



Ph.D. Thesis

Development of new e-Assessment Technologies in Chemistry

**Conducted for the purpose of receiving the academic title
'Doktor der technischen Wissenschaft'**

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Abstract

One of the most important technological developments in the 20th century is the use of computers in many areas of daily life, work, and research. Virtual labs and simulation is a powerful tool to engage students in active learning. The evolution of Information Technology (IT) allows associating real chemical practice laboratories with virtual laboratory sessions. This makes the process of acquiring chemical knowledge a personally scheduled, ubiquitous and continuously accessible process particularly suited also for lifelong education and learning.

Interactive laboratory activities are able to enhance student's understanding of chemical processes and practical skills. Many useful techniques have been developed in this area during the past few years. In this thesis some additional contributions to this research field are presented.

IChemExam is one of the tools of IChemEdu, which is a self assessment area to check knowledge required performing the experiments. Besides the most common answering methods such a multiple choice selections and checks for numeric values, the Vienna group has developed new tools to answer and proof question via input of chemical structures. This research is the extension of the IChemExam and IChemLab, in the field of apparatus assemblage and online assessment (e-Assessment) for it. In brief 'eAT Virtual Chem Lab' (**eAssessment Tool for Virtual Chem Lab**) is tool where examiner can set an exam to check apparatus assembling knowledge and understanding of students by setting an online exam. Apart from assessment tool it is also an e-Learning tool, which can be used for training the students and technicians good laboratory practices.

Zusammenfassung

Die Integration der elektronischen Datenverarbeitung in den Alltag zählt zu den wichtigsten technisch-gesellschaftlichen Errungenschaften des 20. Jahrhunderts. Der Entwicklungsstand heutiger IT (Information Technology) erlaubt es die chemische Arbeit im Laboratorium mit virtueller Laborpraxis zu verknüpfen. Die virtuelle Simulation eines Labors ist daher ein geeignetes Mittel, um Studenten zu eigenständigen Problemlösungen anzuleiten. Den Forderungen nach stetiger fachlicher Weiterbildung entsprechend können, weitgehend an persönliche Umstände angepasst, chemische Kenntnisse erworben werden.

Die interaktive Laborpraxis vermag dem Studenten ein eingehendes Verständnis von chemischen Abläufen und praktischer Laborarbeit zu vermitteln. Diese Dissertation knüpft an dieses - in den letzten Jahren aktives - Forschungsgebiet mit weiterführenden Beiträgen an.

IChemExam ist, als Teil von iChemEdu, zur Selbstüberprüfung der für die Durchführung von Experimenten notwendigen Kenntnisse zuständig entwickelt worden. Neben bekannten Verfahren, die auf multiple-choice-Tests und der Auswertung von numerischen Eingaben beruhen, ist es gelungen, chemische Strukturformeln als Antwortmöglichkeiten zu integrieren. Entsprechend wurden IChemExam und IChemLab mit der Möglichkeit zum virtuellen Apparatezusammenbau und online-assessment (e-Assessment) erweitert. eAT Virtual Chem Lab bietet dem Lehrenden die Möglichkeit, eine online-Überprüfung der studentischen Kenntnisse zu diesen Themenkreisen zusammenzustellen. Weiters ist die Anwendung des Programms auch im Sinne der "good laboratory practice" und der damit verbundenen Fortbildung von Studenten und Laboranten gedacht.

Preface

“If a man will begin with certainties, he shall end in doubts; but if he will be content to begin with doubts, he shall end in certainties.”

- Francis Bacon

More than three years ago, I arrived in Vienna, in a completely different world. But it was a new beginning in science for me. It was the world outside, the stars above us, which has led me to science. The seeds were laid early on by my maternal grandfather, who took me on journeys around the globe, through time and to the stars, almost every evening during my summer vacations. I pay my apologies to him for not being with him when he showed the last twinkling star of his life. The PhD study in Vienna allowed me to follow this new-born interest. ‘Doing’ a PhD is not always easy. Long nights have to be spent for research, often without much sign of progress. Especially ‘writing up’ a thesis can be tough times and what was hoped to be finished in two weeks appears to take for ever. But then, there are also the times of harvest, when results just seem to ‘drop out’ of the computer or when the thesis gets finally printed.

‘Getting’ into the young field of chemo-informatics was an exiting and tough journey. Many people have contributed to this thesis. I would like to take this opportunity and thank my advisor, Prof. Fröhlich who supported me throughout my PhD studies, gave me the freedom essential for research and always pointed out the progress that I had made.

I would also like to extend my gratitude towards Heinz Krebs and Florian Untersteiner for their advice and help on several occasions. I would also like to

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To my parents, who have always supported and motivated me in all of my endeavors. To Jaywant, who showed unwavering faith in me even when I doubted myself the most, and who sat beside me when I was working late nights with patience, grace, and love - all for my sake. I must say he showed me the dream of Ph.D. and always walked along with to reach the destination. Being a computer professional it was difficult task for me to deal with chemistry, Jaywant always attended all my queries at his working desk and at dining table as well.

I also would like to thank ÖAD- Österreichischer Austauschdienst for awarding me scholarship under ÖAD-Stipendium für Angehörige aus Entwicklungsländern to support my PhD at Institute of Applied Synthetic Chemistry, Vienna University of Technology.

At last but not least I dedicate my thesis to my mother, Late Meerabai Kadam, who brought me to this world. At this moment I really miss her a lot for not being with me to celebrate my success any more.

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List of Abbreviations

AACS	Apparatus Assembly connection String
ACD	Advanced Chemistry Development
BB	Bubbler
CAA	Computer Aided (or Assisted) Assessment
CASD	Computer-Assisted Synthesis Design
CASE	Computer-Assisted Structure Elucidation
CBA	Computer Based Assessment
CGI	computer generated images
DA	Distillation Adapter
eAT Virtual Chem Lab	eAssessment Tool for Virtual Chem Lab
HOCS	Higher-order cognitive skills
HTML	Hyper Text Markup Language
IT	Information Technology
JRE	java Runtime Environment
LAN	Local Area Network
LOCS	lower-order cognitive skills
MCQ	Multiple Choice Questions
MOODLE	Modularly Object- Oriented Dynamic Learning Environment
MRQ	Multiple response questions
QSAR	Structure-Property Relationships
RB	round bottom
SEICO	Spherical Environment Integer Code
SELE	Semantic learning
SMILES	Simplified Molecular Input Line Entry System
TUWEL	TU Wien E-Learning
UID	unique identifiers
WWW	world wide web

Chapter 1: Introduction

1.1 Chemoinformatics

Chemoinformatics is the application of informatics methods to solve chemical problems. Although this term was introduced only a few years ago, this field has a long history with its roots going back more than 40 years. Work on chemical structure representation and searching, quantitative structure–activity relationships, chemometrics, molecular modeling as well as computer-assisted structure elucidation and synthesis design was initiated in the 1960s. These different origins have now merged into a discipline of its own that is in full bloom. All areas of chemistry from analytical chemistry to drug design can benefit from chemoinformatics methods. And there are still many challenging chemical problems waiting for solutions through the further development of chemoinformatics [1].

1.1.1 What is chemoinformatics?

Chemoinformatics is the use of information technology to:

- manage chemical information, and
- solve chemical problems

In 1998, Dr. Brown gave his original definition of chemoinformatics as follows [2]

“The use of information technology and management has become a critical part of the drug discovery process. Chemoinformatics is the mixing of

those information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and organization.”

Whereas we see here chemoinformatics focused on drug design, Greg Paris came up with a much broader definition [3]

“Chemoinformatics is a generic term that encompasses the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information.”

