CHED Committee on Computers in Chemical Education

Fall 2011 CCCE Newsletter

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Papers

Paper 1: **XCITR – Explore Chemical Information Teaching Resources**

Guenter Grethe[1], Grace Baysinger[2], Rene Deplanque[3], Gregor Fels[4], Ira Fresen[3], Andrea Twiss-Brooks[5], Gregor Zimmermann[3]

In 2005, the Division of Chemical Information of the American Chemical Society (CINF) and the Division of Computer-Information-Chemie (CIC) of the German Chemical Society established a Collaborative Working Group to foster a transnational dialogue in order to develop a shared approach for the access, exchange and management of chemical information. Within the larger context of the overall approach, the working group developed XCITR, an international repository of chemical information educational material to be used by librarians and instructors in chemical information. XCITR makes full use of features in Web 2.0 technology and is meant to be a hub in which instructors at all levels can deposit and access important teaching materials. This paper describes the history, organization and technical details of XCITR supplemented by examples from this freely available source.

1) Consultant, Alameda, CA
2) Stanford University, Swain Chemistry and Chemical Engineering Library, Stanford, CA
3) FIZ CHEMIE Berlin, Berlin, Germany
4) University of Paderborn, Department of Chemistry, Germany
5) University of Chicago, John Crerar Library, Chicago, IL

Paper 2: **Information Competencies for Chemistry Undergraduates**

Grace Baysinger[1]

1) Stanford University, Swain Chemistry and Chemical Engineering Library, Stanford, CA

Paper 3: **The Jmol Virtual Molecular Model Kit: A Resource for Teaching and Learning Chemistry**

Otis Rothenberger[1], Thomas A. Newton[2], Robert M. Hanson[3], Markus Sitzmann[4]

Since 2004, Jmol has become the *de facto* molecular viewer for Web pages, supporting chemical education, chemical research, cheminformatics, and molecular biology. One result of recent efforts to enhance the capabilities of the Jmol applet is the CheMagic O=CHem Virtual Molecular Model Kit: http://www.chemagic.com/vmk. The VMK is a multi-functional molecular model kit capable of doing everything that can be done with traditional "ball and stick" models, and much, much more. Along with a brief history of its development and a brief look behind the scenes, this paper will describe the major features of the VMK and illustrate various ways it may be used as a pedagogical tool.

1) Illinois State University, Normal, IL
2) University of Southern Maine, Portland, ME
3) St. Olaf College, Northfield, MN
4) NIH-NCI/CADD

Paper 4. **Learning ChemistryThrough Inquiry: The Molecular Workbench to the Rescue**

Charles Xie[1]

The Molecular Workbench software (http://mw.concord.org) is a computational tool for investigating atomic-scale phenomena. Its computational engines generate dynamic visualizations of microscopic processes that can be observed, manipulated, and analyzed on the computer screen. As such, the tool empowers students to learn through conducting completely graphical "computational experiments" for ideas otherwise untestable in classrooms. This capacity results in many opportunities of inquiry. It significantly lowers the barrier for learning and teaching abstract concepts in physical science. Instructors can bring a salient dynamic visualization up front without intimidating their students with obscure terminology or difficult mathematics. Worth ten thousand words, such a visual representation focuses students on ideas, not vocabulary or math. The Molecular Workbench software is made possible by the National Science Foundation.

1) Charles Xie, The Advanced Educational Modeling Laboratory, The Concord Consortium, Concord MA

Paper 5: **Activities for International Year of Chemistry Organized and Facilitated by the Committee on Chemistry Education (CCE) in IUPAC**

Mustafa SOZBiliR[1]

This paper aims to highlight the significant activities organized and facilitated by the Committee on Chemistry Education (CCE) of the International Union of Pure and Applied Chemistry (IUPAC) to celebrate the International Year of Chemistry (IYC) many of which are carried out in partnership with others within and outside of IUPAC. Several global and local activities special to IYC 2011 has been organized around world. At the international level, the Global Water Experiment (GWE), jointly organized by IUPAC and UNESCO, became a central flagship unifying activity for IYC 2011 with the hope of reaching hundreds of thousands of young people around the world with hands-on experiments related to the substance water, which is vital to all forms of life on earth. The second activity, carried out in partnership with RSC, ACS, and UNESCO is focused on visualizing and understanding the science of climate change. The project is in the final stages of producing a set of peer-reviewed, interactive, web-based materials to help learners visualize and understand the underlying science of climate change. The third activity was a global stamp competition which was open to all students around the world in 3 age categories (12-14, 15-18 and undergraduates from all subjects (not only chemistry!). Finally another international activity was focused on collecting the ideas for IYC 2011 all over the world with the goal of developing toolkits for national chemistry days and weeks during IYC 2011 to raise awareness of the importance of chemistry as the central science by highlighting the applications of chemistry in daily life. In addition to these international activities several local activities were organized to celebrate IYC 2011 around world. This paper will focuses on describing these activities to the chemistry community.

1)Atatürk University, Erzurum-Turkey, TM and Project Group Chair, IUPAC CCE

Paper 6: **The Analytical Sciences Digital Library**

Thomas M. Spudich[1]

The Analytical Sciences Digital Library (ASDL) is a collection of peer-reviewed, web-based resources related to chemical measurements and instrumentation. Materials in the ASDL collection include active learning materials, animations, case studies, lecture slides, on-line texts, simulations, tutorials, and virtual experiments. Sites are categorized to allow for easy browsing or the collection can be searched using a keyword search function. Each web resource in the main collection of ASDL includes a detailed annotation describing the site and its useful attributes. In addition to providing annotated links to web-based content, the ASDL journal, JASDL, publishes online articles in the areas of e-Courseware, e-Labware, e-Educational Practices. Statistics provided by Google Analytics show a global reach with users from around the globe.

1) Maryville University, St. Louis, MO

Paper 7: **The Dynamic Laboratory Manual: A Software Tool to Support Practical Chemistry Skill Development**

Tim Harrison[1], Nick Norman[2], Paul Wyatt[3]

The Dynamic Laboratory Manual (DLM) is an interactive, web-based laboratory manual, which has been developed by Bristol ChemLabS staff in the School of Chemistry at the University of Bristol in association with a Bristol-based e-learning company, Learning Science Ltd. It forms the centre piece of the Bristol ChemLabS (http://www.chemlabs.bris.ac.uk/) student experience of practical chemistry and has transformed teaching and student learning in a laboratory environment. This paper provides an overview of how the new laboratory experience evolved and why the DLM was developed as well as the staff-student interface supporting software to record marks and absences. The expansion of this educational approach to postgraduate level chemistry and to other disciplines is noted.

1) Bristol ChemLabS School Teacher Fellow, University of Bristol and co-author of Foundation LabSkills products, Bristol, UK

2) Chief Executive Officer of Bristol ChemLabS, University of Bristol, Bristol, UK

3) Director of Bristol ChemLabS, University of Bristol, Bristol, UK

Paper 8: **Clash of the Titans**

Harry E. Pence[1]

The death of Steve Jobs caused me to stop and reflect on how much computing has changed since Jobs returned to Apple in 1997. At that time, computing was Balkanized into many medium-sized companies, most of which were competing for market share in specialized niches. Now we live in a time when a few large corporations dominate many aspects of the computer marketplace, and Steve Jobs played a key role in many of these changes. Competition continues to be intense, but the competition is increasingly among four major companies, Apple, Amazon, Google, and Facebook. Each of these has dominated one or more aspects of computing, and now each is increasingly competing with the other three to gain control over as much of the computing space as possible. What do all these changes mean for Chemists?

1) State University of New York, Oneonta, NY

Attachment	Size
abstractsfall2011cccenl.pdf	81.62 KB

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Home

XCITR - Explore Chemical Information Teaching Resources View Edit Track

XCITR – Explore Chemical Information Teaching Resources

Guenter Grethe[1], Grace Baysinger[2], Rene Deplanque[3], Gregor Fels[4], Ira Fresen[3], Andrea Twiss-Brooks[5], Gregor Zimmermann[3]; [1]Consultant, Alameda, CA; [2]Stanford University, Swain Chemistry and Chemical Engineering Library, Stanford, CA; [3]FIZ CHEMIE Berlin, Berlin,Germany; [4]University of Paderborn, Department of Chemistry, Germany; [5]University of Chicago, John Crerar Library, Chicago, IL

Introduction

In 2004, the Division of Chemical Information (CINF) of the American Chemical Society (ACS) as part of its outreach mission and the larger ACS strategy of international communication decided to establish a collaborative working group (CWG) with the Chemistry-Information-Computers (CIC) division of the German Chemical Society (GDCh) to foster a transnational dialogue in order to develop a shared approach for the access, exchange and management of chemical information. To our knowledge, this represented the first attempt within ACS to create an international divisional collaboration other than an exchange of scientific publications. The ultimate goal of CWG is to be the hub in which the international chemical information community comes together to share, debate and reach consensus on important issues in chemical information.

The working group met for the first time in 2005 at the Spring ACS meeting in San Diego to discuss potential areas of collaboration and to explore areas of common interest among them the availability and distribution of instructional material in chemistry. The intensive needs of users of electronic chemical information have made it very difficult for instructors to cope with the large variety of available data sources containing increasingly vast amounts of data and many different searching tools and user interfaces. Available resources for teaching materials are also widely scattered. After continued discussions during 2005 in the US and Germany, the group decided in 2006 at the ACS meeting in San Francisco to build an international repository of chemical information educational material which later was named XCITR (Explore Chemical Information Teaching Resources) - http://www.xcitr.org. A prototype was first demonstrated at the 2009 ACS meeting in Salt Lake City and the program was launched in 2010 at the 6. German Conference on Chemoinformatics (6th GCC) in Goslar, Germany, followed in 2011 at the ACS meeting in Anaheim.

The XCITR Project

As a successor to the Clearinghouse for Chemical Information Instructional Materials created by Gary Wiggins at Indiana University in the mid-1980’s, XCITR is seen not only to meet the needs of librarians and instructors in chemical information, but also chemistry professors, instructors in other disciplines related to chemistry, information specialists, students, high school teachers, and even technical writers. XCITR is envisioned as a hub in which librarians, instructors and information providers can deposit and access important and useful teaching materials. Additionally, educational materials about library services and collections are also welcome. Following the first meeting in 2005, CWG met at every subsequent ACS meeting, once at Stanford University and several times in Germany. Partial financial support was obtained from the Innovative Project Fund Grant administered by the ACS Council Committee on Divisional Activities (DAC) and GDCh. The earlier meetings dealt with the organizational structure of the working group and ways of communication, defining an outline of the project, deciding on a platform and interface, and discussing policy issues. To test various options, FIZ CHEMIE Berlin in 2008 generously provided the server for the project and technical support. From the beginning, the use of open source technologies was considered mandatory and different content management systems, including DSpace and Drupal, were discussed and tested. In order to make full use of Web 2.0 functionalities the group finally decided on Drupal and technical development of XCITR started in 2009. Additionally, many other issues had to be resolved before development could start. Principal among them was the format and content of metadata elements to describe the submission to the repository. At a minimum, the metadata had to describe resource, target audience, system requirement and IP rights. Metadata had to follow standard definitions and contain controlled vocabularies. These discussions took up several meetings and were based on metadata used in similar repositories. Metadata will be discussed in the next section. Quality of submissions is overseen by an editorial board consisting of six members from the CWG. A built-in workflow scheme monitors contributions from initial submission to publication. Contents can be provided as documents (Word, PowerPoint, Excel, and PDF files), embedded videos (from www.youtube.com) or slideshows (from www.slideshare.net), and as external web based instructional materials by providing a link. Piwik is being used as a web analytics tool and Artisteer for the layout. Google Analytics was considered for capturing statistics but privacy concerns made Piwik a more preferable choice.

