Newsletter: Using Computers in Chemical Education Fall 2001

ACS Division of Chemical Education :--Committee on Computers in Chemical Education

Chair : Don Rosenthal Who we are and what we do.

Welcome! The Newsletter is FREE! To be notified when new issues are available, please subscribe.

To view much of the material presented in the Newsletter you need the free players, QuickTime, Macromedia Shockwave Player (includes Macromedia Flash Player), or for all Macromedia downloads.

Our leadoff article by Michael J. Sanger shows us some of the animaions he has created and shares with us the problems and successes using them with students.

'I will review the research on the use of computer animations in chemistry instruction and summarize what we have learned so far. Before I do that, however, I will explain why computer animations were incorporated into the chemistry classroom and why they were expected to be an useful instructional tool. '

ComputerAnimations in Chemistry: What We Have Learned

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Using Color - Part II

Multimedia Tutorial #6

Harry E.Pence

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Harry continues his series on how to make our lecture presentations more interesting and effective. 'The use of color in chemistry lectures has become so common and convenient that it is easy to forget that about 12 million Americans, most of whom are male, suffer from some form of color blindness. Red or green color blindness is most common and since it involves the X chromosome, it is much more common in men than in women. '

First Impressions of Flash 5:

Review by Editor
Brian Pankuch
Chemistry Department
Union County College
Cranford, NJ 07016

Flash 5, available for a free demo from Macromedia, is the latest version for creating animated Web material. Having some experience with other Macromedia products, Dreamweaver, Director, etc., I was hoping to be able to use the program with a minimum of fuss. The interface is similar to the other Macromedia products and I enthusiastically jumped into creating an animation I had planned to do in Director.

More Adventures as a Web Adviser:

Brian Pankuch
Chemistry Department
Union County College
Cranford, NJ 07016

I was the web advisor for Tom Spiro's course on the Chemistry of the Environment during Spring 2001. Tom decided to use a lot of expertise available at Princeton, so many of the

lectures were given by top environmental researchers. Some on work that hasn't been published yet. Unfortunately I was teaching my own courses when most of the talks were given but the ones I was able to attend were very informative. In particular Mario Molina, Nobel Prize in chemistry 1995 for work on stratospheric ozone, painted a historical picture of what life was like in the early 1900's without refrigeration.

INTERIM UPDATE ON SEARCH ENGINES

Harry E.Pence

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Almost every one is aware that there has been a high shake-up in the dot.com world. Many technology and Internet companies have cut staff or even gone into bankruptcy. According to a story being passed around on the Internet, "If you bought $1,000 worth of Nortel stock one year ago, it would now be worth $49. If you bought $1,000 worth of Budweiser (the beer, not the stock) one year ago, drank all the beer, and traded in the cans for the nickel deposit, you would have $79. My advice to you is to start drinking heavily." For those of us who did not invest heavily in the tech bubble, it is important to know what effect these changes have had on the WWW search engines.

Animations in an Instrumental Methods Chemistry Class?

Thomas G. Chasteen

Department of Chemistry
Sam Houston State University

Tom has an amazing collection of animations he has created and considerable experience in using them with students. He also makes them available to us, just ask.....'So once we get over the fear of requiring our students to get as involved as possible with modern computers in their chemistry courses, using computers to help teach specific topics is a natural extension. In my senior-level instrumental analysis course I use animations inside and outside of the course to teach instrumental techniques or particularly important or conceptually difficult points.'

Multimedia Tutorial #6

Using Color - Part II

User-Friendly Presentations for those with Limited Color Vision

Part of The Alchemist's Lair Web Site
Maintained by Harry E. Pence, Professor of Chemistry, SUNY Oneonta, for the use of his students. Any opinions are totally coincidental and have no official endorsement, including the people who sign my pay checks. Comments and suggestions are welcome (pencehe@oneonta.edu).

Last Revised Sept 18, 2001

Using Color - Part II, User-friendly presentations for those with limited color vision, Harry E. Pence, SUNY Oneonta, Oneonta, NY, pencehe@oneonta.edu

(This article appeared in the Fall 2001 issue of the Computers in Chemical Education Newsletter.)