Clearly, the transformation of data into information and of information into knowledge is an endeavour needed in any branch of chemistry not only in drug design. We therefore share the view that chemoinformatics methods are needed in all areas of chemistry and adhere to a much broader definition [1]

“Chemoinformatics is the application of informatics methods to solve chemical problems.”

1.1.2 History of chemoinformatics:

The history of chemoinformatics is reviewed in a decade-by-decade manner from the 1940s to the present. The focus is placed on four traditional research areas: chemical database systems, computer-assisted structure elucidation systems, computer-assisted synthesis design systems, and 3D structure builders. Considering the fact that computer technology has been one of the major driving forces of the development of chemoinformatics, each section will start from a

brief description of the new advances in computer technology of each decade. The summary and future prospects are given in the last section [4].

1.1.2.1 Birth of chemoinformatics

In 1946 King et al [5] published an article illustrating the use of IBM's business accounting machines in carrying out the construction of the rotational spectra of asymmetric rotors by the evaluation of mathematical equations for line position and line intensity. This may be the earliest work of application of computer technology in chemistry, and thus, the year 1946 may be regarded as the birth year of chemoinformatics.

1.1.2.2 Named as chemoinformatics

In the middle of the 1990s, there were some arguments about the best name for the newly emerging discipline of computer applications in chemistry. At that time, there were already societies of chemometrics [6]. Two journals had the word chemometrics in their names: Chemometrics and Intelligent Laboratory Systems [7] and Journal of Chemometrics [8]. On the other hand, although there were neither societies of computer chemistry nor journals with the names containing the term "computer chemistry" (The Journal of Computer Chemistry was launched in 2002 in Japan⁴), this term was quite widely used by chemists whose main research was focused on the development of chemical database retrieval systems and chemical expert systems. There were several institutes with the term "computer chemistry" in their names, such as Computer-Chemistry-Centre, [9] Erlangen, Germany. Two books were titled Computer Chemistry. [10, 11]

Therefore, some chemists liked chemometrics, while others preferred computer chemistry for the name of the new discipline. Surprisingly, neither chemometrics nor computer chemistry won the game; instead, both lost to a newcomer chemoinformatics.

1.1.3 Chemoinformatics : Counterpart of Bioinformatics in chemistry

In 1976, the word bioinformatics (or in Dutch “Bioinformatica”) first appeared in the name of a research group called “Bioinformatics Group” at University of Utrecht, The Netherlands. The first paper using the term bioinformatics was published 2 years later by Hogeweg from that group. [12] They defined bioinformatics as “the study of informatic processes in biotic systems”. With the explosion of publicly available genomic information, such as that resulting from the Human Genome Project, [13] in the middle of the 1990s bioinformatics has become very popular not only in the scientific community but also in the general audience as well. This has led to the coining of the counterpart of bioinformatics in chemistry: chemoinformatics. It is generally accepted that the term chemoinformatics was first introduced by Dr. Frank Brown in the Annual Reports of Medicinal Chemistry in 1998.[14] With the publication of Professor Johann Gasteiger’s Handbook of Chemoinformatics in 2003,[15] chemoinformatics has now become the de facto standard for applications of computer and informatics technology in chemistry. The only thing we should be aware of is that a shorter form of it, cheminformatics, has also been widely used.

1.1.4 Pioneer of Chemoinformatics:

Professor Johann Gasteiger is a pioneer in the field of chemoinformatics. He has played an important role in the formation of the discipline through his significant contributions to several of the important research areas in chemoinformatics in the past 30 years: computer-assisted synthesis design (EROS, WODCA), reaction simulation and prediction (EROS), reaction classification (CORAL, HORACE [16, 17]), 3D structure building (CORINA), simulation of spectra (TeleSpec project [18]), reaction database development (ChemInform), applications of neural networks, and genetic algorithms in chemistry. Professor Gasteiger has also made important contributions to the areas of molecular modeling and drug design. For example, besides the well-known Gasteiger Charges, his group has also developed methods for the treatment of conformational flexibility of molecules (ROTATE and GAMMA) and approaches for the discovery of lead structure, the optimization of drugs, the definition of similarity and diversity of combinatorial libraries,[19] the establishment of structure-activity relationships,[20] virtual screening,[21] data mining,[22] chemotaxonomy,[23] prediction of the metlab- CHEMOINFORMATICS: PAST, PRESENT, AND FUTURE J. Chem. Inf. Model., Vol. 46, No. 6, 2006 2247 olism of drugs,[24] and modeling of biochemical pathways.[25] These methods are based on structure coding techniques (SURFACE, AUTOCORR, ARC) developed in his group.²⁵⁷ Professor Gasteiger is a coeditor of the prestigious Encyclopaedia of Computational Chemistry,[26] and the editor of the authoritative Handbook of Chemoinformatics.¹¹ In addition, he has edited four volumes in the

Software Development in Chemistry series: #1 (1987), #2 (1988), #4 (1990), and #10 (1996). He is also the author of several influential books, such as *Neural Networks in Chemistry and Drug Design* [27] and *Chemoinformatics - A Textbook*. [28] Professor Gasteiger is also a cofounder of the well-known Computer-Chemistry-Centre at Erlangen, Germany. [9] Last but not least, he has been a mentor for many chemoinformatics specialists in the chemical and pharmaceutical industry and in academe. Professor Gasteiger is one of the leading chemoinformatics scientists. His contributions to chemoinformatics as well as other related fields have been widely recognized. He is the recipient of the Gmelin-Beilstein Medal of GDCh (1997), the Herman Skolnik Award of the ACS Division of Chemical Information (1997), the Mike Lynch Award of the Chemical Structure Association Trust (2005), and most recently, the ACS Award for Computers in Chemical & Pharmaceutical Research (2006). [18]

1.1.5 Future prospects of Chemoinformatics

After its development over the last half-century, a variety of chemoinformatics methods has been established and become “must have tools”, such as chemical structure drawing programs and database searching systems. Chemoinformatics has emerged as a new discipline, as indicated by Gasteiger’s *Handbook of Chemoinformatics*. Besides the traditional mainstream areas of chemoinformatics, such as database systems, computer-assisted structure elucidation systems, computer-assisted synthesis design systems, and quantitative structure-activity relationship (QSAR), several new research areas of chemoinformatics have appeared recently, such as *in silico* library design, virtual

screening, docking, prediction of ADME and toxicity, and so on. The scope of this rapidly developing field will certainly continue to expand [4].

Because of the specific focus of this contribution and also the limitations of space, it should be noticed that many of the new chemoinformatics systems have been built on the base of the key technologies (such as chemical structure representation, substructure and maximum common substructure searching,[29] etc.) invented during the development of “traditional” chemoinformatics systems [30].

At the end of the 20th century, almost all the major foundations and theories of chemistry had been well understood and established. Chemistry has already evolved from largely a study of the elements to a study of molecules to currently a study of molecular interactions, especially those involving biomacromolecules. This offers an excellent opportunity for chemoinformatics to grow in this new direction [4].

It can be expected that compuinformatic chemistry will become one of the most active research frontiers in chemistry in the future. It should also be noticed that, in the recent years, the classic two approaches to scientific research, theoretical/ analytical and experimental/observational approaches, have been extended to *in silico* modeling and simulation to explore new possibilities and to achieve new precision. The emerging *compuinformatic science* (including compuinformatic chemistry, compuinformatic biology,[31] etc.), whose major goals are to develop mathematical models, computational and information technologies, and computer programs and apply these programs to studying and

solving scientific and engineering problems, will become a key technology field of the 21st century. It will bring a new generation of much more powerful yet intelligent modeling and simulation methods and other revolutionary technologies, allowing scientists to study real-life complex phenomena and processes that are experimentally difficult, if not impossible, to characterize and to solve.

