 2008a, 2008b; Podolefsky et al., 2010).

Our design approach is driven by two overarching goals: 1) to facilitate the development of an expert organizational framework of one's knowledge about the science, and then, recognizing that the development of this framework requires significant mental effort, to 2) provide scaffolding and satisfying feedback in order to make that effort productive and rewarding for students. Many of our design features are illustrated in the Gas Properties and Acid-Base Solutions simulations shown in Figures 1 and 2. These include:

1. Making the simulations highly interactive, engaging, and open;
2. Emphasizing the connection between science and everyday life;
3. Emphasizing productive visual and conceptual models of experts and using physically-accurate, highly-dynamic visual representations of the physics and chemistry with real-time animated response;
4. Building connections between multiple, linked representations;
5. Productively constraining and scaffolding interaction through selection of controls, feedback, and sim structure, while using minimal explicit guidance in the sim (e.g. minimal text); and
6. Reducing cognitive load and making controls intuitive and easy-to use.

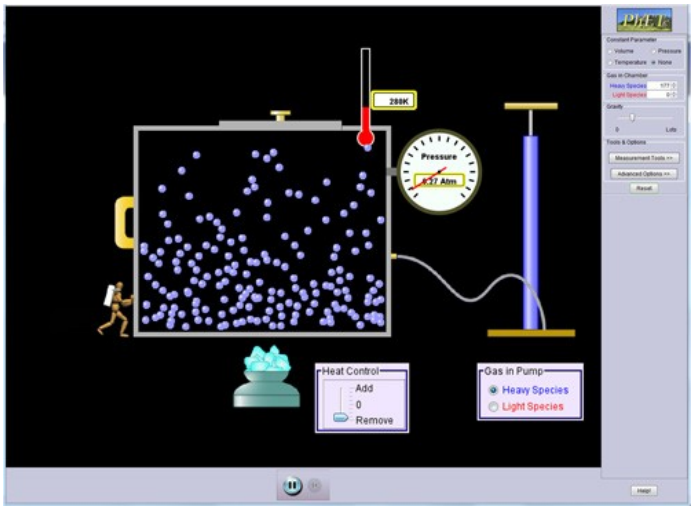

Figure 1: Gas Properties Sim

In our research with college science students, we find that well-designed interactive sims allow and attract students to *actively engage* with the content as scientists do - that is, productively explore a sim through a cycle of self-generated questions where the dynamic, visual feedback from the sim allows students to progressively build, monitor, and correct their understanding as they construct their own mental model of the phenomena. We call this mode of learning *Engaged Exploration*, and it embodies the *process and dynamic* nature of science as a discipline (Adams et al., 2008a; Podolefsky et al., 2010). Note that by engaged exploration, we do not mean pure discovery, which may not provide sufficient scaffolding to support productive student inquiry (Kirschner et al, 2007; Hmelo-Silver et al., 2008).

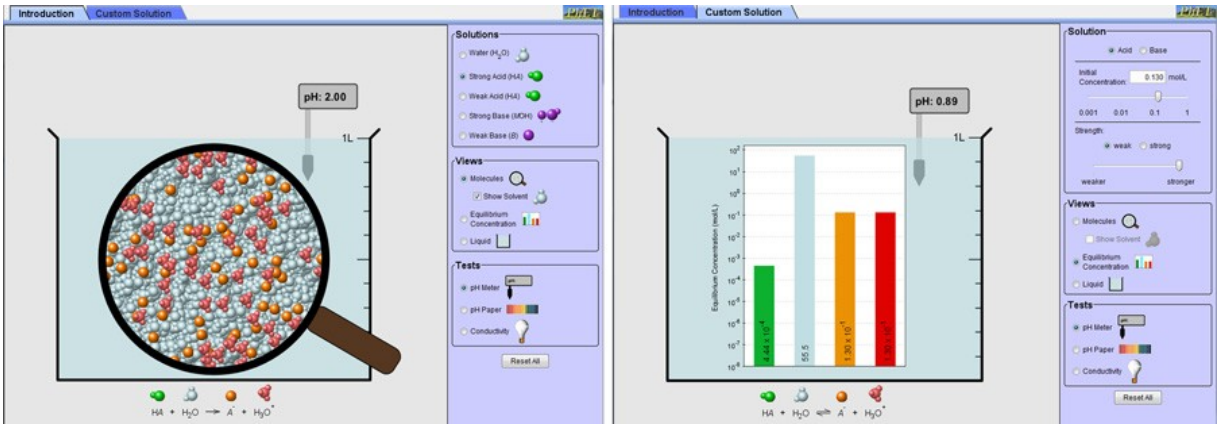

Figure 2: Acid-Base Solutions Sim

PhET sims foster productive exploration through significant *implicit scaffolding* in terms of what the user can and cannot do as well as what the user is and is not shown (Podolefsky et al., 2010). This scaffolding is built into sims through choice of controls, dynamic feedback, visual representations, etc., and can focus students' attention on the most important aspects of the science, illuminate causal relationships, cue interactions, and reduce cognitive load. Simultaneously, implicit scaffolding provides students the freedom to take multiple productive pathways in exploring the content as their understanding evolves.

While a sim can be honed into a highly effective learning tool, how that sim is used in the classroom is critical. Sims can enhance a well-designed curriculum and the efforts of a good teacher, but they cannot replace them. Issues of classroom context, student motivation and prior knowledge, teacher facilitation, and learning goals all play a role in designing effective simulation-based activities. Identifying and understanding effective approaches to embedding PhET simulations in educational practice is an active area of research for our group and our collaborators.

Examples from Chemistry

In the Gas Properties sim (Figure 1), students are invited to interact with a familiar bicycle pump. Immediately upon interaction, they are presented with an expert visual model: a molecular view of air particles as they enter the box, bounce off of walls, and collide with each other. Intuitive click-and-drag manipulation, sliders, and radio buttons are used to change temperature, change

box size, and activate quantitative analysis tools such as a ruler, pressure gauge, or thermometer. As the user manipulates these controls, responses are immediately animated thus effectively illustrating cause-effect relationships as well as linking multiple representations (motion of the objects, graphs, number readouts, etc.). This simulation can be used to support multiple learning goals ranging from visualizing the molecular view of gases, to making predictions using the ideal gas law, to more advanced goals like exploring diffusion rates or the origin of the Maxwell-Boltzmann distribution (by disabling and enabling collisions).