P**lease note! I apologize, but due to a server problem, this link is incorrect. It should read**

http://www.eclipse.net/~pankuch/Newsletter/Pages_NewsF01/NewsletterCCE_Fall_01.html

Our server won't recognize the ~ and replaces it with %7. You may either type in the above link, or amend the link given above.

The previous tutorial in this series was concerned with selecting the best colors for a PowerPoint presentation that would be given to a general audience. The use of color in chemistry lectures has become so common and convenient that it is easy to forget that about 12 million Americans, most of whom are male, suffer from some form of color blindness. Red or green color blindness is most common and since it involves the X chromosome, it is much more common in men than in women. Despite common belief, color blindness does occur in women, although this is relatively rare. Total color blindness is relatively rare in individuals of either sex. There are several sites that discuss the basics of color vision and how this relates to vision problems, including ERGOGERO, a company that does human factors design, the site on the Science and Mathematics of Color by Prof. Tom OHaver (U. of Maryland) and Webvision, a site from the University of Utah Medical School.

Some individuals have learned to cope with color limitations, and others have obtained special lenses that assist color vision, but many people who are color blind do not realize that they have a difficulty. Thus, it becomes the responsibility of the instructor using color to insure that it is done in such a way that no one is penalized, even those who do not have normal color vision. This is true both for lecture presentations as well as web materials.

One of the best ways to start is to try to understand the nature of the situation. If you wish to experience

something of what it would be like to be colorblind, the free Colorfield web site allows a viewer to examine a series of photographs as they would appear if viewed by someone who had Dichromat, one of the main types of color blindness. In this case a single type of color receptor, i.e. red, green or blue visual pigment, is missing. These three types are called Deutan, which is a loss of sensitivity to green light, Protan a loss of red sensitivity, and Tritan, which is a loss of blue sensitivity. Deutan is most common, and Tritan is by far the least common. In each case, moving the mouse across the names of the three types of color limitations converts the image on the right into an approximation of what might be seen with that type of color blindness. Even though the conversions may not be totally accurate, this is a case where the company deserves credit for offering everyone a real service. (Colorfield is trying to sell an inexpensive color adjustment plug-in called Insight that currently works for Photoshop, Fireworks, and several other Macintosh programs. This commercial intent does not detract from the usefulness of their web site.)

Mrs. Christine Rigden, whose spouse is color blind, has created a standard 216-color web-safe palette, which is available for free from her web site, Safe Web Colors for Color-deficient Viewers. Mrs. Rigden also provides color comparisons to show the effect of the main types of color blindness as well as a link to download a replacement palette. Like the Colorfield site, the intention is not to reproduce the experience of color blindness with absolute accuracy, but rather to help a designer understand what colors and color combinations should be avoided whenever possible.

On a more practical note, there are several simple suggestions that will help an instructional designer to make projected text materials more user-friendly to people with all types of vision. Perhaps the most fundamental advice is never to use color as the only visual cue for guiding a user; always provide an alternative cue that is totally color independent. For example, if red (or blue or green) text is being used to indicate emphasis, it should also be underlined to provide a visual cue that is not affected by color vision. Alternately, the emphasized text can be enclosed in a white box so that it will stand out better. It is important to use a text color that contrasts strongly with the background. For example, a medium green text on a pastel green background might be very difficult to see for someone who is less sensitive to green light. It is easy to put a black shadow on any text, and the shadow may help to clarify the text letters. Perhaps most important, be sure to consult with the audience and ask if they are having any problems reading the material.

As noted in earlier tutorials, one of the real advantages of presentation software is the ability to insert images in close proximity to the text. The ease of inserting images is not, however, totally without educational liabilities. All of us have had the experience of seeing an image for the first time and requiring some interval to become oriented and understand what the image shows. The instructor brings to any image a great deal of experience that the students lack, as well as a better understanding of what is important. (This is why the instructor chose the image!) This period when comprehension develops can be slow for all students but even more difficult for those who are color blind. As is demonstrated on the Colorfield site mentioned earlier, some students will not see images in the way that the instructor expects. For this reason, it is always a good rule to verbally describe what the students are seeing when showing an image, and with a complicated image, it is helpful to point out the main features of the illustration. Do not assume that any students will completely comprehend an image at the first viewing! A picture may be worth a thousand words, but usually at least a few words of explanation are helpful for all students.