The XCITR System

The website is open to all users without a login requirement. Users can freely browse, read the documents, and download them for their own use if allowed by license agreements. However, users have to establish an account when submitting material. Using the URL http://www.xcitr.org, the program opens the homepage (Figure 1) which contains several areas which can be activated for browsing. In addition to listing the top 5 submissions based on hits, users can browse the content based on general categories, their sub-topics and specific areas (Figure 2).

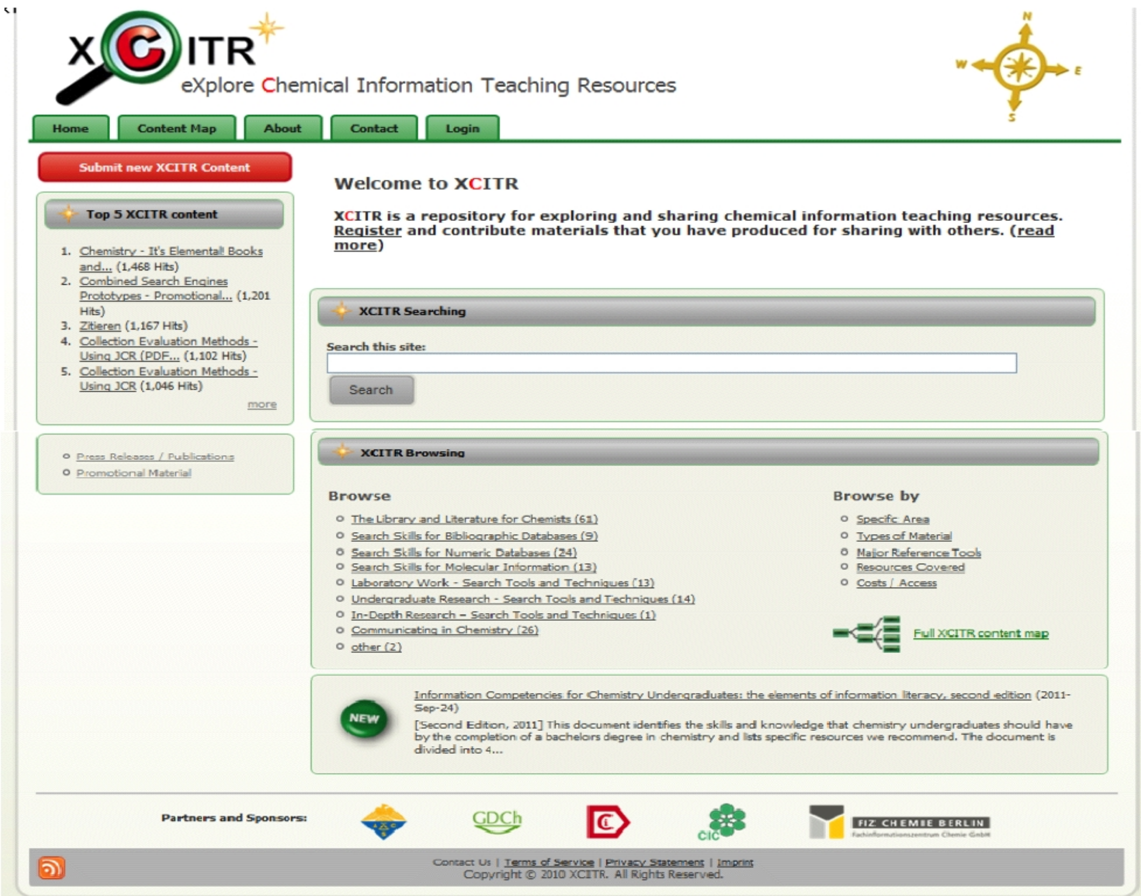

Figure 1: XCITR homepage

The controlled vocabularies of these categories are an essential part of the metadata and must be entered by authors during submission. The page also contains a link to the full XCITR content which is grouped according to subject, subject category, major reference tools, type of material, resources covered, and cost access. The same page can also be opened by activating the tap "Content Map" on each of the XCITR pages. In most cases, any submission is listed in more than one category. A click on any group or subgroup automatically opens the corresponding paper(s) (Figure 3). The homepage also contains a search function and a current awareness field showing the latest submission. The "About" tab opens a page describing XCITR and lists the member of the CWG and their association. Another tab provides a template to contact and leave messages with the technical support of XCITR.

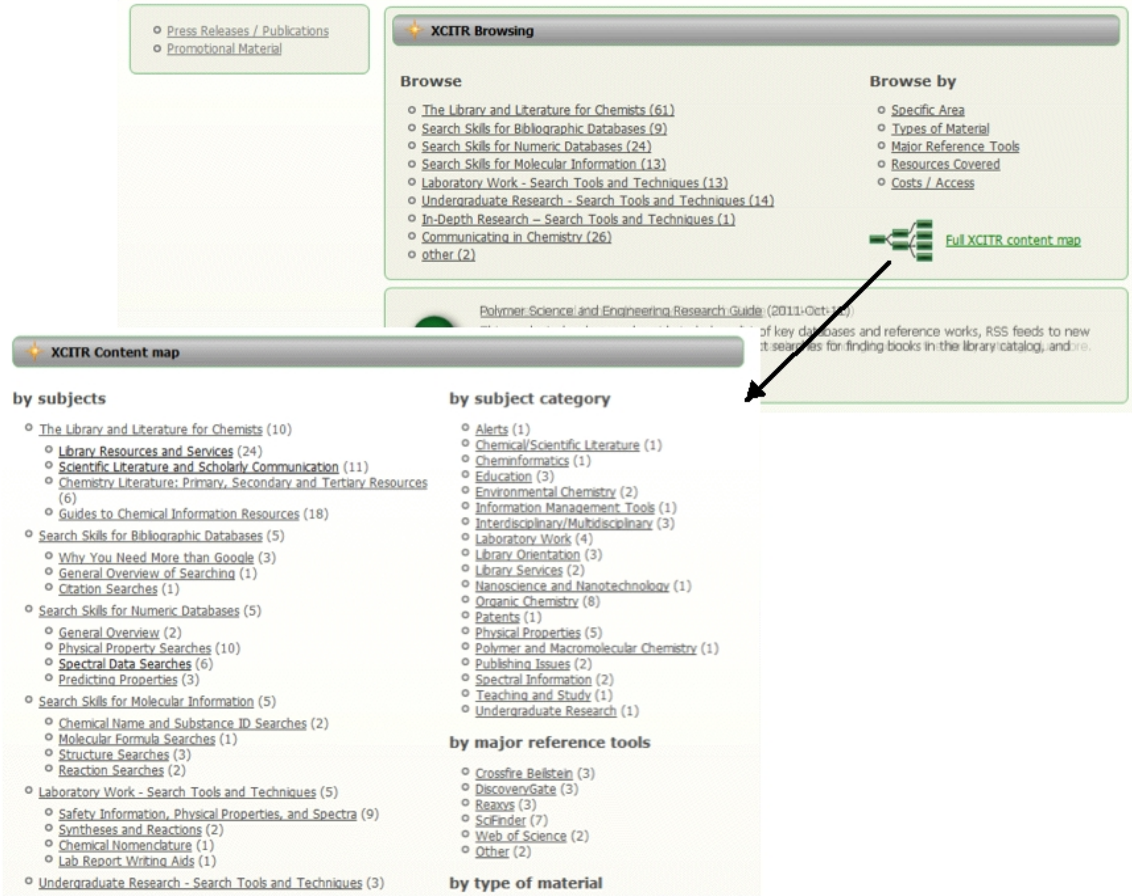

Figure 2: XCITR contents map

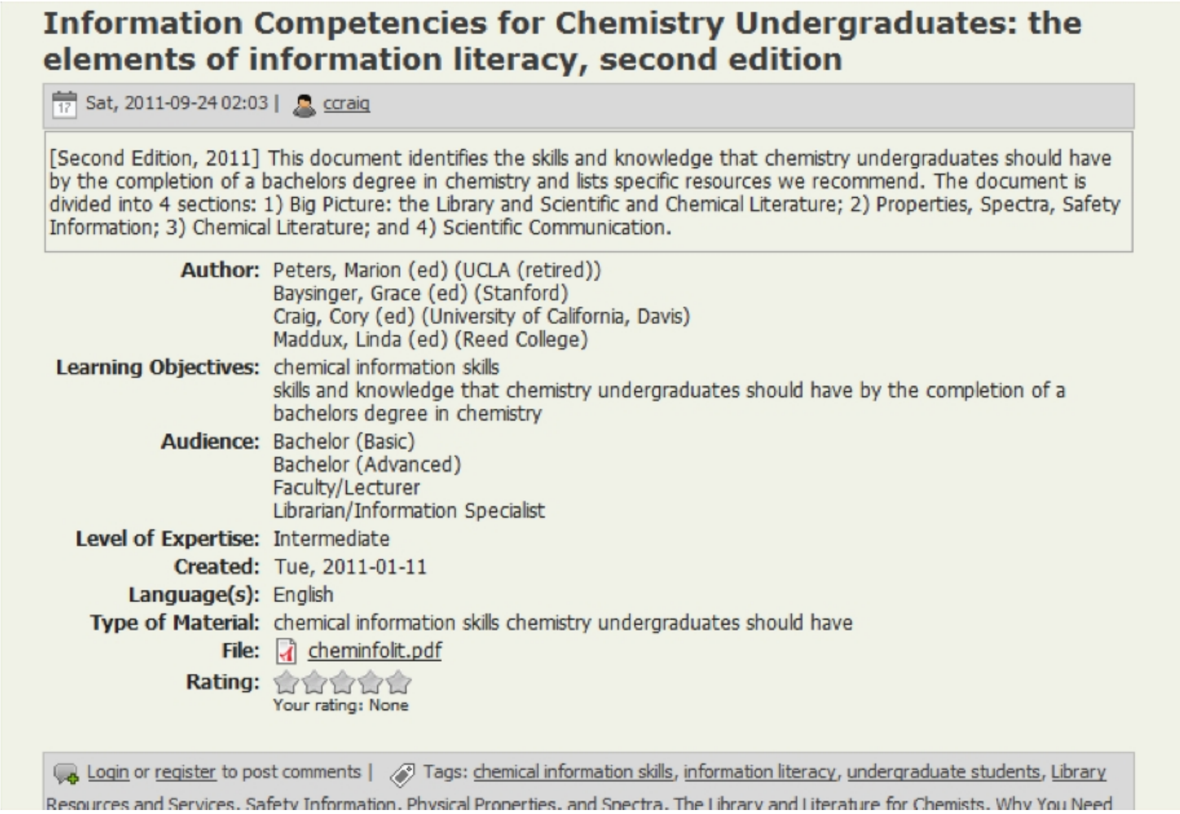

Figure 3: Sample metadata information for XCITR content

All these pages are accessible to any user. Submitting new content to XCITR requires the user to login. Clicking the button "Submit new XCITR content" opens a new page where the user can either login or establish a new account. This opens up the new tabs for accessing the Forum page for discussions and a Calendar page (Figure 4).