The Reactants, Products, and Leftovers sim (Figure 3) is designed to address the well-documented student difficulty in translating between the chemical equation and a molecular view of the reaction (Nurrenbern and Pickering, 1987; Mulford and Robinson, 2002). In this sim, folder-like "tabs" along the top are used as scaffolding, with complexity increasing as students move from tab-to-tab in their exploration. The first tab employs the analogy of making sandwiches to help ground student learning in a concrete and familiar context. In the chemical reactions tab, students select among several real-world reactions like making water or combusting methane. Adjustments to the number of each reactant immediately and dynamically change the molecular view representations of products and leftovers. Finally, a game tab - with 3 difficulty levels and options to hide either the molecular or numeric information - provides an opportunity for students to challenge, test, and refine their understanding. For this simulation, interviews established the game as the critical feature for engaging students in developing a robust understanding of limiting reactants.

In the Acid-Base Solutions sim (Figure 2), students can use real-world lab tools to explore how strong and weak acids and bases differ - they can dip pH paper or a probe into the solution to measure the pH, or insert electrodes to measure the conductivity. Students can also use tools not available in lab, such as a magnifying glass that shows the particles in solution. They can elect to show the solvent, which can help dispel the notion that water is continuous. In the second tab, students can use sliders to change both the concentration and the strength of an acid or base. In so doing, they immediately see the effects on the distribution of particles in solution, and thereby develop a conceptual model of acid and base strength.

We have identified 35 existing PhET simulations as relevant for teaching general chemistry or quantum chemistry. Several simulations address topics of electronic energy levels, photon absorption and emission, and photon energies, including Models of the Hydrogen Atom, Neon Lights and Other Discharge Lamps, Lasers, and Photoelectric Effect. The Nuclear Fission, Alpha Decay, Beta Decay, and Radioactive Dating Game sims address nuclear decay and its applications. In addition to being used to address concepts implied by their names, the Salts and Solubility sim and the Reactions and Rates sim can both be used to address the concept of equilibrium. Some other chemistry sims include pH Scale, States of Matter, Greenhouse Effect, and Density.

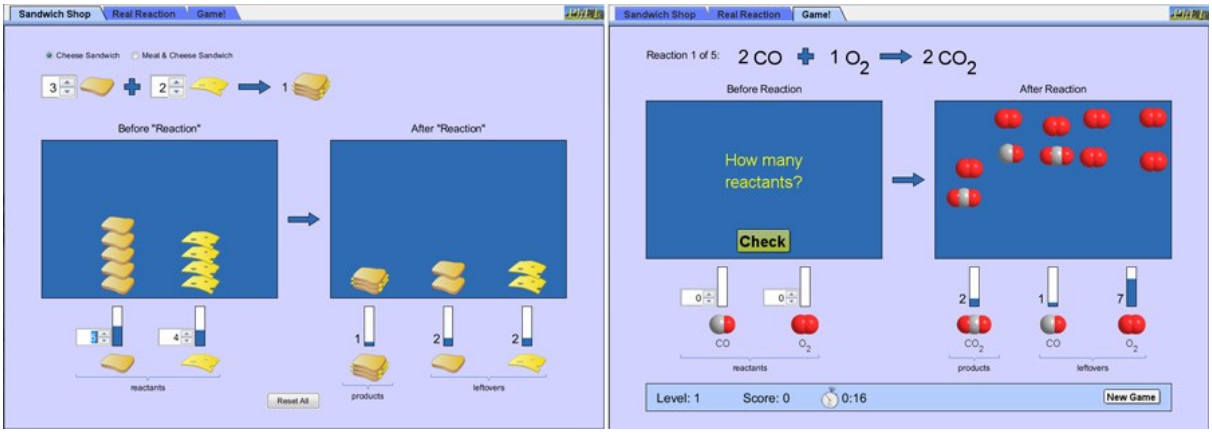

Figure 3: Reactants, Products, and Leftovers Sim

Teacher Resources

All PhET simulations are available for free from our website (http://phet.colorado.edu). They can be run online or downloaded for use without internet. On each sim page, we include a list of main topics, related topics, sample learning goals, and teaching tips. In addition, we provide teacher-contributed activities associated with that simulation from PhET's Ideas and Activities database, a collection of activities written by the PhET team and the community of teachers using PhET. The activities database can be searched by sim, type of activity, grade level, language, and keywords. Activities that align well with current education research findings are highlighted with a Gold Star to guide teachers. Teachers are encouraged to contribute ideas on how they have used PhET sims, or to contribute comments when they have tried an activity with their class.

Accessibility and Usage

One of our ultimate goals is to put valuable new educational technology in the hands of students and teachers at all levels everywhere in the world. This outcome is very difficult to measure, but we have data to indicate that we are making progress towards this outcome. The traffic to the website has increased dramatically over the last several years; Figure 4 shows the number of simulations run per year from 2004 to 2010. Over the past year, there were over 13 million simulations run from our website and over 30,000 full website downloads.

International use of PhET continues to climb. PhET's translation tool makes translating a sim easy for dual-language educators, and we now have sims translated into 51 languages. Not all sims are in every language, but over 2,000 foreign-language sims are hosted on our website. International use now accounts for about 30% of our online simulations use (see Figure 5). In October 2010, we added full translation support for the PhET website, and we now host Arabic and Korean translations of the website and anticipate more languages soon.