The development of the new discipline of chemoinformatics was only possible because quite a few scientists in different areas of chemistry were visionaries who realized the great potential of computer technology as well as mathematics and informatics methods for solving chemical problems. They ventured into unexplored areas and came up with novel solutions. [32] Chemoinformatics, through its development in the past half a century, has reached in the present wide acceptance, and will have a bright future! [4]

1.1.6 Chemoinformatics - A Mature Discipline of Its Own

1.1.6.1 A New Discipline

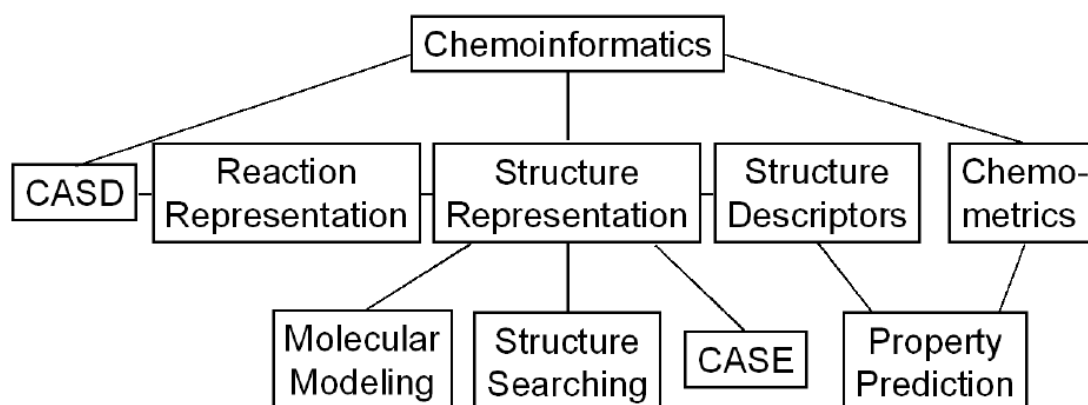


Figure 1: The Various Areas of activities in chemoinformatics

The various fields have grown from humble beginnings 40 years ago to areas of intensive activities. On top of that it has been realized that these areas share a large number of common problems, rely on highly related data, and work with similar methods. Thus, these different areas have merged to a discipline of its own: *Chemoinformatics* [33].

Computer-Assisted Synthesis Design (CASD)

The design of a synthesis for an organic compound needs a lot of knowledge about chemical reactions and on chemical reactivity. Many decisions have to be made between various alternatives as to how to assemble the building blocks of a molecule and which reactions to choose. Therefore, computer-assisted synthesis design (CASD) was seen as a highly interesting challenge and as a field for applying artificial intelligence techniques. In 1969 Corey and Wipke presented their seminal work on the first steps in the development of a synthesis design system. [34] Nearly simultaneously several other groups such as Ugi and coworkers, [35] Hendrickson [36], and Gelernter [37] reported on their work on CASD systems. Later also at Toyohashi work on a CASD system was initiated. [38]

Quantitative Structure Activity/ Property Relationship(QSAR/QSPR)

Building on work by Hammett and Taft in the fifties, Hansch and Fujita showed in 1964 that the influence of substituents on biological activity data can be quantified. [39] In the last 40 years, an enormous amount of work on relating descriptors derived from molecular structures with a variety of physical, chemical, or biological data has appeared. These studies have established Quantitative

Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) as fields of their own, with their own journals, societies, [40] and conferences.

Chemical Structure Representation

In the early sixties, various forms of machine readable chemical structure representations were explored as a basis for building databases of chemical structures and reactions. [41] Eventually, connection tables that represent molecules by lists of the atoms and of the bonds in a molecule gained universal acceptance. Connection tables were also used for the Chemical Abstracts Registry System which appeared in the second half of the sixties. [42]

Chemometrics

Initially, the quantitative analysis of chemical data relied exclusively on multi linear regression analysis. However, it was soon recognized in the late sixties that the diversity and complexity of chemical data need a wide range of different and more powerful data analysis methods. Pattern recognition methods were introduced in the seventies to analyze chemical data. In the nineties, artificial neural networks gained prominence for analyzing chemical data. [43] The growing of this area led to the establishment of chemometrics as a discipline of its own with its own society, [44] journals, and scientific meetings.

Molecular Modeling

In the late sixties, R. Langridge and coworkers developed methods for visualizing 3D molecular models on the screens of Cathode Ray Tubes. At the same time, G. Marshall started visualizing protein structure on graphic screens. The progress

in hardware and software technology, particularly as concerns graphics screens and graphics cards, has led to highly sophisticated systems for the visualization of complex molecular structures in great detail. Programs for 3D structure generation, for protein modeling, and for molecular dynamics calculations have made molecular modeling a widely used technique.

Structure Searching

A connection table is essentially a representation of the molecular graph. Therefore, for storing a unique representation of a molecule and for allowing its retrieval, the graph isomorphism problem had to be solved to define from a set of potential representations of a molecule a single one as the unique one. The first solution was the Morgan algorithm for numbering the atoms of a molecule in a unique and unambiguous manner. [45] This provided the basis for full structure searching. Then, methods were developed for substructure searching, for similarity searching, and for 3D structure searching.

Computer-Assisted Structure Elucidation (CASE)

The elucidation of the structure of a chemical compound, be it a reaction product or a compound isolated as a natural product, is one of the fundamental tasks of a chemist. Structure elucidation has to consider a wide variety of different types of information mostly from various spectroscopic methods, and has to consider many structure alternatives. Thus, it is an ambitious and demanding task. It is therefore not surprising that chemists and computer scientists had taken up the challenge and had started in the 1960s to develop systems for computer-

assisted structure elucidation (CASE) as a field of exercise for artificial intelligence techniques. The DENDRAL project, initiated in 1964 at Stanford University gained widespread interest. [46] Other approaches to computer-assisted structure elucidation were initiated in the late sixties by Sasaki at Toyohashi University of Technology [47] and by Munk at the University of Arizona. [48]

1.1.6.2 Overview of Topics

The following gives an overview of chemoinformatics, emphasizing the problems and solutions - common to the various more specialized subfields. These topics also constitute the various chapters of the Textbook and of the Handbook of Chemoinformatics. [49, 50]

Representation of Chemical Compounds

Whole range of methods for the computer representation of chemical compounds and structures has been developed: linear codes, connection tables, matrices. Special methods had to be devised to uniquely represent a chemical structure, to perceive features such as rings and aromaticity, and to treat stereochemistry, 3D structures, or molecular surfaces.

Representation of Chemical Reactions

Chemical reactions are represented by the starting materials and products as well as by the reaction conditions. On top of that, one also has to indicate the reaction site, the bonds broken and made in a chemical reaction. Furthermore, the stereochemistry of reactions has to be handled.

Data in Chemistry

Much of our chemical knowledge has been derived from data. Chemistry offers a rich range of data on physical, chemical, and biological properties: binary data for classification, real data for modeling, and spectral data having a high information density. These data have to be brought into a form amenable to easy exchange of information and to data analysis.

Datasources and Databases

The enormous amount of data in chemistry has led quite early on to the development of databases to store and disseminate these data in electronic form. Databases have been developed for chemical literature, for chemical compounds, for 3D structures, for reactions, for spectra, etc. The internet is increasingly used to distribute data and information in chemistry.

Structure Search Methods

In order to retrieve data and information from databases, access has to be provided to chemical structure information. Methods have been developed for full structure, for substructure, and for similarity searching.

Methods for Calculating Physical and Chemical Data

A variety of physical and chemical data of compounds can directly be calculated by a range of methods. Foremost are quantum mechanical calculations of various degrees of sophistication. However, simple methods such as additive schemes can also be used to estimate a variety of data with reasonable accuracy.