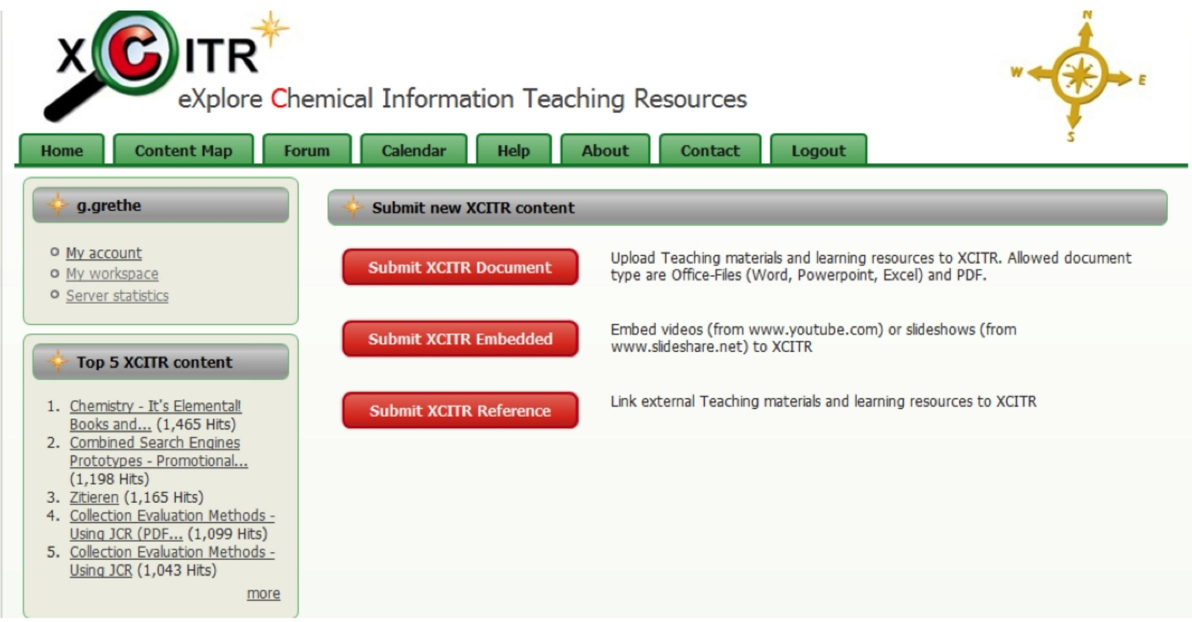

Figure 4: Submitting a resource

Figure 5: Link to an external resource in XCITR

XCITR allows for submitting different types of documents, each of which has its own button (Figure 4). The most common types currently submitted are Microsoft Office files, such as Word, PowerPoint, and Excel, and PDF files (type A). Users can also submit embedded videos (YouTube) or slideshows (Slideshare) (type B). The most recent and very important type is linked to external instructional sources which only require the URL of the material to be given rather than the full document (type C). After calling up a desired document, types A and B show the file extension, for example the PDF document in Figure 3. Type C on the other hand displays a small icon of the homepage which when clicked on leads directly to the desired website (Figure 5). Author(s) must fill out metadata forms for required and optional data. In addition to personal information, most of the other required datafields use controlled vocabularies. Figure 6 shows the fields of the required metadata common to all types of documents and the file type fields (A – C) for the type of documents files submitted. As a legal requirement the author also has to state that he has the right to publish the resources. Authors also specify if an item they are submitting is copyrighted, has a creative commons license or is in the public domain.

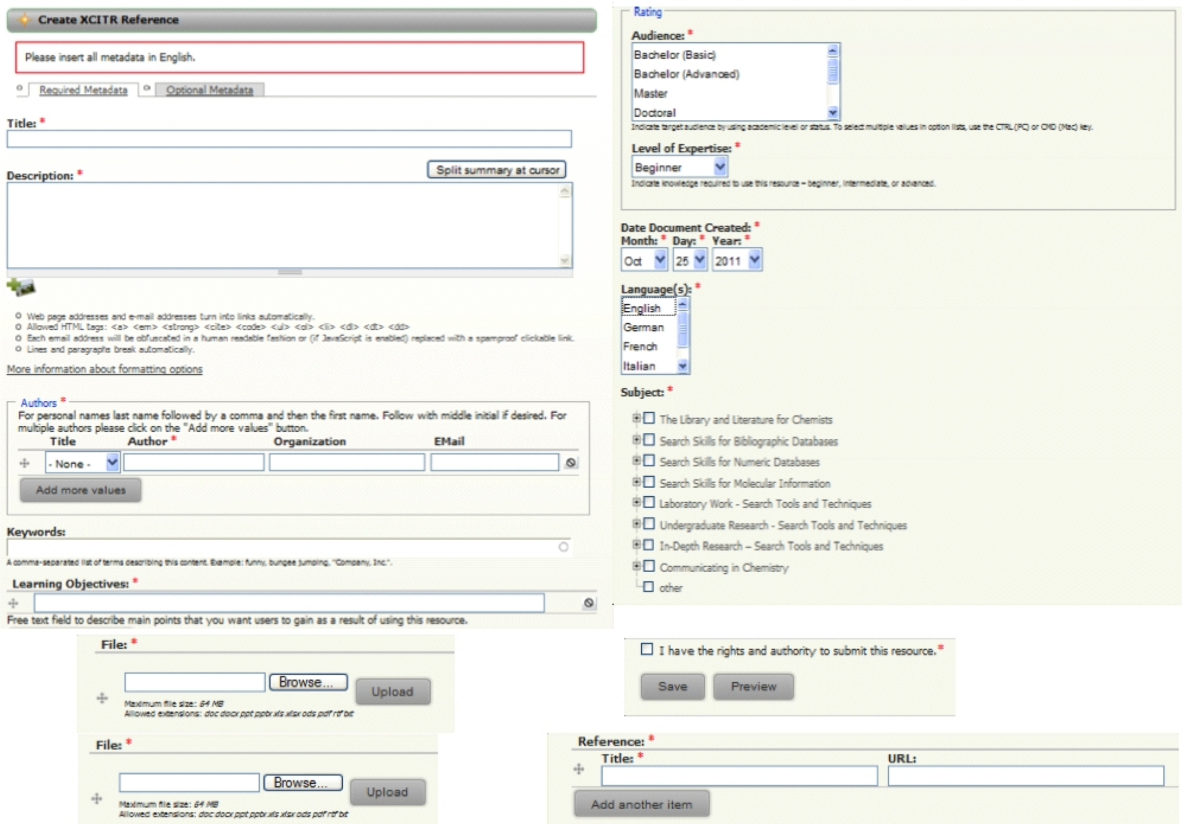

Figure 6: Required metadata for XCITR submissions

Once an author submits a document and indicates it is ready for review, the editorial board will be notified by an automated message system to review the submission. Documents have to meet the general criteria of being usable as instructional material to teach chemical information and related topics and peer review of the document as such is not required. Furthermore, all required metadata have to be submitted. In order to shorten the review process and to speed up publication, CWG decided that only one member of the editorial board is required to review the document, agree to publication, suggest revision or indicate rejection. A special workflow page has been established for the editorial board to check on the progress and history of the review. Authors are notified when their submission is published and publicly available.

Conclusion

After many years of organizational discussions, refining and evaluating content management (CMS) systems, XCITR represents a good example of international collaboration. Over 50 submissions have been made to date and the user data are at an upswing. The Piwik data show some very interesting usage statistics and it is encouraging that the top five documents show over 1,000 hits each. We can confidentially look into the future and assume that XCITR will become a valuable tool for all instructors in chemical information and related areas. We urge all readers to access the site, become familiar with it and use it.

Attachment	Size
fig2p1fall2011cccenl.jpg	385.89 KB
fig3p1fall2011cccenl.jpg	340.65 KB
fig4p1fall2011cccenl.jpg	253.75 KB
fig5p1fall2011cccenl.jpg	476.81 KB
fig6p1fall2011cccenl.jpg	448.35 KB
fig1bp1fall2011cccenl.jpg	590.5 KB

Press Release: September 2011 Information Competencies for Chemistry Undergraduates

Information Competencies for Chemistry Undergraduates

click here to download a printable pdf version of this paper
click here to download a printable pdf version of the document from XCITR

Updated September 2011, the 2nd Edition of *Information Competencies for Chemistry Undergraduates: the Elements of Information Literacy* is available at http://units.sla.org/division/dche/il/cheminfolit.pdf. It is issued jointly by the Special Libraries Association, Chemistry Division and the American Chemical Society, Division of Chemical Information.

The *Information Competencies* include skills and knowledge that students should have by the time they graduate. Knowing how to navigate the scientific and chemical literature will help make them more successful in their undergraduate careers, help prepare them for graduate school, and help them be more competitive in the job market.

This document is divided into four sections:

1. Big Picture: The Library and Scientific Literature

2. Chemical Literature

3. Properties, Spectra, Crystallographic, and Safety Information

4. Scientific Communication and Ethical Conduct

Each section includes specific skills that students should develop and identifies recommended resources. Recommended resources are free unless indicated by a **$$**. Resources listed are provided as suggested titles as some resources may not be available at an institution. Students do not need to know every recommended resource but should acquire enough skills to find information using available resources. Resources can be in any format but ideally students should be proficient using both print and online resources.

Educators and librarians who work with chemistry undergraduates are the intended audience for this document. It can be used to:

a) Improve chemistry undergraduate instruction.

b) Facilitate acquisition and assessment of information literacy skills by chemistry undergraduates.

c) Provide a list of recommended resources for libraries working with chemistry undergraduates.

d) Serve as a bridge between the ACS Guidelines for Bachelor's Degree Programs by the ACS Committee on Professional Training; and Information Literacy Standards for Science and Technology and Information Literacy Competency Standards for Higher Education, by the Association of College and Research Libraries, a Division of the American Library Association.

e) Assist as a resource for developing subject-specific information literacy standards in related scientific disciplines.

The "Information Competencies" document in combination with XCITR (eXplore Chemical Information Teaching Resources) http://www.xcitr.org/, a repository for exploring and sharing chemical information teaching resources, provides two current resources for those engaged in chemical instruction for undergraduates.

Comments regarding the document may be sent to: cheminfolit@ucdavis.edu, a listserv established for timely notification of URL changes and other inquiries or comments.

Submitted by Grace Baysinger, Stanford Chemistry and Chemical Engineering Librarian, Co-Editor of the 2nd Edition of the Information Literacy Guidelines

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Home

The Jmol Virtual Molecular Model Kit: A Resource for Teaching and Learning Chemistry

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The Jmol Virtual Molecular Model Kit:
A Resource for Teaching and Learning Chemistry

Otis Rothenberger, Illinois State University; Thomas A. Newton, University of Southern Maine; Robert M. Hanson, St. Olaf College; Markus Sitzmann, National Institutes of Health

Background

Until 2009, the Jmol applet was used primarily as a model display and animation tool. During the 2009 calendar year, a group of Jmol users and developers added a molecular editor to the Jmol applet capability (1). The authors of this report worked as part of that team, creating a Web-based small molecule model kit and providing enhanced applet development. The model kit served as a source of ideas as well as a testing platform for the overall project. It also provided a Web application, the Jmol Virtual Molecular Model Kit (VMK) that was released simultaneously with Jmol v.12.0.RC15 in 2010: chemagic.com/vmk or chemistry.illinoisstate.edu/osrothen/vmk.