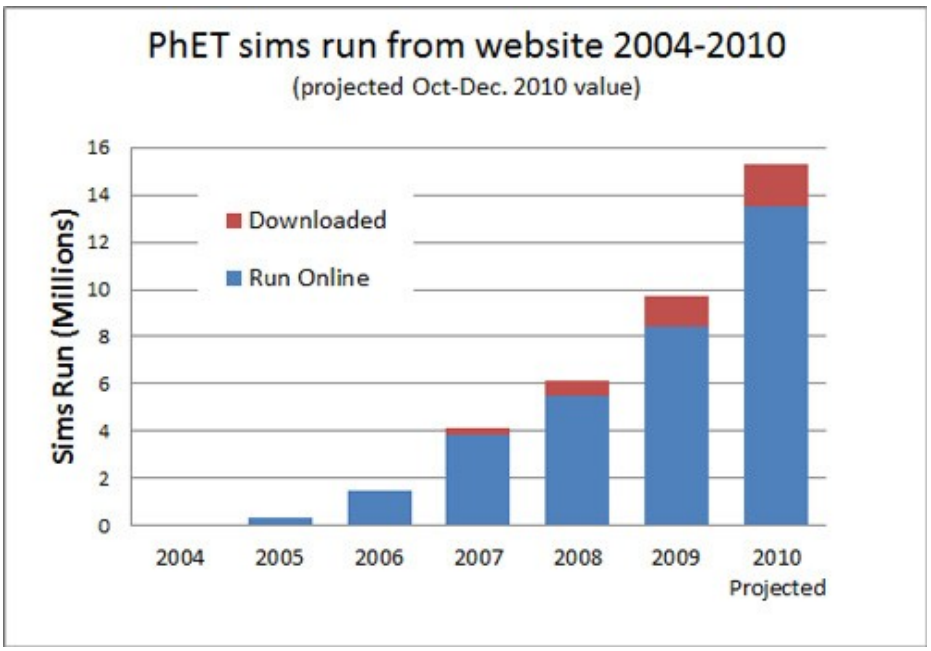

Figure 4: PhET Usage Statistics

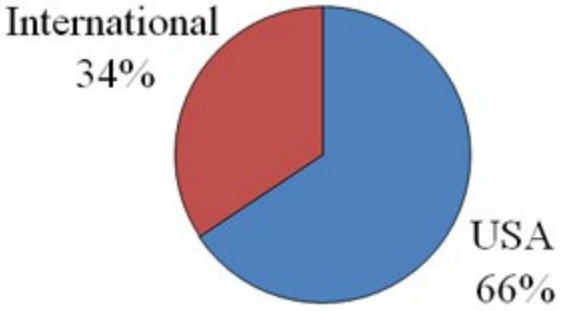

Figure 5: Domestic versus International Use

Conclusion

The PhET project aims to be a comprehensive resource for educators by providing free, research-based, interactive simulations along with tips for use and teacher-contributed activities. This resource is most productive in the hands of good teachers using curricula that are well matched to the needs of their students.

Acknowledgements

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References

Adams, W. K., Reid, S., LeMaster, R., McKagan, S. B., Perkins, K. K., Dubson, M., and Wieman, C. E. (2008a). A Study of Educational Simulations Part I - Engagement and Learning. Journal of Interactive Learning Research, 19(3), 397.

Adams, W. K., Reid, S., LeMaster, R., McKagan, S. B., Perkins, K. K., Dubson, M., and Wieman, C. E. (2008b). A Study of Educational Simulations Part II - Interface Design. Journal of Interactive Learning Research, 19(4), 551.

Bishop, M. and Kelly, R. (2009). Bound to fail: challenges faced in the design of molecular level visualizations (Paper 6) Committee on Computers in Chemical Education Newsletter (Web): December 7-9, 2009.

Bransford, J., Brown, A.L., Cocking, R.R. and National Research Council (1999). How People Learn: Brain, Mind, Experience, and School. (National Academy Press: Washington, D.C.).

Burke, K.A., Greenbowe, T.A., and Windschitl, M.A. (1998). Developing and Using Conceptual Computer Animations for Chemistry Instruction, *Journal of Chemical Education*, 75(12)

Clark, R.C. and Mayer, R.E. (2007). *e-Learning and the Science of Instruction: Proven Guidelines for Consumers and Designers of Multimedia Learning*. (Pfeiffer).

Jones, L.L. and Smith, S. G. (1993). Multimedia technology: A catalyst for change in chemical education, *Pure and Appl, Chem*, Vol. 65, No. 2, pp. 245-249.

Jones, L.L., Jordan, K.D., and Stillings, N.A. (2005). Molecular visualization in chemistry education: the role of multidisciplinary collaboration, *Chemistry Education Research and Practice*, 6 (3), 136-149

Kirschner, P.A., Sweller, J. and Clark, R.E (2006). Why minimal guidance during instruction does not work: An analysis of the failure of constructivist, discovery, problem-based, experiential, and inquiry-based teaching. *Educational Psychologist* **41**, 75-86.

Hmelo-Silver, C.E., Duncan, R.G., and Chinn, C.A. (2007). Scaffolding and Achievement in Problem-Based and Inquiry Learning: A response to Kirschner, Sweller, and Clark (2006). *Educational Psychologist* **42**, 99-107

Mulford, D.R. and Robinson, W. R. (2002). An Inventory for Alternate Conceptions among First-Semester General Chemistry Students, *J. Chem. Educ.* , 79, 739-744.

Nakhleh, M.B. (1992). Why Some Students Don't Learn Chemistry: Chemical Misconceptions, *J. Chem. Educ.* 69, 191-196.

National Research Council (2005). How Students Learn: History, Mathematics, and Science In the Classroom. (National Academies Press: Washington, D.C.).

Nurrenbern, S.C. and Pickering, M. (1987). Concept Learning versus Problem Solving: Is There a Difference *J. Chem. Educ.* 64, 508-510.

Podolefsky, N.S., Perkins, K.K., and Adams, W. K. (2010). "Factors Promoting Engaged Exploration with Computer Simulations", *Phys. Rev. ST Phys. Educ. Res.*, 6, 020117

Sanger, M.J. (2009). Computer Animations of Chemical Processes at the Molecular Level, *A Chemist's Guide to Effective Teaching Vol 2*, Pienta N., Cooper M., and Greenbowe T. eds., Chapter 14, pp. 198-211, Prentice Hall.

Tasker R. (2004). Using multimedia to visualize the molecular world: educational theory into practice. In *A Chemist's Guide to Effective Teaching*, Pienta N., Greenbowe T. and Cooper M., eds., Chapter 16, pp. 256-272, Prentice Hall.

Williamson, V. and Jose, T.J. (2009). Using Visualization Techniques in Chemistry Teaching, *A Chemist's Guide to Effective Teaching Vol 2*, Pienta N., Cooper M., and Greenbowe T. eds., Chapter 6, pp. 71-88, Prentice Hall.

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BestChoice: Learning how to teach interactively over the web

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The BestChoice web site (bestchoice.net.nz) was born in 2002 out of a desire to offer additional learning support to students in large first-year university courses. The aim was to create web-based activities that modeled a one-on-one interchange with an experienced teacher. Thus it was intended that content be developed systematically, using both information and question pages, and that users receive instructive feedback in response to their answers.

The activities currently on the web site have 24 000 opportunities for users to interact with the system and receive feedback. A selection (75) of activities is available in a menu accessed by clicking on DEMO MODE at bestchoice.net.nz. The design of these activities, the tools used to create them and the system that delivers them has been driven by the pedagogical requirements of teaching model, direct feedback from our users, and analysis of their usage data. The purpose of this communication is both to introduce you to the nature of the *BestChoice* activities and to share with you insights that have been gained as a consequence of our analyses of their usage by various cohorts of students.