Perhaps the most important aspect of attempts to improve educational access for students who have special problems is the knowledge that these changes may be beneficial even to those who do not appear to need any help. Too often, educational materials are provided in a way that seems to be easiest for the instructor but is not really ideal for any of the students. With a little forethought, an instructor will often find that easily accomplished changes in the way he or she teaches can make the instructional process much more accessible and enjoyable for all students. Probably nowhere is this more true than in the efforts expended to make text and images clearer and easier to understand.

Addenda

During the discussion of an earlier tutorial in this series, I received several suggestions that I carefully set aside for use in the current tutorial. As is often the case, my efforts to insure that these references wouldn't be lost caused me to file them away so well that I couldn't find them when I needed them. Fortunately,

they have recently returned to the light of day, and so I will provide them as addenda.

Fred Senese was kind enough to point out an excellent site on Print Legibility and Partial Sight sponsored by Lighthouse International. This discussion includes the basic recommendations for making all types of printed material more legible. Many of these suggestions, such as color contrast, font selection, and font size, have been discussed in these tutorials, but the site also includes useful ideas about paper finish, margins, etc. that expand the discussion. Lighthouse International also offers an excellent site on Effective Color Contrasts, which supplements much of the current discussion.

On a similar topic, Walt Volland suggested a site titled Color Matters -Vision, which includes some additional exercises that may be of interest. In a separate communication, Liz Dorland pointed out the contradiction that this site does not seem to follow its own recommendations. Walt also pointed out that people with dyslexia may have a different type of color problem, they find black text on white background to cause eye fatigue. He suggests a site entitled Dyslexia - reading through colored filters to better understand how a simple filter can make text more readable.

Finally, during the on-line discussion of this paper, Jim Diamond has pointed out that someone who is red-green color blind may find that the red light of a HeNe laser pointer is almost invisible.

Many thanks to Fred, Walt, Liz, and Jim for their input.

Return to Multimedia Tutorial contents page.

INTERIM UPDATE ON SEARCH ENGINES

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Last Revised Oct. 15, 2001

(This article appeared in the Fall 2001 issue of the Computers in Chemical Education Newsletter.)

Interim Update on Search Engines, Harry E. Pence, SUNY Oneonta, Oneonta, NY, pencehe@oneonta.edu

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INTRODUCTION

Almost every one is aware that there has been a high shake-up in the dot.com world. Many technology and Internet companies have cut staff or even gone into bankruptcy. According to a story being passed around on the Internet, "If you bought $1,000 worth of Nortel stock one year ago, it would now be worth $49. If you bought $1,000 worth of Budweiser (the beer, not the stock) one year ago, drank all the beer, and traded in the cans for the nickel deposit, you would have $79. My advice to you is to start drinking heavily." For those of us who did not invest heavily in the tech bubble, it is important to know what effect these changes have had on the WWW search engines. Even though my students will not do their annual review of search engines for chemistry until next semester, Brian Pankuch and I have agreed that an interim report on recent developments might be helpful.

Search Engine Changes

Surprising enough, despite all the doom and gloom about the tech industry, new search engines continue to come on line. The most interesting of the recent engines is Wisenut, which some writers are claiming will be competitive with Google. Wisenut made its debut in early September of 2001, with a relatively large index (about 850 million pages) and a search algorithm similar to that used by Google to produce more accurate searches. The Wisenut white paper is a PDF file that may be downloaded to obtain more information about this new engine. Perhaps one of the most interesting aspects of Wisenut is the claim that it is designed to handle up to 1 trillion URLs. Since the current estimates of the size of the searchable web are only about two to four billion pages, this suggests that Wisenut plans to stay competitive for some time.

As those who have read my previous reports may remember, I consider Danny Sullivan to be an excellent search engine analyst, so I place considerable weight on the evaluation of Wisenut by Sullivan, which suggests that this new engine will not really challenge Google because there is more money to be made by providing search services to large sites. Sullivan quotes one expert who recently estimated that the annual growth rate for search technology sector will be over 50% per year. Nevertheless, the large index size, interesting features, and plans for continued growth suggest that this is an engine to watch in the future.