VMK Overview

The VMK is designed to provide easy control panel access to Jmol's model editing ability. This means that users can build models directly in the kit's Jmol window. Users can add or delete atoms or groups at will. With the click of a mouse, they can convert, for example, (2R)-2-chlorobutane to its (2S) enantiomer. Changing (Z)-but-2-ene to the E stereoisomer is almost as easy. The kit's MultiUser function allows two or more people to work with the same model at the same time, a feature that enables collaboration between teachers and students.

While the VMK allows users to create models "from scratch", it also offers a rich source of starter models via links to PubChem (2) and the NIH/NCI Chemical Identifier Resolver (3,4), a Web application that translates one chemical identifier, such as an IUPAC name, into another, e.g. a SMILES, InChI, or SDF, thereby enabling the VMK to display models of, and to find information about, more than 30 million compounds! The link to PubChem provides a large library of stored SDF data, while that to Resolver generates SDF data by calculation. Using the embedded JME structure drawing applet (5,6), VMK also allows users to draw 2D structures that can be rendered as 3D models.

As the development of the VMK progressed, a new browser application called AKA that interfaces with PubChem and ChemSpider to construct compound-specific queries used in chemical database searches was created. Figure 1 identifies the principle data connections that VMK and AKA utilize.

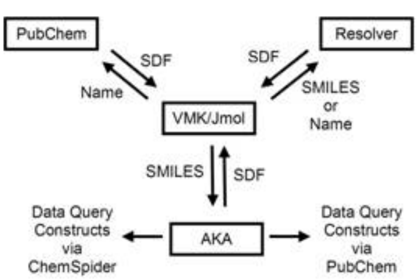


Figure 1-A flow diagram illustrating the communication pathways between the components of the VMK and AKA

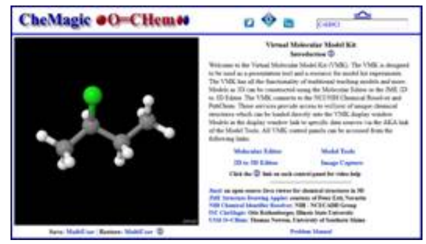
The identifiers in these queries, SMILES, InChI, InChIKey, etc., allow rapid transfer of information from PubChem, ChemSpider, NIST, ChEBI, Wikipedia, and other data sources. AKA sends an initial query to PubChem that returns the structure, formula, and missing identifiers for the identifier that was sent in the initial query. A search algorithm then constructs several identifier-specialized queries that return links to specific chemical database information: chemagic.com/aka.

The Control Panels of the VMK

In addition to the Jmol display window, the VMK consists of five control panels. A brief description of the features of each control panel follows. Clicking the name of a control panel will load a YouTube video demonstrating that panel's functionality.

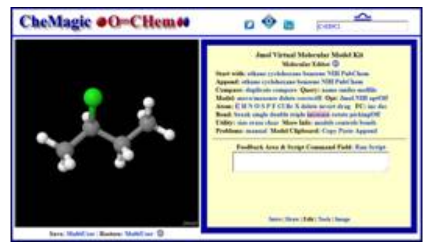
Introduction

- **provides an introduction to VMK and identifies important contributors**
- **provides access to the other control panels**
- **provides a link to the Problem Manual**



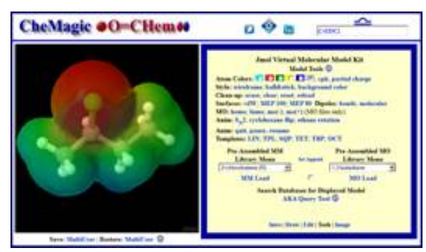
Molecular Editor

- **create, edit, and optimize models**
- **work with multiple models**
- **make structural comparisons of two models**
- **find chemical identifiers such as compound names and SMILES**



Model Tools

- **load pre-assembled models from two local databases allowing display of MEPs, MOs, and partial charges**
- **link models to external searches**
- **display animations and vdW surfaces**
- **load templates for making models of inorganic compounds**



2D to 3D Editor

- **convert a 2D drawing into a 3D model**
- **depict 3D model as 2D JME drawing**
- **compare two drawings to determine their structural relationship**
- **select 2D to 3D optimization method: Jmol (UFF), PubChem (MMFF94), Resolver (CORINA)**

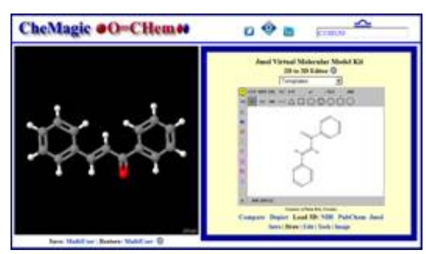
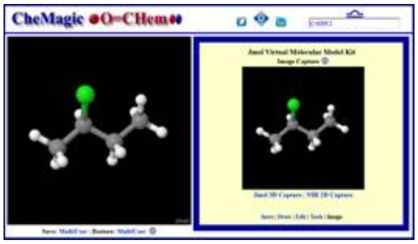


Image Capture

- **copy and save an image of a line drawing of the model that is in the Jmol window**

copy and save an image of the model that's in the Jmol window.

determine R/S stereochemistry of model



The ability to translate 2D structures drawn in JME into fully editable 3D models makes the VMK ideally suited for classroom use. The kit's multi-user feature allows for interaction/collaboration between teachers and students alike.

Additional Information

Data Bases

In addition to PubChem, VMK is connected to a local database of 2000 compounds. This local database will continue to grow. Models loaded from PubChem contain partial atomic charge data, allowing display of partial charges and MEP surfaces

Jmol SMILES

Jmol can create a SMILES for any displayed model. Jmol also uses an approach to SMILES comparison that eliminates the need for canonical SMILES algorithms (7).

Help Files

The Introduction control panel contains a link to a Problem Manual, which at the present time has 12 problems, each of which provides step-by-step instructions about a specific feature of the VMK. Each VMK control panel also has an information help link to YouTube video help.

References

Jmol: an open-source Java viewer for chemical structures in 3D - http://jmol.sourceforge.net/
PubChem SD File Formatted Data - ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_sdtags.pdf
The NIH - NCI/CADD Chemical Identifier Resolver - http://cactus.nci.nih.gov/chemical/structure
NCI/CADD Chemical Identifier Resolver: Indexing and Analysis of Available Chemistry Space, Markus Sitzmann, National Cancer Institute (NCI) - http://www.int-conf-chem-structures.org/fileadmin/user_upload/lectures/ICCS2011_D8_Sitzmann.pdf
JME Molecule Editor - http://www.molinspiration.com/jme/index.html
P. Ertl, Molecular structure input on the web, J. Cheminformatics 2010, 2:1 - http://www.jcheminf.com/content/2/1/1
A Universal SMILES String Comparator: Robert M. Hanson, St. Olaf College - http://chemapps.stolaf.edu/jmol/docs/examples-12/JmolSmilesTest.htm

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fig3p3fall2011cccenl.jpg	8.91 KB
fig4p3fall2011cccenl.jpg	9.9 KB
fig5p3fall2011cccenl.jpg	8.39 KB
fig6p3fall2011cccenl.jpg	8 KB

CHED Committee on Computers in Chemical Education

Learning Chemistry Through Inquiry: The Molecular Workbench to the Rescue

Learning Chemistry through Inquiry: the Molecular Workbench to the Rescue

Charles Xie (charxie@gmail.com), The Advanced Educational Modeling Laboratory, The Concord Consortium, Concord, MA 01742, USA

According to the National Science Education Standards [1], "inquiry into authentic questions generated from student experiences is the central strategy for teaching science." Inquiry involves asking and investigating questions, gathering and analyzing data, and predicting and explaining results. Because of its experimental nature, inquiry is typically taught through hands-on activities.

But atoms and molecules, the core idea in chemistry, are too small to be touched by bare hands. The conceptual abstraction of atoms and molecules and their motion and interaction often leaves instructors few options other than teaching them as facts.

The *Molecular Workbench* (MW) software (http://mw.concord.org) is a computational modeling system that can be used to support inquiry into the molecular world [2]. MW simulations generate dynamic visualizations of microscopic processes that can be observed, manipulated, and analyzed on the computer screen. This simulation capacity offers a powerful means of experiential learning in the absence of direct hands-on opportunities. MW offers completely visual learning experience, which allows the majority of students to learn about the concepts and ideas in atomic-scale science without being bogged down in the difficulty of mathematical and technical details.

The computational engines of MW for simulating molecular motions and quantum waves grew out of contemporary molecular modeling research [3]. As such, MW is not just an animation tool. It has all the predictive and explanatory power delivered by the research-grade computational methods built in it. That power is fundamentally important to enabling "digital inquiry." If we agree on the parallelism between inquiry in science and inquiry in education, why not give students a research tool and make it easy enough for them to use?

One of the concerns from teachers about using professional-grade computational tools in classrooms is that they tend to have complex functionalities for tackling complex relationships. This kind of complexity is often overwhelming to students. MW addresses this issue by introducing a user interface builder that allows curriculum designers to make custom controls for a specific simulation. These controls provide simple, direct user interactions with a simulation and set up a "sandbox" to confine student exploration within a subject. Within this "sandbox," students can investigate one variable at a time.

In his Foreword for a National Research Council's report on inquiry-based learning, Bruce Alberts singled out an important inquiry skill: "One skill that all students should acquire through their science education is the ability to conduct an investigation where they keep everything else constant while changing a single variable. This ability provides a powerful general strategy for solving many problems encountered in the workplace and in everyday life."[4] In many hands-on activities in chemistry labs, however, it is not always easy to find two substances that differ in only one property or vary just one property of a substance at a time. But this is not a problem for a computer simulation.

To be concrete about how this kind of inquiry is made possible in MW, let's look at a couple of examples that chemistry teachers typically teach and discuss how computer simulation can transform our teaching practices. These simulations may be commonplace to some readers. But they provide a good starting point to initiate a discussion.

A phase simulation lab

When learning states of matter, students are often taught in a way as if the three states, gas, liquid, and solid, were separate things. But, in fact, the formation of a phase is determined by only a few factors that are common to materials in any state made of any kind of atoms. An MW simulation shown in Figure 1 was designed for students to discover whether or not they can "cause a phase change" by adjusting one variable at a time. Students can explore four independent variables: atomic mass, atomic radius, interatomic attraction, and temperature. Using the simulation, students will be able to assess the effect of each individual variable. Those that do not have a significant role on phase change are used as distracters that can be ruled out through inquiry.

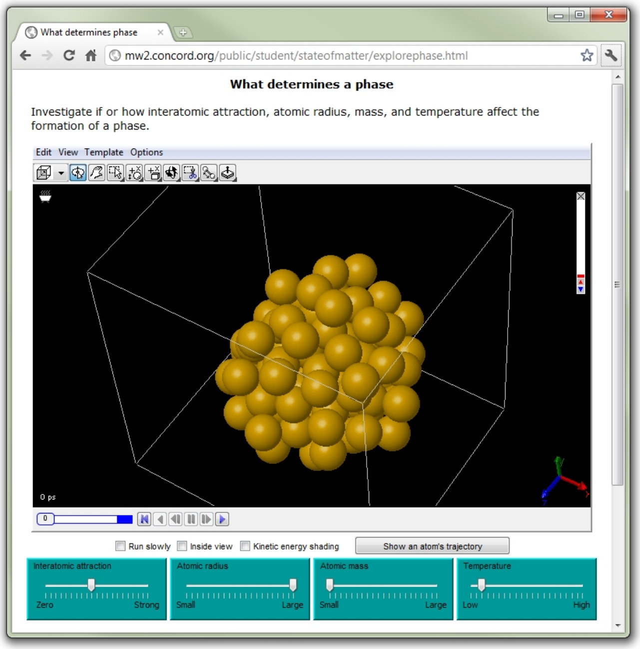

Figure 1. An online molecular dynamics simulation that students can use to investigate if or how interatomic attraction, atomic radius, mass and temperature affect the formation of phases.