THE IMPORTANCE OF HAVING A VERSATILE SET OF AUTHORING TOOLS

Our previous experience with developing computer-based learning activities led us to envisage a text-based system where images were used only when the pedagogy demands. We chose to develop our own authoring tools so that these could be modified as required by the teaching model. In order to achieve the goal that we had set ourselves, the author needed the capability to

- place answers and feedback in the flow of text anywhere on the page

  (so that multi-step problems can be developed on a single screen page)

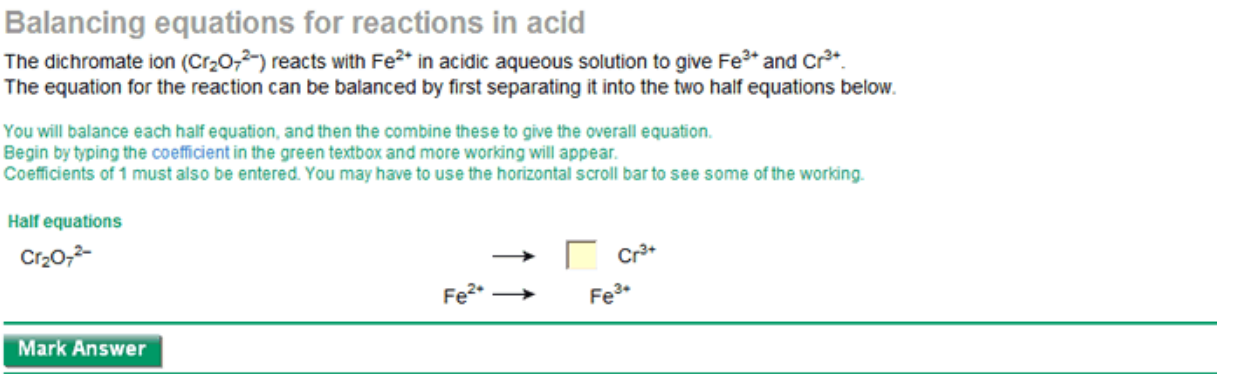
- mix-and-match answer input styles on the page and use any number of these

  (so that the answer style could be chosen to suit the objective of the question)

- hide page sections on loading and have their appearance triggered by a correct response

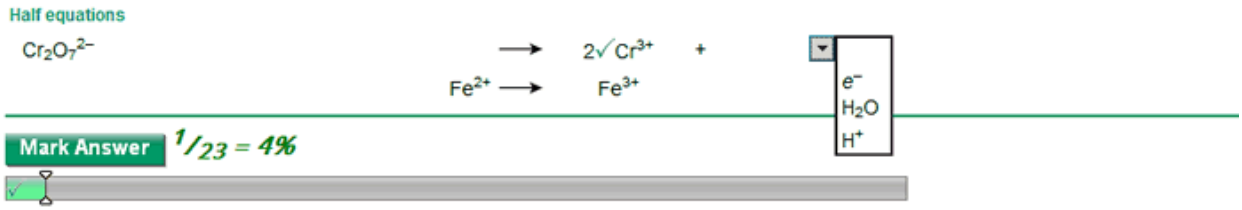
  (so that in development of multi-step problems, the user is not overwhelmed by complexity at the outset)

The necessity for all of this (and more) is illustrated by a *BestChoice* question page for a drill-and-practice exercise where the user constructs and balances the half equations and the overall equation for the reaction between iron(II) ions and dichromate ions. The page loads as shown below.



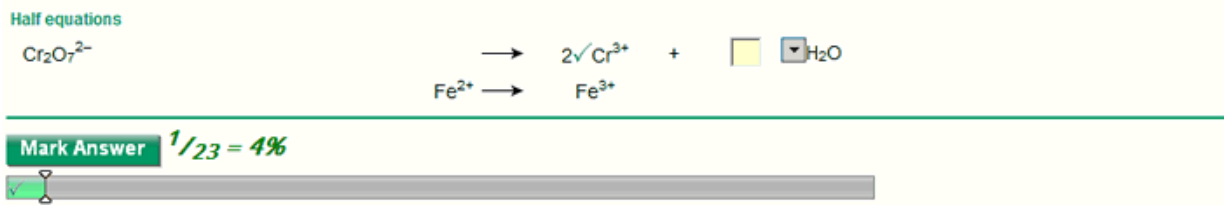
The objective was to create an on-screen version of the pen-and-paper approach (balance atoms other than O and H, balance O, balance H.....). This requires 23 answers. 10 are formulae for the species involved, 13 are numbers.

Students learning to balance redox equations on pen-and-paper would have all chemical formulae available so that they can focus on the balancing. Thus the formulae are on dropdown lists in the corresponding web-based exercise.

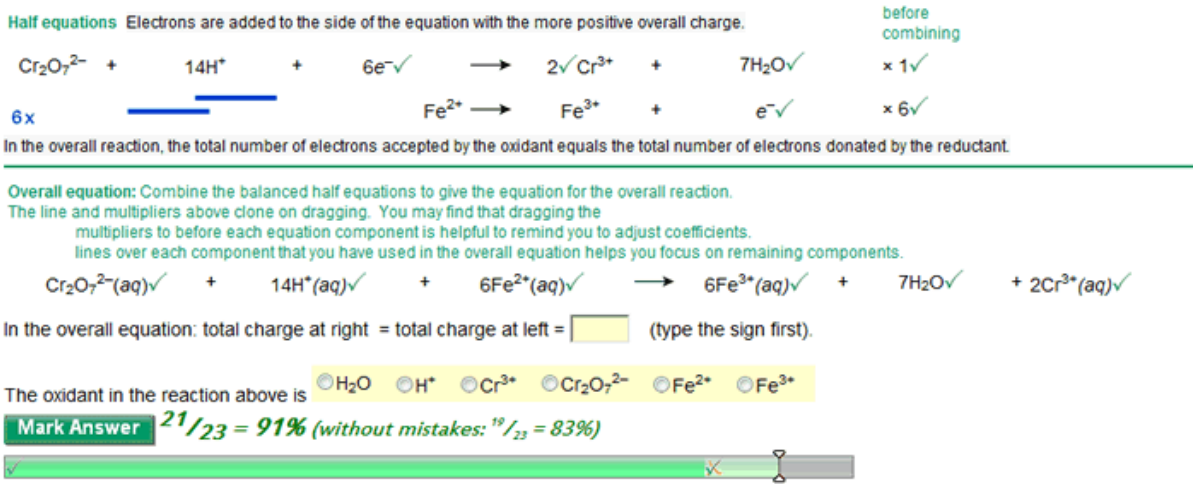


To simulate the balancing sequence, the completion of each part (for example, the balancing of chromium) triggers appearance of the next part (for example, the list from which water would be chosen).

On paper, once the correct formula for a species is written, the stoichiometric coefficient is entered. The screen shot shows that in the web-based balancing, choosing a formula from the dropdown triggers appearance of a text box into which a number can be entered.