Another promising new search engine that has recently started operation is Teoma, which also claims to compete with Google in terms of focused search algorithms. Teoma was created by computer scientists at Rutgers university and uses an algorithm that bundles search results in terms of natural Web communities to create more relevant results. Before Teoma was even out of beta test, however, it was purchased by Ask Jeeves, which is itself a well-known search engine. According to a press release, Ask Jeeves plans to continue to maintain a separate Teoma site and also introduce the Teoma technology into the existing Ask Jeeves engine. Both Wisenut and Teoma will be included in the annual update of search engines for chemistry that will appear in the *Newsletter* next spring.

[Author's comment: Although there was not time to do an extensive comparision of these two new engines, I did do a search on the phrase "ionic solvents" on Google, Wisenut, and Teoma. Wisenut found 38 documents(but claimed 47); Teoma found 24; and Google found 89 (and claimed about 116). It was the opinion of the author that the first ten Google Links seemed more generally useful than the first ten links returned by Teoma, which in turn seemed more useful than the first ten from Wisenut. Finally, it was clear (at least on the day that this test was run) that the Wisenut search was much slower than the other two.]

On the negative side, two of the oldest search engines in existence reported serious financial problems. The parent company of the Excite search engine has filed for bankruptcy, and is trying to sell the Excite.com portal. The engine is still in operating at this time, but it is questionable how long it will continue to be kept up-to-date. Meanwhile, Altavista, another well-known search engine has made another major staff cut (30%) and appointed a new chief executive officer. The Altavista engine continues to operate, but the reports from search engines analysts (see below) suggest that the index has stopped growing in size. It has also been reported that in April Altavista stopped updating the regional sites that it maintains with links for sites in specific countries, mainly in Europe but also countries like Australia, Canada, New Zealand, India, and Korea. And finally, About.com, which is notable for providing human guides who organize and search the web, is reported to be eliminating 300 of its 750 guides.

Changes in the Size of Search Engine Indexes.

The latest report from Danny Sullivan on Search Engine Sizes, dated Aug. 15, 2001, indicates that Google has by far the largest index, followed by FAST, Altavista, and Inktomi, in that order. The graph of search engine size over time indicates that Google is also growing much faster than the competition, including some, like Altavista, that are static. On Aug. 14, 2001, Greg Notess did a similar study on Changes in Search Engine Size that shows that Google, FAST, and Altavista are the three largest engine indexes (in that order)and since April, Google and FAST have increased in size; Altavista and Northern Light have remained about the same size: and MSN, which is powered by Inktomi, has actually decreased in size.

Recently, Greg Notess has compared the results of the major search engines using 25 small, single-word terms. He identified Google as the leading search engine, as might be expected from the size of its index, because it returned the greatest number of hits overall and also found the greatest number of hits on 19 of the 25 individual searches. Based on his results, he ranked Fast in second place and Wisenut, which was mentioned above as a potential competitor to Google, was third. Notess ranked Altavista at sixth but he noted that in two of the searches it did give the best results. Teoma, which is also mentioned earlier, can only display 200 results, and so in most cases it could not be compared with the other engines. See Total Hits from 25 Engines for more complete results.

Acknowledgments

As noted in the earlier reports in this series, the Search Engine Watch web site, maintained by Danny Sullivan, and the Search Engine Showdownweb site, maintained by Greg Notess are excellent resources for anyone who wishes to keep up with current developments in WWW search engines. These sites are a major source for the information in this report.

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Return to Web Tutorial Home Page at the Alchemist's Lair.

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Animations in an Instrumental Methods Chemistry Class?

[Thomas G. Chasteen]

Department of Chemistry

Sam Houston State University

[Chemistry-Based Animations]

Why?

So why would we interrupt our students' lives by requiring them to study a computer-based animation?

Beyond saddling them with the cost of their $90+ instrumental text book, these poor souls are next required to find a modern computer and run a browser, or a Flash Player, or install QuickTime. A color monitor is required and headphones (in a noisy...I mean quiet student lab) might even be required. What a hassle for students who are already struggling--usually in their senior year--with a looming graduation, the attendant resumes, probable relocation, existential angst, etc. Why indeed.