Students can also study how the variables are correlated. For instance, they may find out that the melting point of a solid can be increased by making the attraction among the particles stronger. They can investigate whether substances made of larger or more massive atoms would necessarily have a higher melting or boiling point. This permits teachers to pose questions such as why mercury is a liquid and radon is gas whereas aluminum is solid.

The opportunities of inquiry provided by this simulation would hardly be possible if the molecular dynamics technique had not been used to construct it. Although molecular dynamics is based on only a few fundamental rules that connect the above four variables, it is capable of producing many different emergent behaviors and rendering countless subtle details. The details can further enrich the inquiry experience and lead students to deeper exploration. For example, students can randomly pick a particle and trace its trajectory. They can compare the trajectories of particles in different states. These manipulations of the simulation provide students much more learning opportunities than just telling them how atoms move in different states as many textbooks currently do.

A gas simulation lab

Everyone teaches the Ideal Gas Law. An ideal gas is a hypothetical gas made of randomly moving particles that do not have a volume and do not interact with each other. Have your students ever asked questions such as "What about non-ideal gases? How good is the Ideal Gas Law for real gases?" To answer those questions, you probably would have to pull out the Van der Waals Equation and pray that doing the math would do the trick.

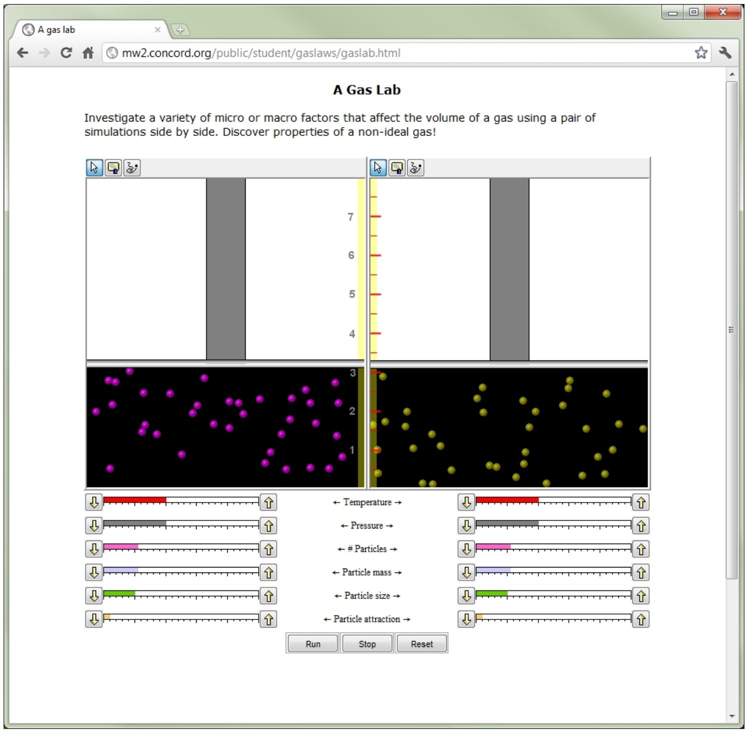

Figure 2. An online molecular dynamics simulation that students can use to investigate how well the Ideal Gas Law approximates real gasses.

Now, there is a better way to teach this. Using an MW simulation shown in Figure 2, investigating non-ideal gases becomes a piece of cake. This simulation uses a pair of gas containers side by side and allows the user to explore if or how six variables affect the volume of a gas: temperature, pressure, number of particles, particle mass, particle size, and particle attraction. It basically covers all the variables in the Van der Waals equation—without saying them explicitly. And there is a variable that is not included in the Van der Waals equation. The simulation reveals exactly why it is not there.

It is noteworthy that this simulation uses a setup of two gas containers that makes it easy for students to compare the results whenever they modify a variable for one gas.

A final note

The Molecular Workbench software has many more existing simulations that cover many topics in science. And best of all, if you are not satisfied with one, you can create your own.

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Attachment	Size
fig1p4fall2011cccenl.jpg	281.73 KB
fig2p4fall2011cccenl.jpg	262.62 KB

Activities for International Year of Chemistry Organized and Facilitated by the Committee on Chemistry Education (CCE) in IUPAC

Activities for International Year of Chemistry Organized and Facilitated by the Committee on Chemistry Education (CCE) in IUPAC

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Introduction

The International Year of Chemistry 2011 (IYC 2011) is a worldwide celebration of the achievements of chemistry and its contributions to the well-being of humankind. Under the unifying theme "**Chemistry—our life, our future**" IYC 2011 offers a range of activities for all ages. IYC 2011 is intended to reach across the globe, with opportunities for public participation at the local, regional, and national level [1].

The concept of IYC 2011 started with the recognition within the IUPAC Bureau that a number of scientific disciplines (e.g. World Year of Physics [2] and International Year of Astronomy 2009 [3]) have achieved significant benefits from securing designation by the United Nations of an international year pertaining to their field of study. The idea of having IYC 2011 has been discussed at IUPAC General Assembly in Turin, Italy in August 2007 and a resolution in favor of the proclamation of 2011 as the International Year of Chemistry was approved. Less than a year later, the UNESCO Executive Board recommended the adoption of such a resolution [4], submitted by Ethiopia, and which subsequently lead to the declaration in December 2008 by the UN General Assembly [5] of 2011 as the "International Year of Chemistry"[6].

IYC 2011 has four main purposes [1]:

- Increase the public appreciation and understanding of chemistry in meeting world needs,
- Increase interest of young people in chemistry,
- Generate enthusiasm for the creative future of chemistry,
- Celebrate the 100th anniversary of the Mme. Curie Nobel Prize and the 100th anniversary of the founding of the International Association of Chemical Societies.

IUPAC and the Committee on Chemistry Education CCE

IUPAC was formed in 1919 by chemists from industry and academia. For nearly 90 years, the Union has succeeded in fostering worldwide communications in the chemical sciences and in uniting academic, industrial and public sector chemistry in a common language. IUPAC is recognized as the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights and more. In recent years, IUPAC has been proactive in establishing a wide range of conferences and projects designed to promote and stimulate modern developments in chemistry, and also addressing education and public understanding of chemistry [1].

CCE is one of the committees of IUPAC. It has four main duties listed below [7]:

- To advise the President and the Executive Committee on matters relating to chemistry education, including the public appreciation and understanding of chemistry.
- To maintain a portfolio of educational projects and to coordinate the educational activities of IUPAC.
- To monitor chemistry education activities throughout the world and to disseminate information relating to chemical education, including the public appreciation of chemistry.
- To develop liaisons with international organizations such as UNESCO, national and regional chemical societies, chemical education committees, and organizations concerned with the public appreciation of science.

CCE is one of the groups which is actively involving in the organization of IYC 2011 educational activities [8]. CCE has worked with partners to collect and bring ideas to the IYC Management Committee [9] about high profile global events that would raise awareness about the importance of chemistry in our lives; such events could be carried out by the public (especially students) in various places around the world. Each country freely organizes their own activities, however, CCE worked out mostly on global activities. These are described below.

Global Activities

Water: A chemical solution - Global experiment for the International Year of Chemistry

Involving the public, and in particular students, in the activities of the IYC is one of the most important goals. Several global and local activities special to IYC 2011 have been organized around world. IUPAC and UNESCO have developed, in partnership with chemical industry and others, a set of activities called the *Global Chemistry Experiment* (GWE) to entice students around the world to learn about how chemistry contributes to one of the most important resources in their daily lives. The global experiment engages students in schools across the world in practical activities around the theme "Water: A Chemical Solution". The chemistry of water as a solution as well as the role of water in society and the environment is highlighted [10]. GWE come a central flagship unifying activity for IYC 2011 with the hope of reaching hundreds of thousands of young people around the world with hands-on experiments related to the substance water, which is vital to all forms of life on earth. GWE was launched on the UN World Water Day, March 20 - 22, in Cape Town, South Africa.

Although water is the most abundant substance on the Earth's surface, about 70% of the planet's surface is covered with water, it is rarely found pure. 97% of the water on Earth is sea water of high salt content and is not adequate for most uses. Therefore the availability of water around the world, in terms of both quality and quantity, requires that practical methods be found for proper treatment. Water fit for human consumption, or potable water, is essential for health and well-being. Purification of potable water demands adherence to a series of quality criteria embodied in physical, chemical and microbiological parameters, all of which require measurement according to prescribed procedures. The Global Chemistry Experiment demonstrates these concepts clearly and simply for students around the world [10].

The Global Chemistry Experiment consists of four component activities; each can be carried out by children of all ages in schools across all continents [11]. The activities are adaptable to the skills and interests of students of various ages and use equipment that is widely available at little or no cost. Short description of each activity is given below. The details for the activities can be accessible through the links given at the references.

Activity 1- *Acidity - pH of the Planet*: Students measure the pH of a local water source and explore the acidity of the water sample [12].

Activity 2- *Salinity - Salty Waters*: The salinity of a salty water sample is measured by evaporation [13].

Activity 3- *Water Treatment – Water: No Dirt, No Germs*: A dirty water sample is first clarified with a homemade filter and then disinfected [14].

Activity 4: *Distillation – Solar Still Challenge*: Students construct and test a solar still, exploring how it works, and then construct a still to their own design [15].

An interactive website [16] developed with help from *European Schoolnet* for the experiment now is in use includes all information for the GWE. Through the registration site school teachers can register their interest in the project and sign up their school to the activities. The data submitted is displayed via a mapping tool displaying the global data, school information including a Google map in color. Currently, as of end of October 2011, over thousand teachers and 24 thousand students were performed the experiment from total of 1174 registered classes in 25 different country throughout the world and submitted data [17].

Global Stamp Competition: Chemistry as a Cultural Enterprise

This activity is aimed to design a national stamp that reflects on 'Chemistry as a Cultural Enterprise', showing the chemical impact on the culture and/or everyday life in participants' country. The competition was open to students all over the world in 3 age categories (12-14, 15-18 and undergraduates/teacher students from all subjects (not only chemistry!) [18]. This activity was launched during the official opening ceremony of the IYC in UNESCO headquarters in Paris, France on January 27-28, 2011. Students uploaded their designs to a publication platform that allowed peer review. The submissions were collected until the June 15, 2011. 247 entries from 18 different countries were received. Most of the entries were from 15-18 age groups and the competition was most popular in Asia Pacific (total number 142 with 105 entries from Malaysia). Both stamps produced on the computer and pictures of stamps, drawn by hand were received. From Western European countries quite a few students' groups collaborated on one design. A panel of experts from IUPAC and all partners judged the entries. The winners of the stamp competition for each age group are given below in Figure 1[19].