Once the half-equations are complete, they are added to give the overall equation. In the overall equation, the order in which the reactants (and products) are chosen from the dropdowns should not matter. In the web-based balancing, this requires that each coefficient-answer is coupled to its formula-answer.



Finally for the completed page to have a text-box appearance, all buttons used to access the dropdown lists, all text-surround boxes and all coefficients of 1 must have disappeared on display of the correct response.

While the page above simulates fairly well the balancing of a redox equation with pen and paper, a significant difference between this exercise and the pen-and-paper one is that in the web-based exercise, incorrect answers are exposed immediately and can be corrected. Thus the user has an opportunity both to learn from his/her mistakes and to proceed to complete a correct balanced equation.

While every page authored informs the authoring of future pages, our priority has been to let the content drive the style of question page created. Some page styles (like the redox equation one) are re-used. However, each system has its unique features and pedagogical possibilities, and the point of *BestChoice* is to go beyond drill and practice to expose the thinking behind the problem, placing a greater emphasis on the problem-solving process than on the overall answer.

THE IMPORTANCE OF COLLECTING DATA AND ANALYSING THAT DATA

The users of *BestChoice* are in equal parts New Zealand high school students, UK high school students and New Zealand first-year university students. 80 000 users have entered 30 000 000 correct answers on *BestChoice* pages. We have learned that students can be a great help in designing systems to teach them. With the best will in the world, we cannot put ourselves in their shoes. We can, based on our experience as teachers, create activities that *we think* that students will like and deliver these in what *we consider* to be a learner-friendly way, but students should be the judge and jury. They are the customers.

With a view to encouraging users to give us feedback, a survey was placed on the last page of every *Bestchoice* activity. Users may enter a Likert scale rating (1 to 6) and/or a text-comment. This is one of the best things that we ever did. 24 000 comments relevant to teaching and learning have been entered along with 122 000 Likert scale ratings. Overall, 79% of the comments are compliments or suggestions, 21% are criticisms. 30% of the Likert scale module ratings are the maximum rating, and 79% of responses are positives.

Completion of the survey is voluntary, so it is important also to collect usage data for all users. A

companion application (*BestChoice Reports*) was developed to view these data. This application is both used by the developers and also made available to teachers of students who are *BestChoice* users.

User comment has informed the approach taken when constructing the activities.
The first activities developed used an enquiry approach. The user was given minimal information on screen pages preceding the question pages, and content was developed through the questions and feedback. Comments from users indicated that they liked the integration of information pages, questions and feedback.

13 Mar 06 I really like this because you have a review and the questions are right after it and everyone knows you need to do alot of questions to know the material. Keep it up!

31 Mar 05 This is really an awesome site, it has helped so much especially with the step by step instructions and the helpful explanations after you get a question right. The exclamation mark when you ask for help is good too cos its like ah hello, its this obvious. I love this site.I can see it is going to help me immensly this year

However, users did not like being asked about something had not featured in earlier information pages.

13 Mar 06 i really liked how there were notes to read throughout the quizes. Maybe for future quizzes notes could be added before the question is asked to give hints as to what the answer will be

This feedback led us to alter our module format to supporting users with information pages prior to the relevant question pages. This type of activity has a better completion percentage and receives more favourable student comment. Students like to be able to flick back to information pages in *BestChoice* without losing their previously-entered answers.

In a similar vein, carefully-worded instructions are important so that users know what to expect when they embark on entering/choosing answers on a question page. Even with experience, the author does not always anticipate the detail of instruction needed as per the comment below that pertains to a recently-authored page. The student was emailed, and it transpired that he had a perfectly valid point, and a further instruction was added.

3 Oct 10 instructions on what is required to be done is highly unclear. This causes some answers to be marked wrong despite the answers technically being correct, only because the answers have been entered incorrectly. I repeat, the INSTRUCTIONS on what the question requires, particularly on HOW the question needs to be answered, are usually unclear and/or incomplete. Highly frustrating...

User comment has had considerable impact on our marking practices
Scores are important to students, even though completion of *BestChoice* activities commonly does not contribute to course assessment. Our first scheme was one mark for each *BestChoice* answer irrespective of whether it was entered correctly on the first attempt or on a subsequent one. Each answer was marked instantly and feedback was displayed adjacent to the answer. The

feedback feature was (and is) very popular. The instant marking was much less popular for reasons pointed out in the two comments below. As a consequence, instant marking is no longer our default marking style.

9 Oct 10 for the last question i think it would be best if the answer didnt auto correct as with the previous ones. Sometimes you dont understand the reaction scheme until youve played with combinations for a while.

9 Oct 10 i prefer it when i can manually press 'mark answer' so i can correct myself when i accidentally click the wrong answer

Additionally, users told us that they did not think that it was fair that they got the same mark for a first-right answer as they did for a changed-right-answer. Thus, in 2007 we put in place the system that currently operates. The overall score is still for completion, but this is now the sum of first-right-answers and changed-right-answers, with the marking bar displaying both of these.

This development, driven by student feedback, has been a huge bonus for our evaluation program because the percentage of first-right answers, in conjunction with the number of Give-Ups, gives us evidence for (a) whether a question is achieving its objective for most users and (b) whether the feedback for a wrong answer is sufficiently instructive to enable most students to recover from their initial mistake.

Survey and usage data guide us in providing scaffolding appropriate for a particular topic. Our intention was to create activities to help students bridge the gap between being presented with information (listening to a lecture or reading a book) and flying solo where they solve multi-step problems or apply concepts without support. Thus *BestChoice* activities ask students lots of little questions that would not normally feature in written exercises. The aim is to probe whether the student understands the background to the system in the problem. This approach means that there are lots of opportunities to give users feedback at a point when they are receptive due to just having engaged with the content. The usage data that accrues give us clues where understanding breaks down.

It is important that the questions asked include content that authors perceive to be the obvious because what is obvious to us is not necessarily obvious to learners. These questions also build student confidence, showing them that they do have some of the prior knowledge required to be successful. However, surprises abound when one takes this approach and then examines the data.

It is pleasing, for example to know that users do not find balancing equations difficult, provided they are given the reactants and products. On the other hand, it was disturbing to find that 30-40% of students do not know that $2Cl(g)$ is a higher energy system than $Cl_2(g)$. Likewise, who would have believed that students who had happily identified tetrahedral, trigonal planar and bent shapes from static pictures of mononuclear species would not cope nearly so well with identifying the same shapes at particular atoms in a multi-nuclear Jmol of an amino acid?

It is important to go beyond simply looking at the data, to using it to inform modifications that may make the question more accessible. This could involve building in repetition where

knowledge of concepts is probed from various perspectives. For example, users can be asked to identify the nucleophile and identify the electrophile many times before they start to get the idea.