We all know the reason why these requirements are not so onerous for these young scientists: **Instrumental analysis is a computer course.** While some instrumental chemical signals might still be feed to an analog (paper-based) chart recorder, for instance from a flame ionization detector signal in a gas chromatograph, the chance of this playing an important part in any of our graduates' futures is insignificant. Obviously gone is the time spent teaching chromatographic integration via the cutting and weighing of paper-based peaks, along with teaching our budding chemists the proper way of handing those small, shiny gram weights necessary to operate chain-operated four-place balances. Gone; all gone. No, instrumental methods of analysis are computer-dedicated methods of collecting data and all that involves, almost exclusively using personal computers networked to one instrument and possibly many.

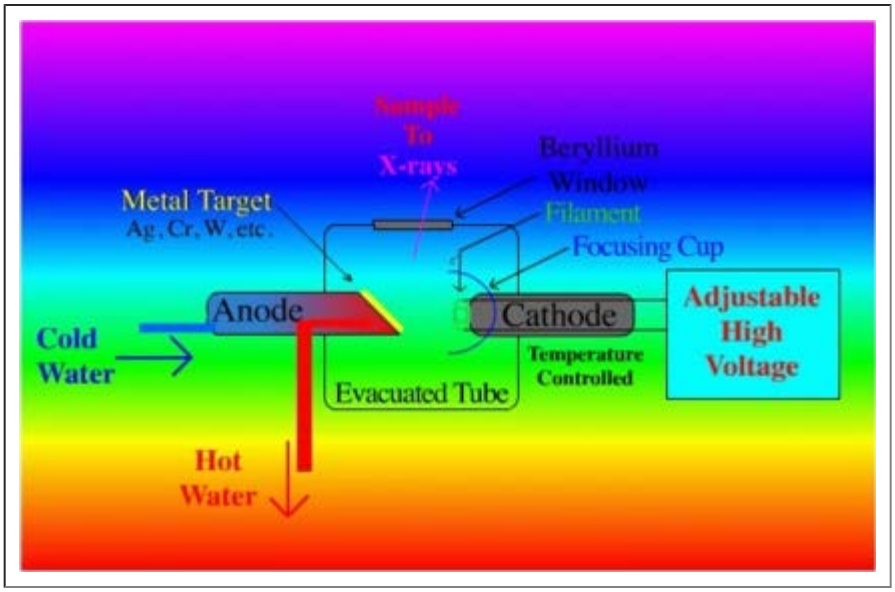

Figure 1. X-ray source in an X-ray spectrometer. Single frame from an animation entitled "X-ray Absorption Spectrometer." Gradient filled background is mercifully not present in the original.

How?

So once we get over the fear of requiring our students to get as involved as possible with modern computers in their chemistry courses, using computers to help teach specific topics is a natural extension. In my senior-level instrumental analysis course I use animations inside and outside of the course to teach instrumental techniques or particularly important or conceptually difficult points.

The advantages of using a schematic movie of the most difficult instrumental method I teach, gas chromatography/mass spectrometry via a Macromedia's Shockwave Flash animation will be briefly discussed below. But first I'd like to introduce an older animation constructed using a simple drawing program and Apple's QuickTime . My use of animation vehicles/programs has been morphing as the program options have changed with time. All of the animations I have created to teach with are listed here in roughly chronological order from the bottom of that page (oldest about 1996) upward in the list to the most recent.

In the "early days" the final file's size was one of the most important variables in each project. The unavailability of broadband ethernets and 56 kb modems that are so prevalent today made the animations files' delivery size **very** important then. As our network connections got faster my projects got larger and larger. As I passed 6 MB in file size (the tilted earth animation for an atmospheric chemistry class in 1999 and then a video taped 15 MB (!) freshman titration in 2000) I realized that except for my students access via our on campus T1 lines (300+ kb/sec), fewer and fewer users would wait for a 6 MB file to download. And this was using all the shrinking tricks: small palette size (fewer pixels), fewer frames per second, and extensive compression using software compressors best suited to the type of images in the animation.

Then came Shockwave Flash. The vector-based nature of this program means that long, complex, full screen animations are possible at a fraction of the size of bitmapped images. And the MP3 sound compression even allows for reasonable sound incorporation in Flash animations, if I could just learn how to synchronize sound with action....

What?