Figure 1a. Vasilena Vasileva (Age 14) Bulgaria

Figure 1b. Muszhafar Hassan Ismail(Age 18) Malaysia

Figure 1c. Peter Yuosef M. Rubio (undergraduate) Philippines

Figure 1. Winners of the Global Stamp Competition.

The jury also selected runners-up stamps too. Runners-up for 15-18 age groups are Stavrou Maria, Spyrou Chrisia and Stylianou Chrysovalento from Cyprus, Luqman Safwan Che Mohd Fauzi from Malaysia, and Kyle Stratford and Max Willinger from USA.

Due to a generous gift of GlaxoSmithKline the organizers were able to send the winners $500 and the runners-up $250 (for the group). All mentioned students received a personal certificate. All other participants got a certificate of participation. A selection of the best designs will be on show during the IYC Closing Ceremony in Brussels. The winners and the runners-up also received additional prizes from their national chemistry societies and local authorities. Moreover Cyprus issued a customized stamp with the runners-up design, and the National Dutch Postal Services did the same with the Dutch winners' design.

Developing Toolkits for National Chemistry Weeks during IYC

This activity aimed to develop toolkits for national chemistry days and weeks during IYC 2011 in order to raise awareness of the importance of chemistry as the central science by highlighting the applications of chemistry in daily life [20]. The project essentially fulfilled the following two objectives:

- To collect information about the planned activities for IYC2011 from countries which already have established national chemistry days or week.
- To develop toolkits to facilitate the widespread celebration of national chemistry days or weeks around the world, particularly in countries that do not have a strong tradition to date of doing so.

In carrying out this project, it is hope that 2011 may be the beginning of on-going celebrations of the importance of chemistry in some new countries around the world.

The task group was collected information about the planned activities for IYC 2011, especially from countries having a strong tradition in celebrating chemistry at national level. The planned activities then published on the project web site to facilitate the sharing of those ideas with other nations, especially those that do not have already established national chemistry day/s or weeks, and that desire guidance for the celebration of chemistry days or weeks during IYC. Currently ideas and activities for IYC 2011 are available at the project web site [21].

Visualizing and Understanding the Science of Climate Change

Understanding and responding to global climate change is one of the defining challenges of the 21st Century. This IUPAC CCE project [22] provides a set of peer-reviewed, interactive, web-based materials [23] to help learners visualize and understand the underlying science of climate change. As a contribution to the IYC 2011, this project results from a three-year collaboration between the faculty and student research team at the King’s Centre for Visualization in Science (The King’s University College, Edmonton, Canada) and chemists and educators from the Royal Society of Chemistry (RSC - UK), UNESCO, IUPAC CCE, the American Chemical Society (ACS - USA), and the Federation of African Societies of Chemistry (FASC). The target populations are 16-19 year old students, teachers at the secondary and first year tertiary levels, and chemistry professionals. The materials are freely accessible to the general public. At present 4 of the planned 9 interactive web based modules are published and accessible through the project web site at www.explainingclimatechange.ca [23], and the remaining 5 modules have been drafted and are undergoing both scientific and pedagogical peer review prior to posting them on the web.

Local Activities

There are some other events that have been done with the help of IUPAC CCE and others at some localities. Among them are the Flying Chemists Program (FCP), Young Ambassadors for Chemistry (YAC) events and Women Sharing a Chemical Moment in Time.

Flying Chemists Program (FCP)

The FCP intends to provide emerging or economically disadvantaged countries means to improve the teaching and learning of chemistry at primary, secondary, and tertiary levels. The FCP provides a country with the expertise and external sounding board to strengthen chemistry education and to assist it in its own development [24]. A very successful FCP program visit was held in February 2011 in Ethiopia in conjunction with an IUPAC CCE project which aims to empower Ethiopian chemists and teachers to modernize chemistry education at secondary and tertiary levels [25]. The Ethiopia FCP program events were scheduled to coincide with the official national launch IYC in Ethiopia, the country that led the way in obtaining designation at UNESCO and the UN. FCP activities bring together at the national level a critical mass of chemistry educators to improve chemistry education, facilitated by external resource persons with expertise in areas targeted by the country, and including experience with previous FCP programs.

Ethiopia carried out a survey of chemistry education at secondary and tertiary level, and then brought together a network of chemists and chemistry educators to review the results and discuss ways to enhance the capacity of the country to provide quality chemistry education at these levels. Particular emphases were placed on laboratory instruction; visualization at the molecular level; designing and implementing contextualized and learner-centered chemistry education; promoting innovative ways of training quality chemistry teachers; and placing chemistry education in rich contexts related to local, national, regional, and global challenges. The FCP visit began with a half-day official launch of IYC in Ethiopia, and after three days of workshops, lectures, and brainstorming, was followed by the 27th Annual Conference of the Chemical Society of Ethiopia. The FCP visit was planned in consultation with both the Chemical Society of Ethiopia and the Federation of African Societies of Chemistry. The FCP program was made possible by supplementing the small amount of IUPAC funding with additional support from the Royal Society of Chemistry (UK), UNESCO, the Governments of Ethiopia and Germany, and the Federation of African Societies of Chemistry [26].

Young Ambassadors for Chemistry (YAC)

The YAC project [27] is a partnership between IUPAC CCE and the Science Across the World (SAW) network [28] to facilitate the flow of ideas between chemistry and society. This project uses the 'train the trainer' model to create public interest in chemistry. YAC has been running for years with several successful activities throughout the world. During IYC four of them were done in Ethiopia, Kuwait, Jordan and Puerto Rico. The YAC event in Ethiopia was held during 18-19 February 2011 in Addis Ababa with the help of Federation of African Chemical Societies (FASC) in University of Addis Ababa [29]. In April two individual YAC events was held in Kuwait and Jordan in April 18 and 20 respectively. YAC in Kuwait was organized by Kuwait Chemical Society and the Yarmouk University organized the YAC in Jordan. The Final YAC event in IYC 2011 was held in Puerto Rico on July 29 during 43rd IUPAC World Chemistry Congress in San Juan in Puerto Rico.

Women Sharing a Chemical Moment in Time

CCE Associate Member Mary Garson from Australia designed and carried out with the support of Fabienne Meyers and others a very successful global activity to celebrate the role of women in chemistry. Women chemists from 44 countries organized morning events on January 18, 2011 through an international networking event entitled "Women Sharing a Chemical Moment in Time". This event was a "prequel" to the official launch of IYC 2011 in 27-28 January 2011. Roughly 5000 women chemist came together to make it one of the largest gatherings of women scientist worldwide. A number of countries held multiple gatherings while some of them just had one gathering [30].

Conclusion

The goals of IYC2011 are to increase the public appreciation and understanding of chemistry in meeting world needs, to encourage interest in chemistry among young people, and to generate enthusiasm for the creative future of chemistry. The activities described above were planned and implemented by IUPAC CCE to fulfill the above goals. It has been a very busy year and it is still continue to be so. Chemists are enjoying the promotion of chemistry and reaching their voices to the far ends of the public. IYC 2011 is not just the celebration of past achievements of the chemistry, but is also a celebration for the future of the chemistry. As we approach officially the end of the IYC 2011, it is time to think about the sustainability of the events carried out during IYC 2011. For this purpose world leading chemists came together on a virtual conference to discuss the sustainable future of chemistry. Next stage of the events should be focused on how to keep this motivation achieved by IYC 2011 events for the sustainable future of our chemistry. As officially declared by the IYC 2011 management committee "Chemistry is our life- our future".

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Attachment	Size
fig1ap5fall2011cccenl.jpg	240.79 KB
fig1bp5fall2011cccenl.jpg	314.59 KB
fig1cp5fall2011cccenl.jpg	139.25 KB

The Analytical Sciences Digital Library, Thomas Spudich

Analytical Sciences Digital Library – a Unifying Force for Analytical Science Education

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The ASDL, as seen with some of the links on its main web page in Figure 1 (http://www.asdlib.org), is more than just a repository of information for the use of analytical chemistry teachers, students and practitioners; it is a site that creates opportunities for input and interactions among the analytical science education community. Interactions within the ASDL on-line community gives chances for continual growth in the adaptation of curricular materials already posted on ASDL and development of new resources that can be shared with others. The ASDL on-line community goes beyond traditional social networking through a variety of tools provided to allow users to collaborate on projects, maintain their own blog spot, develop research and curriculum ideas, syllabi, and online texts, connect with colleagues, and work collaboratively in teams of students and/or faculty. The library Editor-in-Chief is Cynthia Larive, from University of California-Riverside, and the Managing Director is Theodore Kuwana, Emeritus Faculty Member from the University of Kansas. There are several editors and an Advisory Board, and the names of the individuals are here: (http://www.asdlib.org/asdlPeople.php). Note that all of the material in ASDL is peer-reviewed, which gives the user an advantage over the traditional online search engine, such as Google, in that suitable sites have already been identified by the reviewers as being an acceptable resource for the topic of interest. There are resources that will be mentioned here that can be, or have been used in classes such as, but not limited to quantitative analysis and instrumental analysis, which complement or can possibly replace traditional textbooks used for these courses.

Figure 1: The main ASDL web page highlighting several options for the online community.

URL: http://www.asdlib.org

Figure 1: The main ASDL web page highlighting several options for the online community.

Analytical Chemistry 2.0: David T. Harvey, from DePauw University, has submitted an electronic textbook for use to teach a traditional analytical chemistry/quantitative analysis course (http://www.asdlib.org/onlineArticles/ecourseware/Analytical%20Chemistry%202.0/Text_Files.html). The book has been updated from his text, *Analytical Chemistry*, originally published by McGraw-Hill in 1999. He has done an excellent job of continuing to update the material to allow for the book to be used BY ALL for free. The files are in a textbook format for those that would like to create a paper copy of the material to use. If the student would prefer to use the electronic version, the Adobe Acrobat (pdf) files are set up to allow the student to highlight text, insert their own notes. As per discussions with students, they greatly appreciate when they do not have to spend upwards of $200 for a textbook for one course, and this resource provides that option.

LabView for Analytical Chemistry: Mark Jensen, from Concordia College in Minnesota, has submitted a teaching module highlighting digital signal acquisition and processing (http://www.cord.edu/faculty/jensen/LabVIEW/index.html). The author has focused on several different applications, including calculating a signal-to-noise ratio, a boxcar averaging application, generating a noise/power spectrum, an actual analog-to-digital conversion, calculating the Nyquist frequency, an application on ensemble averaging, and digital signal filtering. An example of the analog to digital conversion can be seen in Figure 2. Jensen provides two options, one via the Labview™ virtual instrument format (.vi file), or standalone executable file where the LabView™ runtime engine, that is a free download on the National Instruments webpage. On the ADC web page, Jensen provides a general description of the mathematical equations needed for ADC, gives a copy of the front panel, as well as guiding questions to help realize the issues with selecting the proper range number of bits for an application.

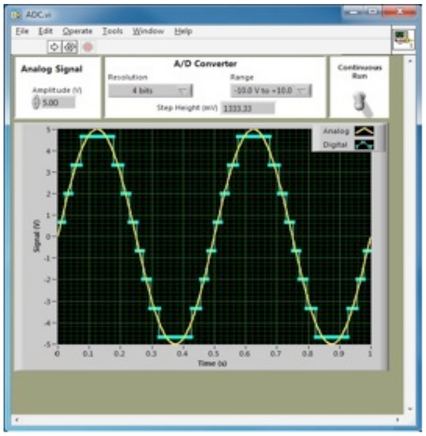

Figure 2: An image of the output of an executable file accessed through ASDL highlighting analog to digital conversion.