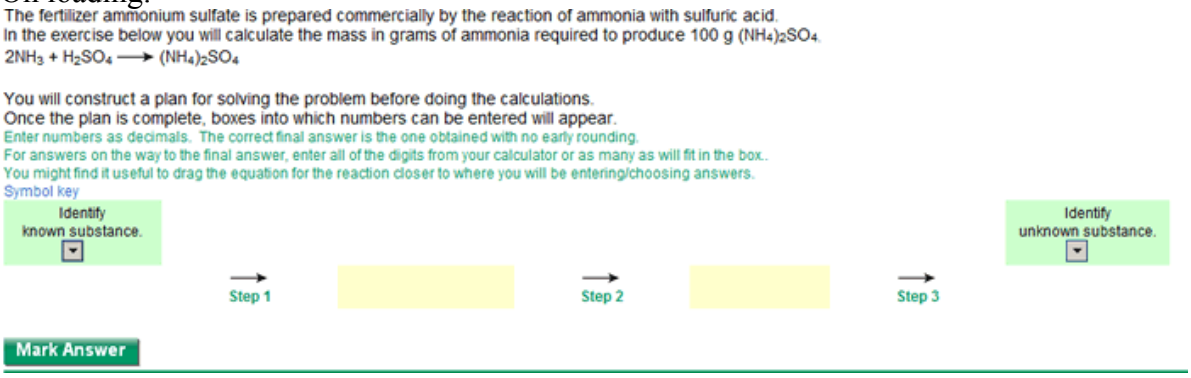
Despite our general emphasis on supporting students, there are areas where, based on usage data, we have removed scaffolding. Stoichiometry is one of these areas. In our early stoichiometry question pages, users worked through problems in a linear way, choosing/constructing the relationships required, entering the given data into the relationships on-screen and then calculating and entering the answers.

Our first attempt to go beyond what was a somewhat over-scaffolded approach was to introduce problem-planning pages before the number-work pages. This was consistent with our philosophy of fostering development of transferrable skills. Users were asked to identify the unknown and known as well as the quantities that needed to be calculated and the relationships required to calculate these. Usage data revealed that students found the planning pages much harder than the numbers pages.

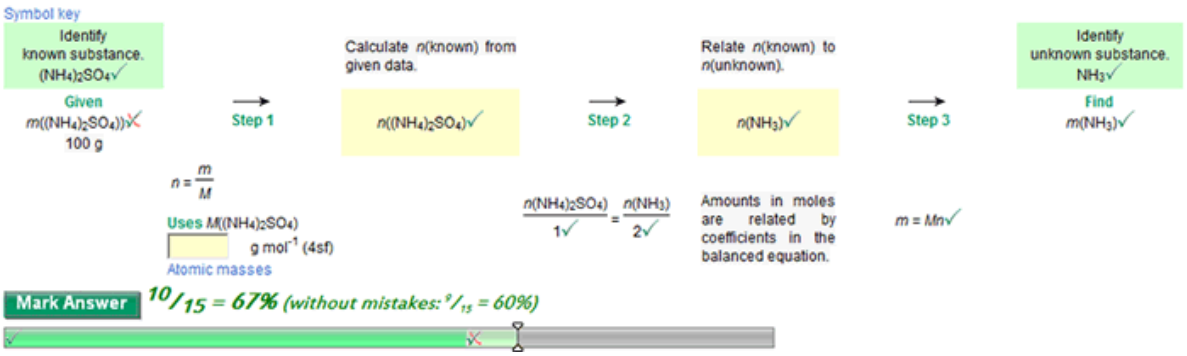
The introduction of planning pages had obviously significantly increased the number of answers that needed to be entered to solve the problem, so the next step was to reduce the scaffolding on the number-entry section, making the assumption that if students had in front of them a simple mathematical relationship (x = yz or x = y/z), and values for y and z, they could calculate the answer. This achieved a reduction in the number of answers to be entered and enabled integration of number-entry and planning sections onto the same page.

We have also moved away from revealing answer fields one at a time (as in the redox equation page), to revealing answers in blocks: first the known and unknown, second all of the intermediate quantities, third all of the relationships, fourth all of the calculation fields. This gives users the possibility of working forward from the known or backward from the unknown. The screen shots show, for one page, various stages in the answering process.

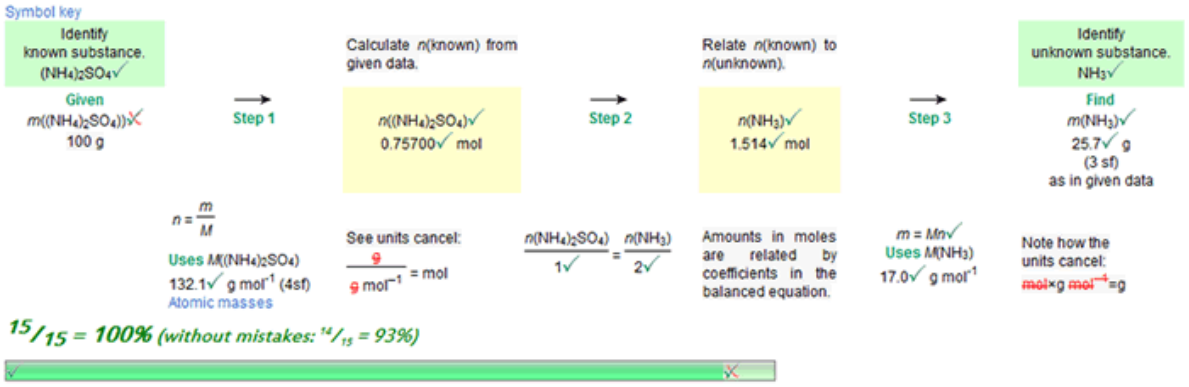
On loading:



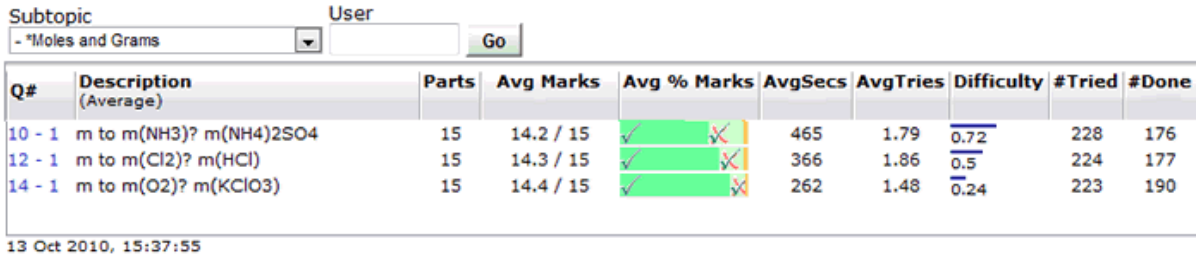
Planning complete:



Calculation complete:
Note the annotations that are displayed on screen as feedback for correct answers.