Example 1: The Double Beam Spectrophotometer

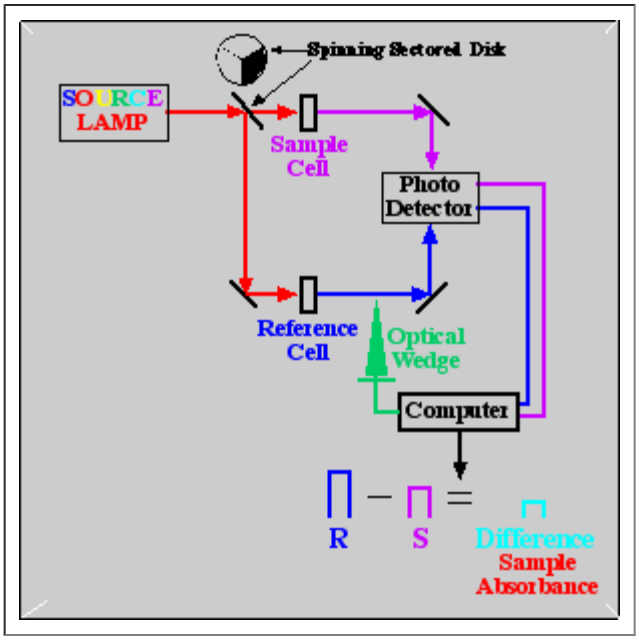

Figure 2. Frame from an animation called "Double Beam Spectrophotometer."

The ideas that I focus in on in the "Double Beam Spectrometer Movie " (a screen shot is in the adjacent Figure) involve, for instance, concepts that are important to the instrument, e.g., double beam "functionality," the separation of reference and sample beams not only in space but in time via the beam splitter. The static textbook drawings though they be many and varied often just haven't been able to get these ideas across to my students.

In the animation the spectrometer's schematic parts are introduced one by one along the light path from source to detector often excluding other instrumental parts for simplicity (look ma, no monochromator) . For me this is the main advantage of constructing my own animations: I can build them up frame by frame from the simple ("this represents a mirror", "this is a beam splitter") to the more complex and all the user has to do is move forward and backward in the animation to "disassemble" or "reassemble" the instrument. And I try to "isolate" the parts that cause the most conceptual trouble for my students. Examples of the build-up technique can be found in these animations: X-ray absorption , gas chromatography , GC/MS , flame and hydride

generation atomic absorption spectrometers for instance. [All the individual animation hyperlinks here and below are to the Flash versions if available. QuickTime or GIF animation versions are available at the link at the top of the page.]

I have also found it difficult to teach some students how the signal is generated by a double beam instrument. The "complete" double beam spectrometer animation provides a moving version of the alternating sample and reference beams with graphical representations of the signal produced by the photomultiplier tube (PMT) as the difference between these signals. [The adjacent image--not actually in the movie--is false in that respect: both beams never fall simultaneously on the detector in this instrument as displayed]. This is another thing I've decided to incorporate in my instrumental animations: an example of the instrument's signal plotted or in some way represented as the instrument generates that signal during the animation. Examples of these adjacent-data-in-the-animation approaches can be found in the Double Beam Spectrometer , Tuneable Monochromator , Flame Ionization Detector , Photoelectric Effect , GC Cryogenic Focussing , and the following GC/MS animation.

Example #2: Gas Chromatography/Mass Spectrometry

The most complex instrumental method I teach in my senior instrumental analysis course is gas chromatography/mass spectrometry. There is much involved in this method in hardware instrumentation, data forms/format, data collection/manipulation, and interpretation. And yet it has become so important in modern instrumental laboratories that I feel it is incumbent upon me to give students a very healthy dose of GC/MS while I have frankly let some more traditional techniques slide (thin layer chromatography, for instance). Our GC/MS laboratory component **encompass three weeks**. When one of my best students a few years ago failed to be able to describe in a clear way the differences between a TIC and an MS on a test's essay, I knew I had to do something. This of course suggests that I didn't hold either myself or the student directly responsible, and I didn't; instead it was an intellectual conspiracy of two, along with our textbook!

Originally constructed in Macromedia's Flash format, this animation has a number of programming features I hadn't learned about yet in my earlier animations, and therefore they are simply missing in the earlier animations. In the case of navigational buttons--to allow the user easy movement inside the animation from scene to scene--this simply was not easily accomplished in my earlier QuickTime animations. The most recent versions of QuickTime allow one to port Flash animations directly into a QuickTime file and keep the navigational buttons and indeed all the Flash features in the QuickTime format.