Calculation of Structure Descriptors

In most cases, however, physical, chemical, or biological properties cannot be directly calculated from the structure of a compound. In this situation, an indirect approach has to be taken by, first, representing the structure of the compound by structure descriptors, and, then, to establish a relationship between the structure descriptors and the property by analyzing a series of pairs of structure descriptors and associated properties by inductive learning methods. A variety of structure descriptors has been developed encoding 1D, 2D, or 3D structure information or molecular surface properties.

Data Analysis Methods

A variety of methods for learning from data, of inductive learning methods is being used in chemistry: statistics, pattern recognition methods, artificial neural networks, genetic algorithms. These methods can be classified into unsupervised and supervised learning methods and are used for classification or quantitative modeling.

1.1.7 Chemoinformatics and the Web

An increasing amount of chemistry information is available on the internet and intranets, often in forms other than traditional, searchable databases (electronic journal articles, web pages, online documents, blogs, RSS feeds and so on). In addition to these forms of data sources, current models of usage of chemical information also include Internet based access in addition to traditional forms such as local Page 7 desktop clients.

One of the fundamental problems that face the chemoinformatics community is the fact that though there are many novel algorithms being developed as well as new data sources being created; they more or less exist as islands. That is, the implementation of these algorithms and the databases containing new data, require that one visit a web page and either download a collection of source files or enter data into a web form which then returns results in the form of an HTML page or in some cases an email. Though this is certainly better than not being able to access these resources at all, such modes of access create bottlenecks for interoperability.

This problem is being tackled in the web community in general by the use of *web services* which allow computational procedures to be accessed through standard web protocols, and the *semantic web* which promises to help interoperability of services and information through the use of standardized markup and ontology languages. We believe that this approach is highly appropriate for chemoinformatics. The chemoinformatics community has developed a number of algorithms for a variety of problems such as structure searching, descriptor calculation, similarity and so on. Many of these are bound to a specific web page or require one to download a program. It would be better if all these algorithms were accessible in a uniform manner (at least those algorithms that perform similar functions) without binding a user to a specific web page interface. Additionally, the development of workflow tools such as Pipeline Pilot [51] and Knime [52] has led to a significant increase in the usability of chemoinformatics tools when handling large datasets. In such a setup, having to

go outside the environment to generate data which must then be imported back into the environment severely hampers the whole idea of a workflow environment. Now, it is certainly possible that a given algorithm might be implemented in a specific workflow tool. However this requires that the developer of the algorithm have access to the workflow program and be familiar with it. Furthermore, this would require reimplementation for each new workflow tool. Clearly, a standardized approach to accessing new algorithms and data sources would easily allow arbitrary workflow tools to include them. Finally, access to a wide variety of algorithms and data sources in a standardized and distributed manner will lead to novel uses of such resources that may not have been considered by their designers. For example, structure searching algorithms have a well defined function, but when coupled to new data sources (such as journal articles or blogs), one can envision new resources that go beyond the traditional view of searching structure databases for similar compounds. The explosion of innovation around the Google Maps API should serve as an inspiration as to what is possible when computational capabilities are made highly accessible. The vision for chemoinformatics described above depends on the presence of an infrastructure. At this point, such an infrastructure is not widely available, though many of the underlying technologies have been available for some time. In the following sections we describe approaches taken by the CICC to achieve the vision of a distributed collection of chemoinformatics resources that cover both algorithms and data sources. [53]

1.1.8 Applications

The range of applications of chemoinformatics is rich indeed; any field of chemistry can profit from its methods. The following lists different areas of chemistry and indicates some typical applications of chemoinformatics.

1.1.8.1.1 Drug Design and Discovery

- The computer is used to analyze the interactions between the drug and the receptor site and design molecules with an optimal fit.
- Once targets are developed, libraries of compounds are screened for activity with one or more relevant assays using High Throughput screening.
- identification of new lead structures
- optimization of lead structures
- establishment of quantitative structure-activity relationships
- comparison of chemical libraries
- definition and analysis of structural diversity
- planning of chemical libraries
- analysis of high-throughput data
- docking of a ligand into a receptor
- de novo design of ligands
- modeling of ADME-Tox properties
- prediction of the metabolism of xenobiotics
- analysis of biochemical pathways

1.1.8.1.2 Chemical Information

- storage and retrieval of chemical structures and associated data to manage the flood of data
- dissemination of data on the internet
- cross-linking of data to information

1.1.8.1.3 All fields of Chemistry

- prediction of the physical, chemical, or biological properties of compounds

1.1.8.1.4 Analytical Chemistry

- analysis of data from analytical chemistry to make predictions on the quality, origin, and age of the investigated objects
- elucidation of the structure of a compound based on spectroscopic data

1.1.8.1.5 Organic Chemistry

- prediction of the course and products of organic reactions
- design of organic syntheses

1.1.8.1.6 Theoretical Chemistry

- Solving of molecular mechanics and dynamics
- Ab initio calculation
- Semi-Empirical method of solving equation

1.2 E-Learning

1.2.1 Definition:

Learning using electronic means: the acquisition of knowledge and skill using electronic technologies such as computer- and Internet-based courseware and local and wide area networks. [54]

This definition addresses:

(The what) Training delivered in digital form, (The how) content and instructional methods to help learn the content, and (The why) to improve organizational performance by building job-relevant knowledge and skills in workers.

1.2.2 What is e-Learning?

The current trend is 'e' with everything: e-commerce, e-science, and e-learning. Since this prefix is associated with the advent of wide-scale Internet usage, it makes sense to define e-learning as being any form of education which uses the Internet.

e-Learning is an umbrella term that describes learning done at a computer, usually connected to a network, giving us the opportunity to learn almost anytime, anywhere [55].

e-Learning is not unlike any other form of education - and it is widely accepted that e-Learning can be as rich and as valuable as the classroom experience or even more so. With its unique features e-Learning is an experience that leads to comprehension and mastery of new skills and knowledge, just like

its traditional counterpart.

Instructional Design for e-Learning has been perfected and refined over many years using established teaching principles, with many benefits to students. As a result colleges, universities, businesses, and organizations worldwide now offer their students fully accredited online degree, vocational, and continuing education programs in abundance.

e-Learning refers to learning that is delivered or enabled via electronic technology. It encompasses learning delivered via a range of technologies such as the internet, television, videotape, intelligent tutoring systems, and computer-based training.

e-Learning is a subset of the larger worlds of both “information technology” and “education and training”. It can be valuable when used as a part of a well-planned and properly supported education and training environment, but e-learning is not a magic bullet that neither replaces nor renders obsolete existing pedagogical theories and approaches. Many learning and technology professionals believe that e-learning will have “arrived” when we stop referring to it by a separate name and begin considering it as an integral part of a complete learning environment.

1.2.3 The whole Picture of E-learning

e-Learning projects fail because the characteristics that need to be addressed aren't...and other characteristics are given too much emphasis. e-Learning itself isn't really a unique field. It's a combination/extension of many other existing

fields. As such, what happens in technology/learning theory/web design/network analysis, etc. impacts and shapes e-learning?

Successful e-learning requires a "whole picture" approach. [56] The diagram below lists the "critical success factors" for e-learning within an organization:

- Starting
- Doing
- Enabling
- Evaluating
- Managing
- Resources



Figure 2: Areas of activities

1.2.3.1 Starting

e-Learning can be initiated program wide in a corporation or institution...or at an

individual level with a trainer or instructor. At the enterprise level, the primary needs are determining the value and impact of elearning – strategic assessment, viability and readiness assessment. Categories include: overview (benefits/negatives, what is elearning), beginning (converting to online, integrating technology with teaching), and readiness (organizational, learner, and instructor).