We have data from a variety of cohorts for a three-problem sequence, the one above and two others based on reactions with different stoichiometries. The screen shot shows, for a class of first year university students working through the sequence, that % first-right answers and % completion improve, and time taken diminishes.



Q#	Description (Average)	Parts	Avg Marks	Avg % Marks	AvgSecs	AvgTries	Difficulty	#Tried	#Done
10 - 1	m to m(NH3)? m(NH4)2SO4	15	14.2 / 15	✓ ✗	465	1.79	0.72	228	176
12 - 1	m to m(Cl2)? m(HCl)	15	14.3 / 15	✓ ✗	366	1.86	0.5	224	177
14 - 1	m to m(O2)? m(KClO3)	15	14.4 / 15	✓ ✗	262	1.48	0.24	223	190

13 Oct 2010, 15:37:55

While the data above are encouraging, the general area of stoichiometry continues to challenge us as both % completions and survey feedback on this type of activity are somewhat below *BestChoice* norms. We continue to experiment with different approaches.

In conclusion
The possibilities that the web offers for experiments in instructional design, like *BestChoice,* are beyond what can be imagined. There is so much potential to complement, extend and inform

conventional modes of instruction. Our voyage of discovery in the area of interactive learning has given us a different perspective on teaching and learning, and enabled us to connect with our students in ways that we would not have previously thought possible. The result is a reciprocal learning situation where in reward for our efforts to support their learning, students support us by providing good suggestions and encouraging comments, such as those below.
12 Oct 10 Extremely helpful in discovering my weaknesses in this topic and also at helping me overcome them.
6 Oct 10 That was really good! I had no idea on this topic, and by slowly going through it, I was learning then practising and now I mastered it! Thanks!

We would encourage to have a look at *BestChoice* (bestchoice.net.nz). In addition to the 75 learning activities mentioned above, there are two presentation modules in the DEMO mode menu, under the heading BCCE. These show in more detail how we use our data. The blue text on the pages are links to more information or data (sometimes at the bottom of pages). If you choose to SIGN UP in order to have a more valid user experience, Choose Other as your Institution and check out the General courses.

Lastly, if you are involved in any web-based education initiatives, do set up automatic data collection. It is like opening your eyes after years of working blind.

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"DIY molecules": a web application to build your own 3D chemical structures

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Introduction

Perceiving molecules as three-dimensional entities is an essential ability to be acquired by students in chemistry and biochemistry. Nowadays plenty of tools are available that allow students to visualize 3D models of chemical structures and even to interact with them on the computer screen using mouse, keyboard and user interface controls like buttons or pull-down menus.

Useful as they are, most of these tools depend on the availability of computer files that contain the atomic coordinates, and optionally other properties, for each molecule under study. These files may or not be readily available, or easy to locate, for an instructor or a student. Hence it is interesting to have a tool that allows anyone to build a model on demand for any envisioned structure. Furthermore, the processes of building one's own structure and conceptually connecting it with the resulting 3D geometry or making small changes and seeing the results adds good educational value to the experience. This method is also amenable to being used for student assignments or tests.

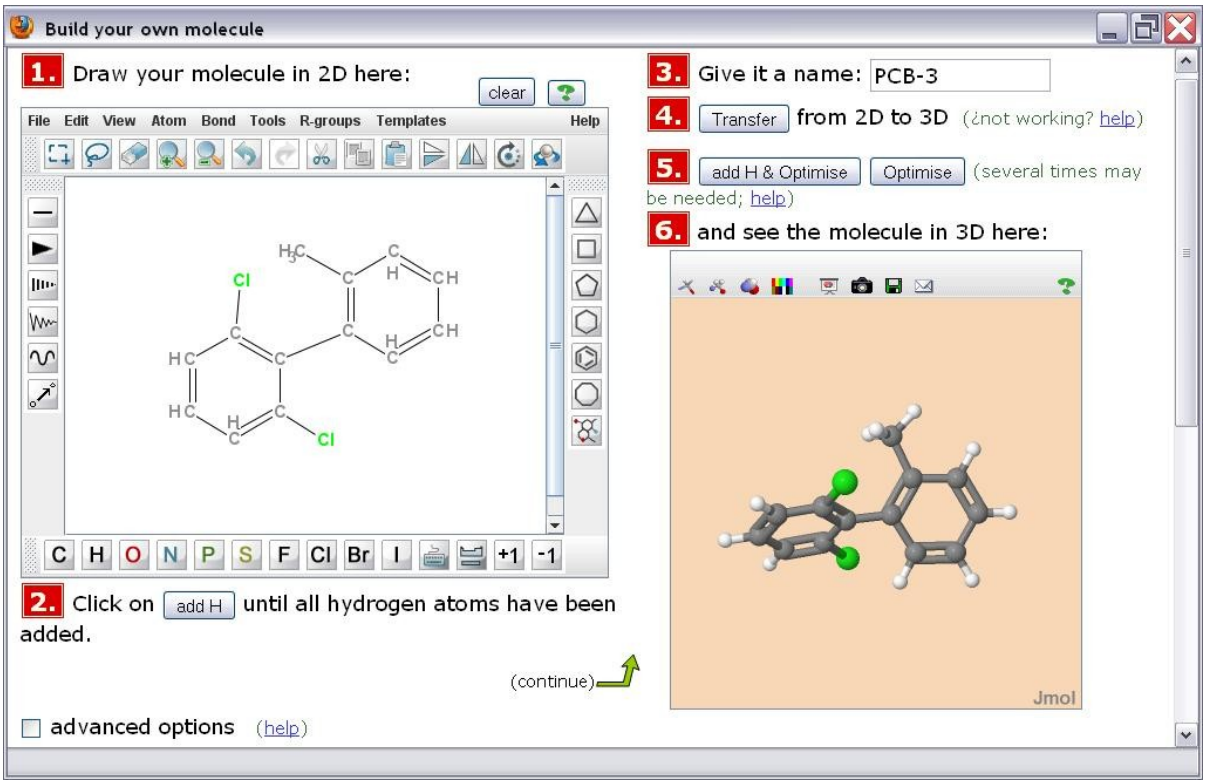
Existing procedures to build models of molecular structures typically require separate software to draw structures and display results, saving of intermediate files, local installation of appropriate software, and learning how to use it. Therefore, although valuable, they hold a limitation for general and widespread use.