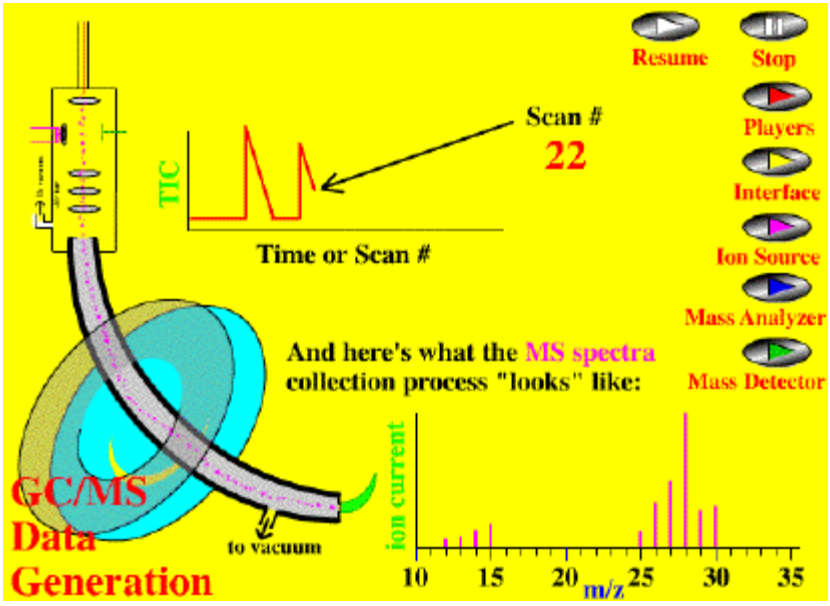

Figure 3. Frame from an animation entitled "Gas chromatography/mass spectrometer."

The adjacent Figure is a snapshot from the most complex scene in the GC/MS animation (the latter scenes in my animations naturally often show all instrumental parts working together). Yet this image also involves all of the most important features of a GC/MS run: ionized fragments streaming into the mass separator, fragments being detected, the total ion chromatogram (TIC) being generated, and an earlier scan's mass spectrum (MS) being displayed. When students see this on a PC's monitor they are, frankly, often blown away, not being able to understand what data stems from what process or how the parts integrate. This animation was my response to the confusion I saw on my students' faces.

Obviously as the fundamentals of the instrument are mastered, introduction and study of more complex relationships become possible. For example with GC/MS, space/time in the course previously dedicated to getting the TIC/MS

differentiation across can be used to investigate, for instance, more complex fragmentation patterns, formation of metastable peaks, or the benefits of different ionization methods. In atomic absorption spectrometry (AAS), facile understanding of the fundamental relationships between light absorption and a linear signal generation, frees us, for instance, to study the benefits of hydride generation atomic absorption spectrometry or graphite furnace AAS.

When and Where?

These animations are often introduced in my class using a computer-feed projector. In that venue, lots of starts and stops, forwards and backwards, and judicious pauses of the animation are used to teach the material and as a group we parse out the the functions of all the instrument's parts. If there is sound I almost always turn that off!

Since the files are also available on the web (and actually getting smaller as time goes on using vector-based programming), the students are also encouraged to investigate the animations out of class. If the situation is appropriate, animations are sometimes used during tests--(often stripped of the instrumental labels)--with essay-based questions about component relationships or functions.

Conclusions

I have finally been able to comfortably approach concepts in a senior level instrumental analysis course using animations, teaching that didn't "go" so well before.

Like most of our efforts to improve our teaching I have as "proof" of this teaching technique's success only a feeling about my students, a feeling of their more complete understanding of these complex instruments. It's kind of like **the opposite** of what I feel like when one of my better students, on the third test of the semester, completely misunderstands a newly worded complex question. Well if **she** doesn't get it, you can bet the more average student won't and as you grade the rest of the test set that initial hypothesis is born out. Sometimes I just throw out the question altogether.

With these animations, I feel that my testing is more thorough and my intellectual demands more rigorous. Everyone in the class seems to do better with these kinds of tools, the teacher and the students.