URL for simulation: http://www.cord.edu/faculty/jensen/LabVIEW/Simulations/Simulation%20Pages/ADC.html

Contextual Problem Approach: Lake Nakuru, Kenya: A team of faculty (http://www.asdlib.org/LakeNakuruPDFs/Guide%20to%20Instructors_1_17_2011.pdf) from across the United States has been able to construct a module highlighting an environmental problem in Lake Nakuru in Kenya (http://www.asdlib.org/lakeNakuru.php), where flamingos had been dying by tens of thousands since 1993. The goals of the module include being able to identify the problem with respect to what was killing the flamingos, generating a sampling plan, understanding the instrumental techniques used to identify and quantify the analyte (currently gas chromatography-mass spectrometry), as well as method validation of the EPA method 525.2. Also included is an instructor's guide which provides focused information to help instructor guide the students in each section. Note that this module has been constructed during ASDL curriculum workshops funded by NSF, typically during the summertime.

Some of the other resources in the library which not described in depth include (1) a forensic science lab-book contributed by Rob Thompson from Oberlin College that includes instructor and student procedures for the analysis of alcohol, arson, drugs, explosives, glass, gun-shot residue, fabric, paint, and pen ink (http://www.asdlib.org/onlineArticles/elabware/thompson/Home1.html); (2) a resource where Way Fountain, Dawn Riegner, from the United States Military Academy, and I provided links (most through ASDL, http://www.asdlib.org/onlineArticles/ecourseware/Spudich/Spudich_ASDL_Chem520.pdf) for several topics and learning objectives seen in instrumental analysis; (3) an interactive learning (http://www.asdlib.org/onlineArticles/ecourseware/Bullen_XRD/XRDModule_index.htm) module on X-ray Diffraction by Heather Bullen from Northern Kentucky University; (4) an online community (http://community.asdlib.org/) for analytical chemists to post blogs for classes, video exchanges, and the list goes on with possibilities. Note there several hundred different resources available through ASDL.

Over the years, there are several items of interest that have been generated about the use of the library for teaching. In using the active-learning modules, it was noted that the students were motivated when having to participate in this environment, more so than in a traditional lecture. The material focuses on student centered learning, is adaptable in a variety of teaching environments, problems are inter-dispersed within the material. Some of the issues are time and tailoring for individual classroom environments. All of the information is electronic (even using an iPhone) and available free of charge.

Future goals include completing textual material for the remainder of the analytical curriculum, develop more inquiry-based collaborative learning projects, more instructor guides and focus new contextual modules to include (1) an extension of the Lake Nakuru project focusing on toxic metals, (2) effects of acid rain on several environments, and (3) performance enhancing drug testing to include steroids analyses.

Attachment	Size
fig1p6fall2011cccenl.jpg	37.88 KB
fig2p6fall2011cccenl.jpg	31.48 KB

CHED Committee on Computers in Chemical Education

The Dynamic Laboratory Manual: A Software Tool to Support Practical Chemistry Skill Development

The Dynamic Laboratory Manual: E-Learning Software to Support Practical Chemistry Skills Development

Tim Harrison, Nick Norman, Paul Wyatt, University of Bristol, Bristol, UK

Introduction

The problem identified with the traditional undergraduate laboratory experience was that students typically arrived at the laboratory to carry out an experiment without a clear idea of the practical techniques they would be using, the skills they would require, or the chemistry behind the practical. Experience had shown that it was often only *after* the laboratory, during a write up, that they would generally start to work out what it was they had been doing throughout their period of very expensive laboratory time. Added to this, students are often expected to perform poorly stimulating, repetitive tasks that appear to have little relevance to the skills set needed by a 21st century chemist. Students would clearly get much more from the laboratory experience if they were to know what they were going to be doing before they arrived and pre-laboratory preparation is the key to achieving this. When Bristol was awarded the grant to become the UK's Centre for Excellence in Teaching and Learning in practical chemistry this matter was addressed, along with the desire to also incorporate other aspects of e-learning and e-assessment into the laboratory experience. One of the main innovations in Bristol ChemLabS has therefore been to shift the balance of work done outside the laboratory to *before* rather than *after* the practical class so that students are much better prepared and therefore more confident in their practical work. Key to the realisation of these two main ambitions has been the development of the Dynamic Laboratory Manual (DLM).

Pre-laboratory Work

As part of the ChemLabS experience, students are now required to work through some background information about the experiment before they arrive at the laboratory (figure 1). All the information they need for a particular experiment is contained in the DLM and they do not need, for example, to have had particular lectures in advance of any given experiment. An important part of the pre-laboratory work centres around a set of multiple choice and multiple completion questions. These are assessed and form part of the overall assessment for that experiment, but also provide immediate and informative feedback on any wrong answers given. Students are given two attempts but since the questions are taken from a question bank, the second set of questions will not be same as the first. Likewise, different students will get different questions.

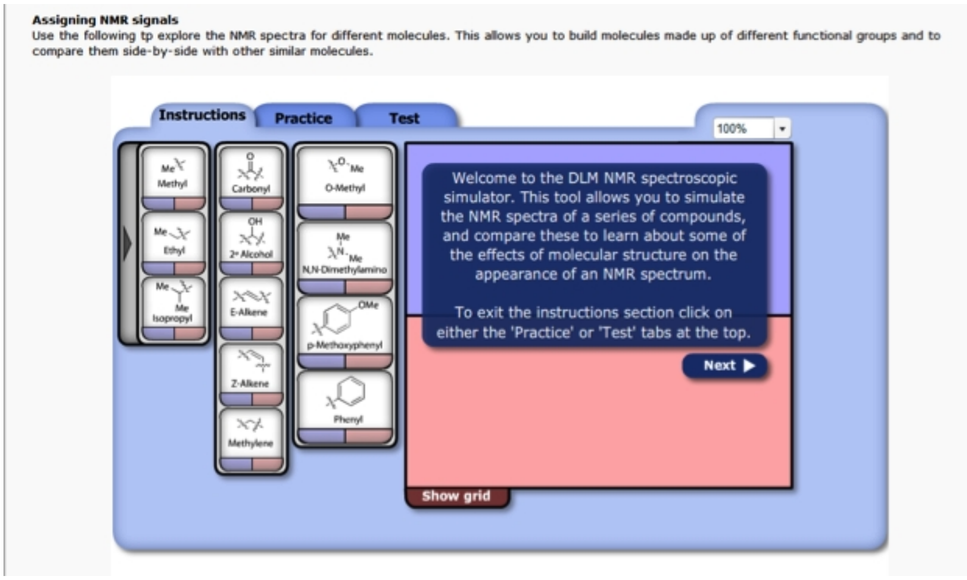

Figure 1 Tutorial on NMR where students can compare the NMR signals of a series of compounds that the student designs.

In addition, information about each experiment comes in a variety of rich formats which includes Flash-based simulations/virtual instruments and video (figure 2).

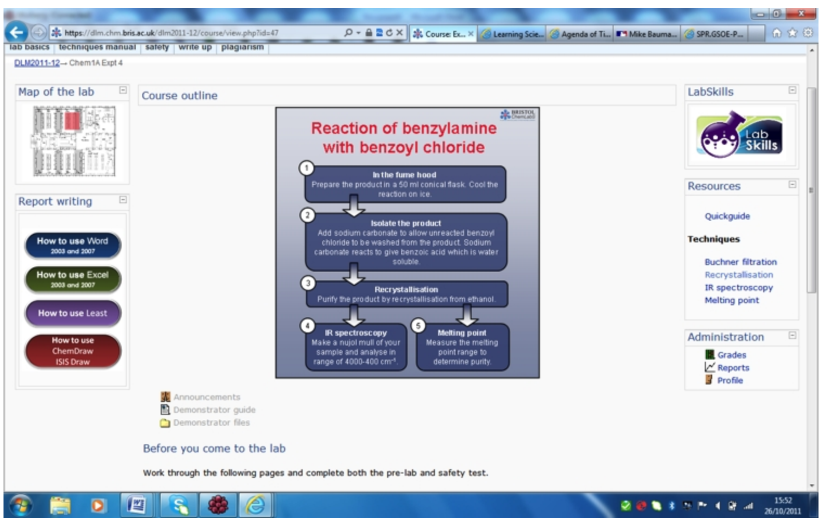

Figure 2 A screen shot of part of a first year practical showing experiment flow chart and allowing access to e-learning tools for report writing tutorials, practical techniques support and a downloadable practical outline.

In the Flash based simulations/virtual instruments a complicated piece of equipment or instrumentation is represented in a diagrammatic form which has interactive valves or switches etc. (Figure 3). The correct use of the equipment can be learned by following a set of instructions and although it is likely that many students will merely play with the valves initially, even this will educate them about the function of the apparatus. Mistakes, which might be quite serious or costly with the real equipment, can therefore be made with no adverse effects; students just start again and have another go.

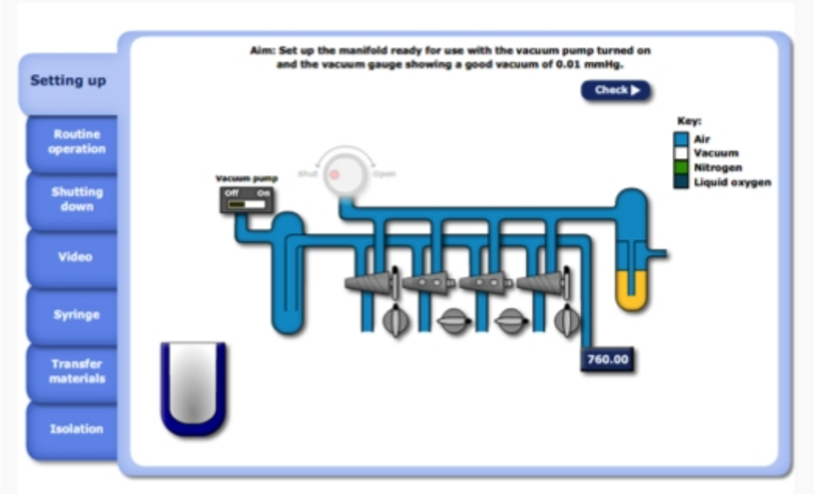

Figure 3 An animation of a Schlenk line, for working in inert atmospheres, is an example of a more advanced undergraduate simulation.

Some techniques are best illustrated with video and students find this a very useful way to get a clear idea of what they will need to do in the laboratory. Many students have limited prior experience of glassware and general laboratory apparatus and seeing, for example, how to set up a Büchner filtration gives them confidence and saves them from having to ask a demonstrator. The videos are sectioned into 20-40 second clips with a brief written explanation of why what is being done is done! Students therefore learn what a particular set of apparatus is supposed to do, have more confidence when it comes to using the real thing, and a much better idea of the chemistry that is being explored in the experiment. Moreover, demonstrators are now free to engage in more productive activities with the students such as in-lab assessment. A demonstration of many aspects of the DLM is available at http://www.chemlabs.bris.ac.uk/DLM.html.

Virtual instruments/equipment and video clips are embedded within each experiment but are also gathered together in a Techniques Manual which is available as a general resource throughout the students' time in Bristol including any periods of industrial or overseas placement. It is important to stress that video and simulation are in no way intended to replace the laboratory experience; their role is to augment it.