With all this in mind, an application has been devised that will allow anyone to draw molecules and build their 3D model easily in a single workspace. We have called it "Do-It-Yourself Molecules".[1] This application runs within a web browser without the need for installing special software, does not use a web server and so can be used locally (even from a read-only device like a CD-ROM) as well as through the internet, under most operating systems. It follows a step-by-step approach and brief instructions are provided within the same page, so the learning curve should be smooth and quick.

User interface and design

All operations are done in a single window and page within the web browser. The interface integrates numbered steps, a panel for sketching the chemical structure in 2D, a few buttons to drive the generation of an energy-optimized 3D conformation, and a panel where such 3D structure is displayed and available for examination and interaction.

For cases when the structure generated is not what was intended, like a wrong stereochemistry, some tools are implemented to allow a fix or to force guidance in generation of the model. Such "advanced options" will not be needed in most cases and are initially hidden to avoid user confusion or distraction.



Software implementation

Building the application in a webpage provides the advantages of an environment familiar to most users and widespread access without installation, under any operating system that supports Java; it may also be used both online and offline. All software elements involved are available for free and open source. The DIY application itself is offered under a Creative Commons Attribution – Noncommercial – ShareAlike License.

The more polished variant —and currently recommended— of the DIY application uses a JChemPaint applet[2] for drawing the structure. This has the advantages of being more powerful, more chemically comprehensive, and localized to several languages. Among other features, it includes an ample set of pre-made structures in the form of "templates", that can be used as such or as a basis for the drawing.

We are also experimenting with alternatives for drawing the 2D structure, like JME, JSDraw, jsMolEdit, SketchEl, Doodler and Kemia.[3] Although they are in general less powerful and many are still not fully developed, some offer the advantage of a smaller file size, which accelerates access to the application over slow internet connections. These alternatives may also be tested in the DIY website.

Rendering of the three-dimensional model relies on the Jmol applet.[4] This is a powerful piece of software that, apart from display, offers user interactivity, generation of an image, and output of atom coordinates to save or send the resulting model. It is also localized into many languages. The DIY application is currently using the unsigned version of the applet to avoid Java security warnings that may deter users; this imposes the need for some convoluted mechanisms to save results to disk. A more straightforward access policy for file input/output, if so desired, may be achieved by switching to use of the signed Jmol applet.

Most importantly, Jmol is responsible for the computation of the optimized 3D geometry from the 2D sketch. For this, it uses the Universal Force Field (UFF[5]). Additionally, Jmol can optionally add implicit hydrogen atoms not present in the drawing. Having a full set of hydrogens is essential for a correct 3D optimization. The 2D editor JChemPaint still suffers from a bug that, in some cases, fails to properly add all implicit hydrogens and so this step cannot be automatically implemented in the 2D editor side. Currently, the two options are maintained as user-driven methods: either add the hydrogens in the 2D drawing or add them in the 3D model just before geometry computation.

Connection between the different modules —2D editor, 3D rendering, exported molecular data or image, submission…— is achieved using JavaScript code included in the page source. Particularly, the exchange of molecular data between 2D and 3D panels uses MOLfile[6] output and input, handled by JavaScript.

The application also includes a PHP script that will send the resulting 3D model (as text in MOLfile format) to the instructor's email address. For this to work, the DYI application files must reside in a web server that supports the PHP language and sending email with it; this is a requisite fulfilled by commonly used server installations. As an alternative, the student could save the model to local disk and then attach the file to an email message written manually in his/her usual email client.

Practical uses

The interface is simple enough that any occasional user may quickly get acquainted with it and start producing 3D models. It can so be used as support for the instructor during lectures, or be given to students for their own practice or, ideally, for working on assigned exercises. With this is mind, a mechanism has been implemented to allow sending the resulting 3D model to the instructor by email.

The process of drawing the flat structural formula and seeing it immediately converted into a model in 3 dimensions may by itself have enough formative value for students. Furthermore, the system offers easy chances to play and test variations of the structure initially planned. Apart from this, the optimization of the flat structure towards a 3D conformation is displayed in real time, adding great pedagogical value, as the user sees the bonds stretching and wiggling until the model reaches a proper stereochemistry. Along the same line, one of the advanced options allows to pull atoms with the mouse and see immediately how they struggle to fit back into proper positions compatible with the stereochemistry —but not necessarily the same they had initially—.

In addition to the basic functionality, some utilities are included. The displayed 3D model can be duplicated in an enlarged window (that can be resized up to full screen), useful e.g. for detailed inspection of the structure or for projection in a classroom. Also, a still image or snapshot of the 3D model can be captured and then it may be copied or saved to file.

Availability

The DIY application is freely available for use.[1] The interface is offered in either English or Spanish; translation into other languages could be easily arranged. Installation of a copy on a server, or even locally in a computer room, is straightforward (one just needs to copy several files, under 9 MB in total). All the software used is open source and cross-platform, and the application is offered under a Creative Commons license (Attribution – Noncommercial – ShareAlike 3.0).

References

1. Do-It-Yourself Molecules: from 2D to 3D. A. Herráez (2010) http://biomodel.uah.es/en/DIY/ [accessed 17 Oct. 2010]

2. JChemPaint: an open-source editor for 2D chemical structures, http://sourceforge.net/apps/mediawiki/cdk/index.php?title=JChemPaint

3. JME Molecular Editor, http://www.molinspiration.com/jme/
JSDraw, http://www.chemene.com:8080/ccd/jsdraw/
jsMolEdit, http://chemhack.com/jsmoleditor/component/content/frontpage
SketchEl, http://sketchel.sourceforge.net/
Doodler, http://web.chemdoodle.com/
Kemia, http://kemia.github.com/

4. Jmol: an open-source Java viewer for chemical structures in 3D, http://www.jmol.org/

5. UFF, a rule-based full periodic table force field for molecular mechanics and molecular dynamics simulations. A. K. Rappé, C. J. Casewit, K. S. Colwell, W. A. Goddard III, and W. M. Skiff (1992) J. Am. Chem. Soc. 114, 10024-10035. doi:10.1021/ja00051a040
See also:
http://web.archive.org/web/20060110100545/http://franklin.chm.colostate.edu/mmac/uff.html [accessed 17 Oct. 2010]
http://towhee.sourceforge.net/forcefields/uff.html [accessed 17 Oct. 2010]

6. The MOLfile, originally from MDL, is a widespread file format for 2D and 3D molecular structures compatible with many software programs.
http://www.symyx.com/solutions/white_papers/ctfile_formats.jsp