1.2.3.2 Enabling

The Enabling stage refers to the teaching and learning technologies used to make any aspect of the learning design, development, and delivery process more efficient. Wikis, blogs, authoring tools, collaboration/groupware tools, social software, are considerations at this level. Technology, in the context of elearning, should enable and provide support for the learning (and resource development) components of the whole picture. Technology is used primarily to *increase the effectiveness* of learning...or to *increase access to* learning. Various groupware tools allow people to connect with each other in spite of geographical distances. Authoring tools improve the effectiveness of learning by providing engaging, interactive content.

1.2.3.3 Doing

The third stage of elearning (and where a company spends the bulk of its time after successfully initiating a program) is focused on Doing elearning - designing, developing, delivering, and assessing the learning. At this level, the content is being created, delivered and learning is being assessed. An intense focus on the

learner is critical for success. Components of this stage include instructional design, content management, usability, accessibility, learning objects, selection of media, assessment, adoption/promotion, and plagiarism/ethics.

1.2.3.4 Evaluating

The next stage is evaluating. Evaluation, in this model, refers to the actual elearning program, not the learners. The elearning initiative is evaluated against the standards defined as important during strategic planning stage. Most corporations will use a variety of techniques (analytics) in evaluating the success of a program. It might be compliance training, ROI, improved business performance, or any other predefined target.

1.2.3.5 Managing

The Managing stage represents the challenges in managing, organizing, and sustaining an elearning initiative. For example, at this level, standards might be a consideration - Which standards to pursue? Or finding a way to stay current on developments in the field. Other categories include: change management, knowledge management, communities, and copyright.

1.2.3.6 Resources

The final category of the elearning model is focused on Resources. Developing technologies may impact elearning, and awareness of these is important. As well, research and resource sites are valuable in exploring the full depth of learning. These are also represented in this stage of the model. Resources are divided into

two areas: technology and general. This aspect of the model is largely used for reference.

1.2.3.7 Final thoughts

The whole picture view of elearning is dynamic - it changes in response to trends in technology and practices. This model will continue to evolve and expand.

1.2.4 Features and benefits of e-Learning

"Good teaching is good teaching, no matter how it's done."

The old adage still rings true, and e-Learning brings with it new dimensions in education. Some of the unique features of e-Learning are listed below.

1.2.4.1 Features of e-Learning

- Learning is self-paced and gives students a chance to speed up or slow down as necessary
- Learning is self-directed, allowing students to choose content and tools appropriate to their differing interests, needs, and skill levels
- Accommodates multiple learning styles using a variety of delivery methods geared to different learners; more effective for certain learners
- Designed around the learner
- Geographical barriers are eliminated, opening up broader education options
- 24/7 accessibility makes scheduling easy and allows a greater number of people to attend classes
- On-demand access means learning can happen precisely when needed

- Travel time and associated costs (parking, fuel, vehicle maintenance) are reduced or eliminated
- Overall student costs are frequently less (tuition, residence, food, child care)
- Potentially lower costs for companies needing training, and for the providers
- Fosters greater student interaction and collaboration
- Fosters greater student/instructor contact
- Enhances computer and Internet skills
- Draws upon hundreds of years of established pedagogical principles
- Has the attention of every major university in the world, most with their own online degrees, certificates, and individual courses

1.2.4.2 Benefits of e-Learning

There are many significant advantages for the student who learns online. Here are just a few to consider:

1.2.4.2.1 Convenience and Portability

- Courses are accessible on your schedule
- Online learning does not require physical attendance
- Learning is self-paced (not too slow, not too fast)
- You're unbound by time - courses are available 24/7
- You're unbound by place - study at home, work, or on the road
- Read materials online or download them for reading later

1.2.4.2.2 Cost and Selection

- Choose from a wide range of courses to meet your needs
- Degree, Vocational, and Certificate programs
- Continuing Education
- Individual courses
- Wide range of prices to fit your budget
- Go back to school to get a degree, learn a new skill, learn a new craft, or just have fun!
- From art to zoology you can do it all online in a price range to fit your budget.

1.2.4.2.3 Flexibility

- Online learning accommodates your preferences and needs - it's student-centered
- Choose instructor-led or self-study courses
- Skip over material you already know and focus on topics you'd like to learn
- Use the tools best suited to your learning styles

1.2.4.2.4 Higher Retention

- Online learning will draw you to topics you like and enjoy. Studies show that because of this and the variety of delivery methods used to reach different types of learners, retention is frequently better than in a traditional classroom.

1.2.4.2.5 Greater Collaboration

- Technology tools make collaboration among students much easier. Since many projects involve collaborative learning, the online environment is far easier (and often more comfortable) to work in since learners don't have to be face-to-face.

1.2.4.2.6 Global Opportunities

- The global learning community is at your fingertips with online learning. The technologies used give online instructional designers the ability to build in tools that take you to resources you may never see in a traditional classroom.

1.2.4.3 e-Learning Trends

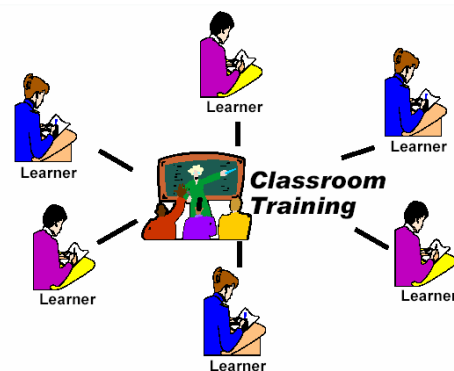
"The next big killer application for the Internet is going to be education.

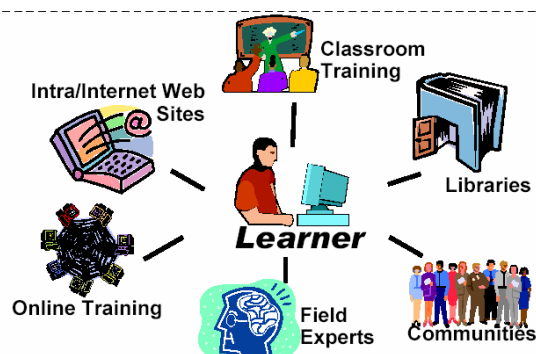
Education over the Internet is going to be so big it is going to make e-mail look like a rounding error."

John Chambers

CEO Cisco systems

Old Paradigm
The instructor is viewed as the center of all knowledge. The classroom is seen as the place where all knowledge disseminates. And the course is viewed as the preferred format for learning.





New Paradigm

The employee/learner is viewed as a knowledge seeker, with constantly changing learning needs and time frames. The web becomes a vehicle for accessing a total knowledge architecture, with information provided in a variety of formats.

Figure 3: Old and New Paradigm

Learning in Chemistry

Little of the new research directions and the increased understanding of the learning process have found their way into the contemporary chemistry classroom or laboratory [57 17]. Chemistry education has, however, much to gain from research. The qualitative researchers of learning distillation in a chemistry laboratory course point out that the traditional curriculum, with its combination of lecture courses and detailed successful laboratory prescriptions, is not succeeding in achieving the ultimate goal at the university level, the students' own conscious thinking [58 18]. The challenges for chemistry education research are a complex interplay between the global perspective of the process of learning and a logical perspective of the content. The researchers must be familiar with the field of cognitive science as well as chemistry. Communication of research results should include enough information to enable an understanding of

chemists, whose training and education have been based on the behaviourist perspective. [59 19, 60 20]

From the perspective of socio-cultural learning comprehension, teaching chemistry has to be seen as the socialization of students into a community of practitioners, chemists, and as making chemistry meaningful within a student's cultural milieu. [61, 21] Because chemistry is an experimental science the laboratory should be a place for practising the ways of a chemist, and laboratory activities should be an essential part of the curriculum. Laboratory experiences have been purported to promote core scientific educational goals: comprehension of scientific concepts; the development of scientific practical skills and problem-solving abilities; and interest and motivation. According to recent studies, the 'cookbook' chemistry in laboratory classrooms doesn't promote the development of higher-order thinking processes and doesn't motivate students to choose the next courses. [62 22] How can students be engaged in both chemistry theory and practise, in conceptual development and in acquiring laboratory skills? Are authentic investigations a meaningful way enabling to compare and discuss gathered data within the socio-cultural contexts of chemistry? [63 23] What about new learning environments [64 24– 66 26] using ICT? Are these environments engaging students in an active learning process of chemistry from their own starting points? Changing realities requires an organisational openness, including the teacher's predisposition for trying new instructional innovations [67 27].