Laboratory safety is also addressed. In the past students have had to sign a safety form declaring that they understand the risks and hazards associated with the chemicals and apparatus for a particular experiment and the precautions which need to be taken. Unfortunately, some students were prone to taking a rather flippant attitude towards the safety form which was never a very satisfactory state of affairs. As part of the DLM, students are now asked a variety of questions, many of them scenario-based, concerning safety and the hazards associated with the chemicals used for each experiment. These questions are in the form of multiple choice or multiple completion questions and students must score a minimum of 80% before they are allowed to start the lab. Students are thus forced to think about hazards and safe practices. They are told the correct answers at the end of their attempt and they may have a second attempt but the questions are taken from a data bank and will therefore not necessarily be the same.
A list of all the undergraduate experiments may be found at: http://www.chemlabs.bris.ac.uk/undergrad-experiments.html.

The Staff/Student Interface

Using bespoke software linked to the DLM, academic staff and demonstrators are able see how the students have performed in the pre-lab and safety tests. In the case of safety data, a student who scores less than 80% has this mark in a red box whereas a student who has passed has their score shown in a yellow box or in a green box if they have scored 100%. The laboratory teaching fellows and postgraduate demonstrators can see at a glance which students need to be spoken to at the start of the laboratory and their tutors can keep a track of the development of their tutees at any point. The students can also see their individual performances throughout their degree.

DLM Developments in Postgraduate Training and Other Disciplines

The value of the DLM approach in supporting undergraduate practical work has led to an extension of the DLM concept to support research training for postgraduate students in two Doctoral Training Centres (DTCs) at Bristol. In the Chemical Synthesis DTC (http://synthesisdtc.chm.bris.ac.uk/), these include advanced tutorial packages on NMR spectroscopy, X-ray crystallography and glove box use. For undergraduates in other disciplines, the Faculty of Medical and Veterinary Sciences at Bristol has also developed DLMs through its eBioLabs programme to support laboratory teaching in Biochemistry, Physiology and Pharmacology, and Cellular and Molecular Medicine (http://www.bristol.ac.uk/ebiolabs/).

Such is the impact of the DLM that Bristol ChemLabS won the UK-based Times Higher Education Award for Outstanding ICT Initiative of the Year in 2010.

The Future

In addition to the DLMs described above, commercial versions of the Chemistry DLM have been developed with Learning Science Ltd as the LabSkills brand including A-Level Chemistry LabSkills and Foundation Chemistry LabSkills. A-Level Chemistry LabSkills supports the practical component of A-Level chemistry (a UK-based pre-university qualification) whilst Foundation Chemistry LabSkills is designed for first year laboratory teaching at university foundation level. Details of these products can be found at http://www.labskills.co.uk/. More recently an agreement between the University of Bristol, Learning Science Ltd and Cengage Learning Inc will see LabSkills technology incorporated into online learning resources designed for freshman chemistry courses in the USA. A-Level Biology LabSkills and A-Level Physics LabSkills are under development.

Attachment	Size
fig1p7fall2011cccenl.jpg	111.16 KB
fig2p7fall2011cccenl.jpg	184.14 KB
fig3p7fall2011cccenl.jpg	66.69 KB

Clash of the Titans

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The death of Steve Jobs caused me to stop and reflect on how much computing has changed since he returned to Apple in 1997. At that time, Microsoft ruled the world of desktop computers; MySpace was the predominant social network site and Facebook had just been registered as an online domain; Nokia was the big name in cell phones having released the first mobile phone to enable wireless email and internet connection in 1996; Larry Page and Sergey Brin, Ph.D. students at Stanford, had just announced a new search engine, called Google; several companies had introduced tablet computers but none had achieved much popularity; and Amazon was beginning to establish itself as a leader in online book sales, having served 1.5 million customers that year. There was intense competition within various types of computer applications, but that competition was still fragmented among several different companies.

At about this time, I began writing a series of articles for *this Newsletter* with the title, "What is the best search engine for Chemists?" When I began writing, there was a plethora of different search engines available, and this seemed like a topic that might be helpful to my colleagues. With passing time, however, Google became so dominant that my focus narrowed to the competition between Google and Microsoft. Despite Microsoft having spent over six billion dollars on Bing, their latest attempt to dominate search, Google has continued to dominate, and this competition never became the Clash of the Titans that I expected [1]. The articles I wrote were predicated on the assumption that the main way Chemists would access online information was by using search software on desktop or laptop computers. This assumption is no longer viable; mobile devices are becoming the new standard for many tasks, including search, that were traditionally done on desktop and laptop computer.

The real clash of the Titans may already be underway, but contrary to my expectations, the battle to determine which company will control the future of personal computing is being fought over mobile devices, like phones and tablets, rather than search. Apple and Google have pushed aside the early leaders in cell phone technology, including Motorola and Nokia, to become the innovation leaders. Recently Nokia, the Finnish mobile company, has agreed to replace its mobile operating system with that provided by Microsoft. It remains to be seen if the Nokia/Microsoft combination can overcome the technological lead of Apple and Google. The companies competing with the iPhone, mainly use the Android operating system, created by Google. Google is in the process of buying Motorola Mobility, presumably to secure the treasure trove of mobile patents held by Motorola. Recently, both Nokia and Microsoft have released new phones, but this news was largely lost in the blizzard of publicity for the iPhone 4s. The dark horse in the race is Amazon, which already dominates ereaders with the Kindle, and has now released a low-priced tablet, the Fire. The important message from these developments is that some very innovative companies with large amounts of cash are going to be focused on the development of mobile computing in the next few years.

In addition, more and more young people have smartphones and use them to access the World Wide Web (WWW). Globally, there are about three cell phones for every computer, and in the year 2008, for the first time sales of smartphones were greater than the sales of laptop computers [2]. A recent study by the Pew Trust reported that "87% of smartphone owners access the internet or email on their handheld, including two-thirds (68%) who do so on a typical day. When asked what device they normally use to access the internet, 25% of smartphone owners say that they mostly go online using their phone, rather than with a computer. [3]" The report notes that these percentages are higher for some groups, including those younger than 45. A recent article in *The Chronicle of Higher Education* indicates that 40% of college students use the Internet on mobile devices every day, and students increasingly expect that all their college services will be available from their phone [4].

Taken together these developments suggest that mobile computing use is continuing to expand rapidly and that increasing numbers of the students in our Chemistry classrooms will be carrying mobile devices that are connected to the World Wide Web. Currently, the use of mobile devices is at about the same point that electronic calculators were a couple of decades ago. There are still many teachers who may remember the efforts to ban electronic calculators from the classroom. It is clear that these efforts were un successful, and it is likely that similar attempts to ignore or ban classroom use of mobile devices will fail. It is time to begin thinking about how the mobile ecosystem can be integrated into Chemistry teaching

It is possible that some of the antipathy towards these devices arises from a misunderstanding based on the word phone. A modern cell phone is no more like a conventional telephone than a modern automobile is a horseless carriage. Both the automobile and the smartphone have capabilities that much greater than their antecedents. The cell phone has become a powerful, handheld, web-enabled, image processing computer. It is the most powerful research device created since the desktop computer, and many of our students already recognize this. It is true that cell phones can serve as a communications device that may be a distraction in class, but focusing on this aspect is no more productive than focusing only on the fact that automobiles create junkyards when they are discarded. In each case the problem is real but is solvable and does not represent a reason to ignore the potential usefulness of these technologies. In addition, banning smartphones at this stage is probably as likely to succeed as was the attempt to ban all electronic calculators.

Recent research suggests that users are already changing their mental habits to take advantage of the computer software, like Google [5]. There is a tendency to use the computer to offload information that is needed less often. This is consistent with transactive memory theories proposed by Daniel Wegner thirty years ago, namely that humans often depend on shared memories to complement their own remembering. For example, a husband might depend upon his wife to remember some facts, or, in the modern day, a student might use the computer as an auxiliary memory, where facts could be recovered as needed [6]. In a similar way, classroom work might discriminate between essential facts, that must still be learned, and less critical information, that can be looked up on a computer as needed.

When thinking about the classroom of the future, it is better to think in terms of the mobile ecosystem rather than specific devices, like smartphones. Many young people seem to be quite satisfied to watch videos and read text on a phone screen, but those of us somewhat further along in years may well appreciate the larger screen on a tablet computer, like the iPad. As the recent explosion of interest in tablet computers demonstrates, the world of computer devices is constantly changing, and so there may be some new device is the offing that will be more attractive. The mobile ecosystem can be defined as the combination of mobile devices, apps, operating systems, physical objects, and networks that integrates information retrieval and communications. Of course, there will still be some jobs that are better done on a laptop or desktop computer.

Apple has recently released the latest version of the iPhone, the 4s, which expands the already impressive capabilities of the previous versions. In addition to a faster dual core chip and improved camera, the new version includes a "personal assistant," Siri, which understands verbal commands, so that you can now tell your phone, "Remind me to turn on the coffee maker when I get to work," and the phone will not only remind you, but the Global Positioning System in the phone will know when you get to work and remind you then. Siri accepts vocal commands to search the web for information. The search is currently directed to Wikipedia or WolframAlpha, but it is quite likely that soon this capability will be expanded to Google or Bing. If Apple decides not to do this, some other smartphone maker will surely seize upon this as a competitive advantage.

How will this change the chemistry classroom? Several faculty are already trying to answer this question. For example, McDonald recently reported in this Newsletter , that she was using smartphones in her high school classroom [7]. There are already a large number of chemistry-related apps available [8] including Chemspider, which is an excellent data base of chemical information [9]. Williams has made a number of presentations about using the Mobile Internet for Chemistry, and many of these are available on Slideshare, including one titled, " Taming The Wild West Of Internet Based Chemistry You Can Help [10] and another on Mobile Chemistry and "Generation App" [11]. Some entire campuses have whole-heartedly made a commitment to mobile technology. For example, Abilene Christian University, a small college in Texas, is entering its fourth academic year of implementing mobile technologies, like iPhones, iPods, and iPads, across the campus, and according to a recent survey, "89 percent of faculty members bring mobile devices to class; 84 percent regularly use the devices in class; and half of faculty report using the devices in every class [12]." Private communications from some of the Chemistry faculty involved in this effort suggest that they are enthusiastic about this change.

Cloud computing does not require commitment to mobile devices but access to the computing cloud does expand the capabilities of mobile computing. Many of the same major corporations are behind this initiative as are behind mobile technologies, Apple, Google, Microsoft, Amazon, etc. Software like Google Docs and Dropbox create opportunities for even undergraduates to learn about manipulation of large data sets [13]. Hey et al have argued that this is an essential skill for science students in the Digital Age [14].

Earlier in this online session, there was considerable discussion of the future of lecture as a teaching method. If mobile learning becomes as widely adopted as expected, all the current methods will probably need some revision. In some cases, like the traditional stand and deliver facts lecture, extensive adjustment will be needed. When students will carry in their pockets the equivalent of a major research library, classroom work can, and should, go beyond focus on individual facts. There will be many different ways to use mobile devices, but at this stage it is critical that these possibilities be explored.

The Clash of the Titans is coming soon to a classroom near you, and, unlike the movie of the same name, it will not be a spectator event; don't bother to bring popcorn. Some of the largest and most innovative companies in this country will be trying to convince you to explore new ways for teaching and learning, and your students are already using their products. It looks like interesting times ahead for chemical education, and I should continue to have plenty to write about, even if the Microsoft-Google battle over search never meets my expectations.

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