Recent studies have expressed many ways in which laboratory activities can

be implicated to meaningful learning in chemistry, [68 28– 75 35] putting more responsibility for learning on the learner, and giving fewer specific directions. The new perspective of the learning process can also be transferred to the teaching field of computer-aided chemistry [76 36], which is currently called e-learning. In the empirical part of the present study, the realization of the new ideas of laboratory learning are examined first as a learner's personal experience in authentic laboratories with the tutelage of experts and second as the quality of conceptual learning tutored in a network environment during the introductory chemistry laboratory course. The nature of this research caters to individual needs and highlights individual differences in motivation and conceptual understanding, which are deemed significant in socio-cultural learning, and specifically in chemistry learning as well [77 37].

The present study has used the five-level SOLO Taxonomy in the analysis of learning quality, and thus also in the analysis of the effectiveness of the changes in the learning process. The subject of chemistry seems complex to a novice learner because there are 15 many concepts that can be observed at the macroscopic level in the laboratory, but can only be explained at the particulate, microscopic level and described at symbolic levels [78 38]. When practices are changed the essence of evaluation is the making of judgements: does this practice facilitate learning? Has this attempt at improving been effective? Many teaching models lack effectiveness in the transmission of concepts. E-learning has for example been successfully used in chemistry laboratory experiments to facilitate students' conceptual understanding by simulation models, [79 39] and learning objectives have been evaluated by the four levels of learning [76 36].

1.2.5 Learning environment of chemistry

The traditional lecturing in chemistry may be compatible for some low-order thinking skills, but incompatible with most high-order cognitive skills. [80 147] In school, the chemistry information and skills normally learned are separate knowledge structures and do not spontaneously transfer into a new situation where the knowledge is applied. The skills required by the information society, problem solving and decision making, are often separated from the relevant content as well as objects of thought and action.

1.2.5.1 Laboratory class environment

The abstract theory contents of chemistry have been discussed in education problems: teaching contents that have been reduced and eliminated. Changing the level of difficulty has been criticised by the higher level of education and by students who seek challenges. [81 149, 82 150] The emphasising of content in the teaching and planning of science education doesn't consider the process of learning and the development of the natural research skills of the learner. Higher order thinking skills, process and research skills are more functional for learners than individual knowledge proceeding from the explosion in the growth of information. [83 151– 86 154] Developing process and research skills are needed: First, more well-built learning environments than traditional classrooms; second, the ideas of essential theory contents; third, active practical and cognitive working individually and socially.

Chemistry has been studied and learnt by experiments in nature and in

laboratories. Mechanical and imitative activities have not, however, necessarily resulted in learning. [87 155] Experiments are significant when the type of activity has been selected carefully and the meaningfulness of the task has been well internalized. [88 156, 89 157] Then the empiricism is the part of the analysed wholeness of the chemistry domain and a learner will be motivated by the task on the basis of his /her earlier cognitive structures of chemistry. But is laboratory work in school education effective? Have the work content and the laboratory skills of goals been selected usefully? According to research results, motivation and the ability to get through courses have been increased even at the university level by connecting theory with practice, for example, in the teaching of analytical chemistry to agronomists: samples to be analysed related to agronomy from the substrate of plants [90 158]. Those who are applying the contents of chemistry do not perceive abstract information as necessary unless it has been embedded into applications of their own domain. Even when the work of a school laboratory tries to mirror the work of a natural scientist, for a learner it is most important content is to help him or her understand the concepts of natural science. Do we still teach the techniques that have long since been automated in the world outside of school or have become meaningless in some other way? Sufficiently strong connections to scientific research motivate students, provide an illustration of the nature of science and collaborative learning, develop communication skills, dissolve the boundaries between disciplines and dismantle the barriers between the real world and school. Actual scientific research, from planning to success or failure, with all its phases of imagination, creativity, techniques, persistence, collaboration, disappointment and difficulty must become familiar as early as

comprehensive school. [91 159] By gradually increasing the openness of a laboratory task, the learner gets a more realistic picture of the nature of science and also ends up needing to use common, shared information in the solving of a problem.

1.2.5.2 Authentic environment

Systems' thinking in the contemplation of a learning situation considers holistically the cognitive structures of culture in the learner's memory and the culture situation outside the learner. Learning is like the other functions of a human tuned into the time, place and situation where it occurs. One goal of a cognitive model in education development is to create a dynamic system which breaks the solitude of classrooms and gives a basis for the adaptation of a changing situation. One promising aspect is authentic learning in which the goals of learning are equal, both thinking and communication and contents and skills. [92 165] Authentic tasks with the most possible comprehensive contexts of a learning subject simulate the real world and facilitate learning. [93 166, 94 167] The study findings indicate that students develop higher-order process skills through non-traditional laboratory experiences that provided the students with freedom to perform experiments of personal relevance in authentic contexts. [95 168]

In classrooms, knowledge is chiefly characteristic symbolic knowledge. However, the majority of a skilled employee's knowledge is tacit, implicit and mute. Alongside this, strategic knowledge, learning – and problem solving strategies, ought to be the goals of learning. The active accomplishment of an

analysis problem drawn from an authentic environment, with the aid of an expert, provides an opportunity to experience the existence of such knowledge and to apply the domain subjects. The complex knowledge learnt in a real world situation shall be anchored comprehensively into cognitive structures and doesn't leave inert: it shall be applied in practice.

1.2.5.3 E-Learning environment

- E-learning is based on reliable technology, but is pedagogically oriented
- E-learning is a social process and should facilitate interaction and collaboration between people
- E-learning implies organisational change and teacher/tutor training.

Technologies give indirect ways for an instructor to awaken a learner's active cognitive working: asking, explaining, comparing, outlining, analysing etc. At the same time, by using interesting internet links, videos and repetition materials a learner can take into account his/her own pre-existing knowledge, skills, beliefs, and concepts that significantly influence what he/she notices about the environment and how he/she organises and interprets it. This, in turn, affects his/her learning with understanding: the abilities to remember, reason, solve problems, and acquire new knowledge [96 59, 97 61]. Besides authentic working tasks for learners by e-learning technology, it is possible to create connections to experts and to the authentic tasks of society. First in the cognitive perspective the aim is to create processes and structures that are assumed to function at the level of individuals. Second in the situate perspective the aim is to focus at the level of interactive systems that include individuals as participants, interacting

with each other and with materials and representational systems. [98 9, 99 102]

Via synergy it may be possible to affect the learner's will and the desire to commit one's self to an active learning process.

An e-learning environment empowers the learner in every situation: at school, at university, at work, at home. The new technology diversifies and gives new possibilities to modify learning environments similar to authentic environments, too. The education organisations of Finland have, at every level, made their own Knowledge Society Strategy and renew it every few years. The vision by 2005 made extensive use of the first-rate action practices of networked teaching and research in universities [100 174, 101 175] The e-Learning Initiative taken by the European Commission in Brussels has led to The e-Learning Action Plan [102 176] and the allocation of funding for several projects, an action to boost the change from traditional education to systematic application of ICT for the provision of flexible learning and competence building- designing tomorrow's education in Finland also. The background behind the change in higher education was the signing of the Declaration in Bologna in 1999 on establishing the European Area of Higher Education by 2010. The new learning environments of chemistry may be characterized by the aims of the virtual university: [103 177]

- Up-to-date (reflectivity, velocity)
- Good achievability (openness, flexibility)
- Good productivity (effectiveness, competency)
- High quality (research, teaching)

The current learning materials placed into Internet don't resourcefully

facilitate a self-regulating learner into the possession of chemistry knowledge and skills. To increase effectiveness, active experiments and studies of environments with new kinds of contents are needed, taking into consideration the characteristic, macro and micro levels and also the symbolic language of the chemistry domain.

Chemists traditionally were overwhelmed by the amount of chemistry data and research information published and the lack of coherent access to on-line data. However, the recent linking of all the computers of the world into a vast global information system, "the internet", in particular through the medium of the World Wide Web, has brought information easily to the chemist's desktop. Using the World Wide Web access as a tool, information is presented in a user friendly manner. Documents are presented containing not just text, but also images, animations, movies, sounds, databases, and most recently "hyperactive" molecules and virtual reality chemical information. In effect on-line multimedia. Using electronic forms and questionnaires the progress of students can be monitored and the teaching material tailored to their needs.

1.2.6 E-Learning Tools

Typical tools for e-learning include web-browsers, computer-based assessment, chat rooms, e-mail, whiteboards, groupware, video conferencing, web-cameras, portals, web-pages, online library catalogues, simulations and micro worlds. The ubiquity of web-browsers has led to many of these tools being made available via a web-page, but many are applications that were Internet applications before the advent of the World-Wide-Web (WWW).

Polychem

Polychem is a comprehensive interactive multimedia chemistry tutorial and simulation tool that helps teachers and students by providing literally hundreds of hours of student activity. The software is not like those programs that provide a nice but short demonstration on a single topic. The full program occupies 500MB on CD, there are hundreds of screens.

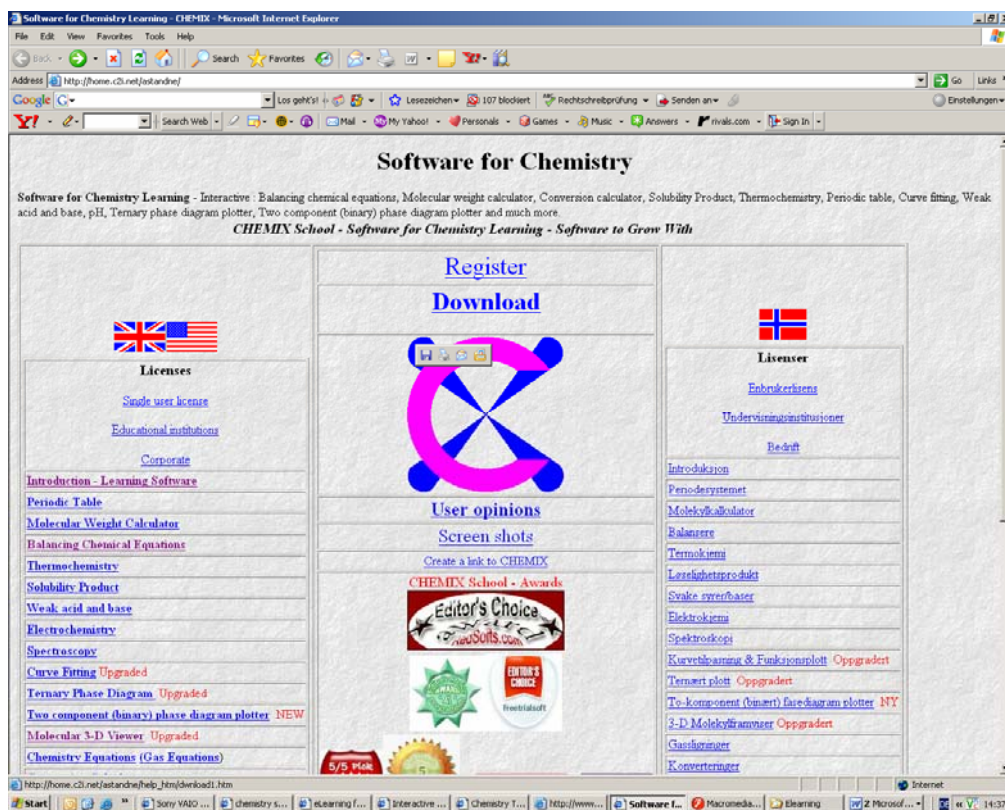


The software contains literally dozens of topics, simulations, videos and activities at senior high school/ college level provided on a CD that is playable on both PC and Mac formats. The software has been developed over the past ten years and has been the subject of a number of research studies. These have enabled the software to develop, and determined the ways that it can be used to best

advantage by students and teachers [104].

Chemix

CHEMIX is an interactive educational software tool developed by a chemist (and teacher) for students, teachers and chemists for help and assistance in study/work. As a stand-alone product it covers a wide range of topics in the area of chemistry.



By the property of interactivity CHEMIX will instantaneously respond to inputs. As an educational tool it will at help increasing the frequency of the repeated process - trial and error - the most common way of learning.

A popular place for using CHEMIX is in the laboratory, where it functions as a standard calculation tool. This is a place where time consuming and often

repeated manual calculations with advantage can be replaced by a help-tool in which performs efficient and secure calculations.

In the classroom CHEMIX is useful for students who after learning to do problems (in which also are included) by hand, can use CHEMIX to help verify their results. It can even be used for correcting erroneous calculations and answers in which often are found in the literature.

The problems/lessons supplied with this software, are intended and levelled for the first-year university level; many of the lessons are also suitable for high school courses.

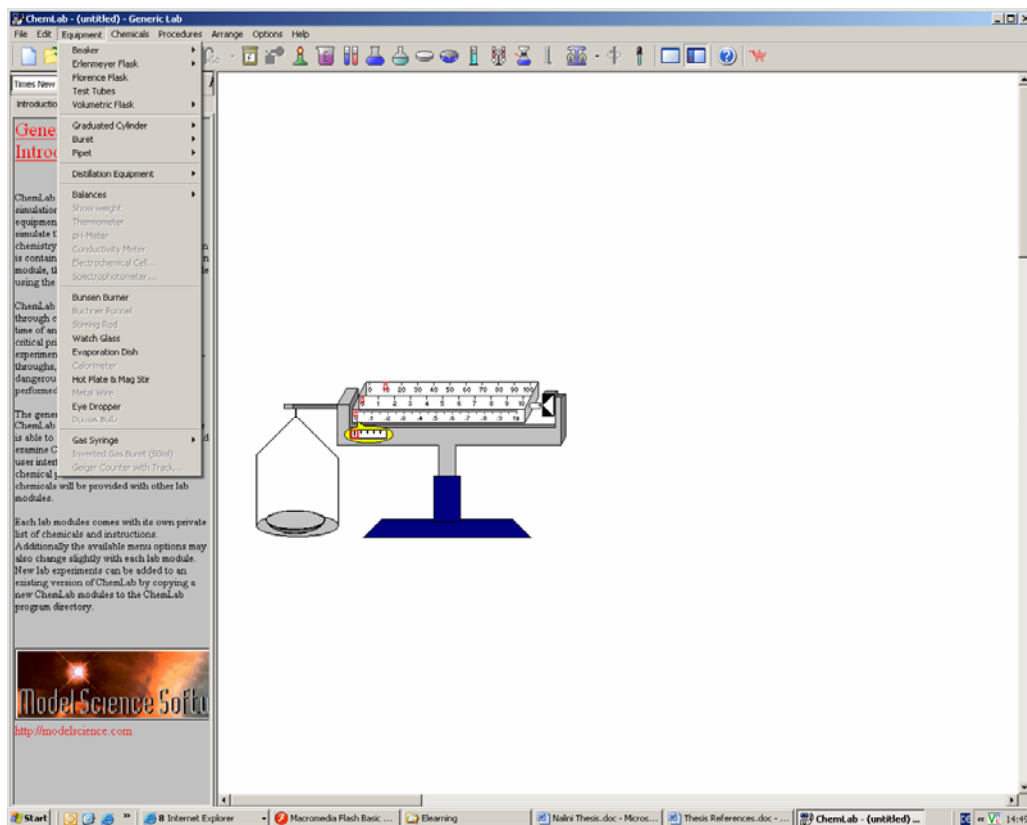
The thorough understanding of the physical and chemical principles involved in a problem is essential in order to apply intelligently the mathematics used in the solution of the problems. Therefore, it is provided to have some basic chemical and physical knowledge before fully taking advantage of CHEMIX learning and censorial capability [105].

ChemLab

ChemLab for windows is an interactive simulation of a chemistry lab. Common Lab equipment and procedures are used to simulate the steps involved in performing a chemistry lab experiment. Each lab simulation is contained in a separate loadable simulation module, thus many different labs are possible using the common lab interface.

ChemLab allows users to quickly run-through chemistry Labs, in a fraction of the time of an actual Lab, while emphasizing the critical principles and techniques of experimental chemistry. It is ideal for lab run-throughs, demonstrations, pre-lab

work, dangerous labs and labs which cannot be performed due to time limitations.



The generic lab module provides a basic ChemLab simulation. In this module the user is able to explore the available equipment and examine ChemLab's various procedures and user interface. You will note that the only chemical provided is water. Different chemicals will be provided with other lab modules [106].

Advanced Chemistry Development. Inc.

Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company offering solutions that truly integrate chemical structures with analytical chemistry information. ACD/Labs' innovative software packages aid chemical research scientists worldwide with spectroscopic validation of structures,

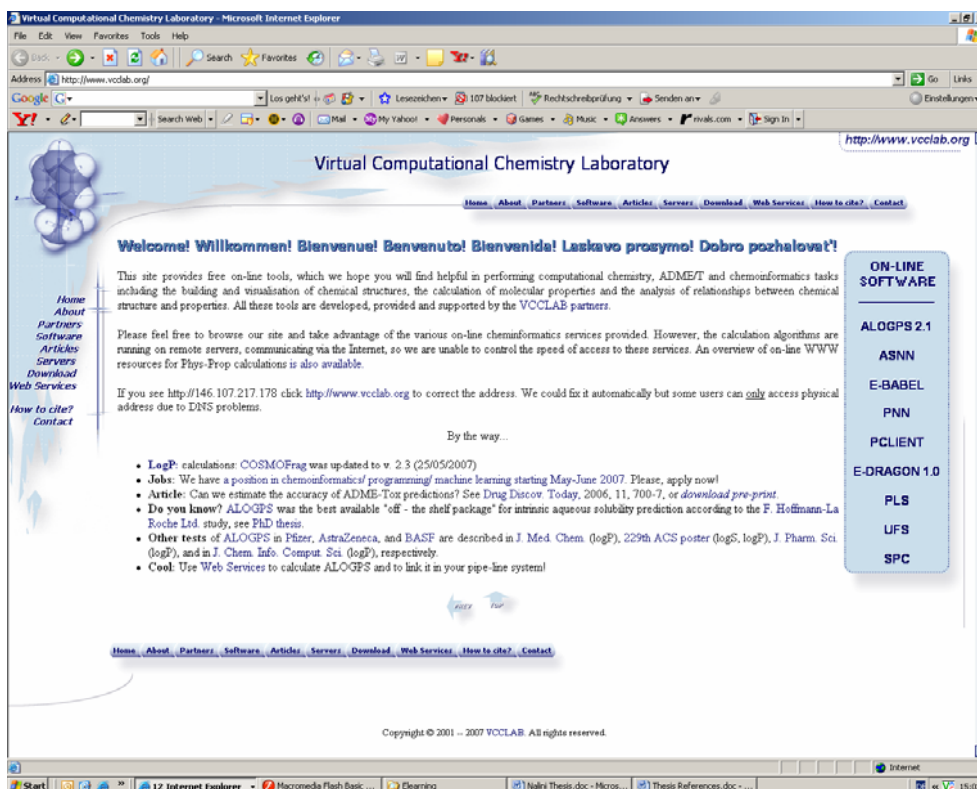
elucidation of unknown substances, chromatographic separation, medicinal chemistry, reformulation of novel drug agents, systematic nomenclature generation, and chemical patenting and publication. Combined, ACD/Labs' solutions create an analytical informatics system (ChemAnalytics®) that provides dramatic feed-forward effects on the chemical and pharmaceutical research process.



Founded in 1994, and headquartered in Toronto, Canada, ACD/Labs employs a team of over 140 dedicated individuals whose continual efforts carry ACD/Labs' innovative technologies into pharmaceutical, biotech, chemical, and materials companies throughout the world. [107]

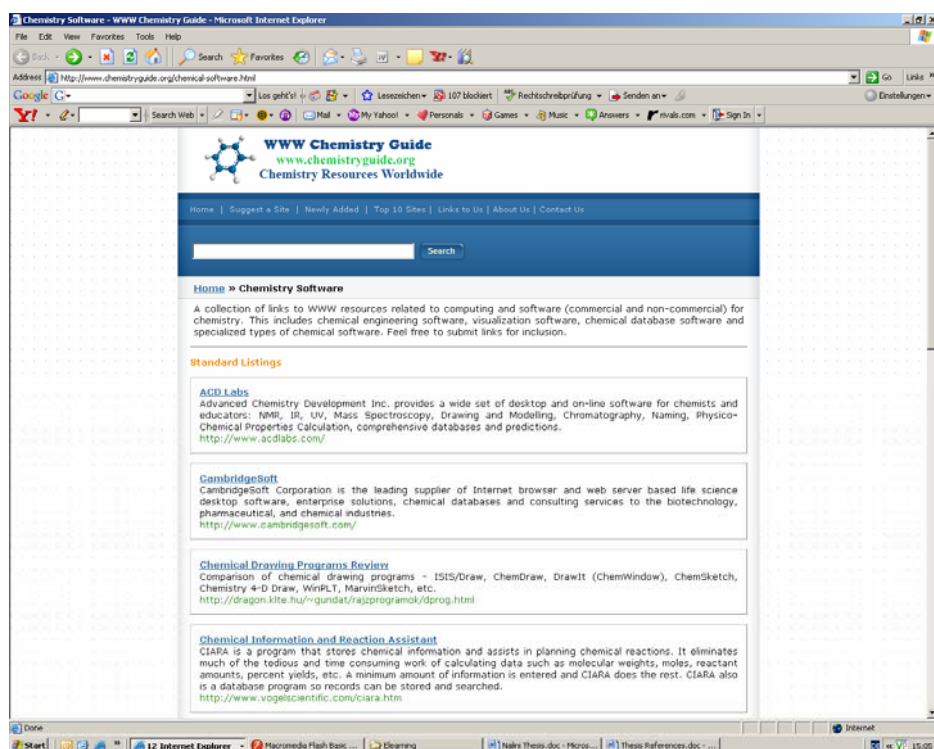
Virtual Computational Chemistry Laboratory VCCLAB

The overall objective of this project is to develop multi-platform software allowing the computational chemist to perform a comprehensive series of molecular properties calculations and data analysis on Internet. The software will be based on three-tier architecture that is becoming widespread to provide client-server services over the world [108].

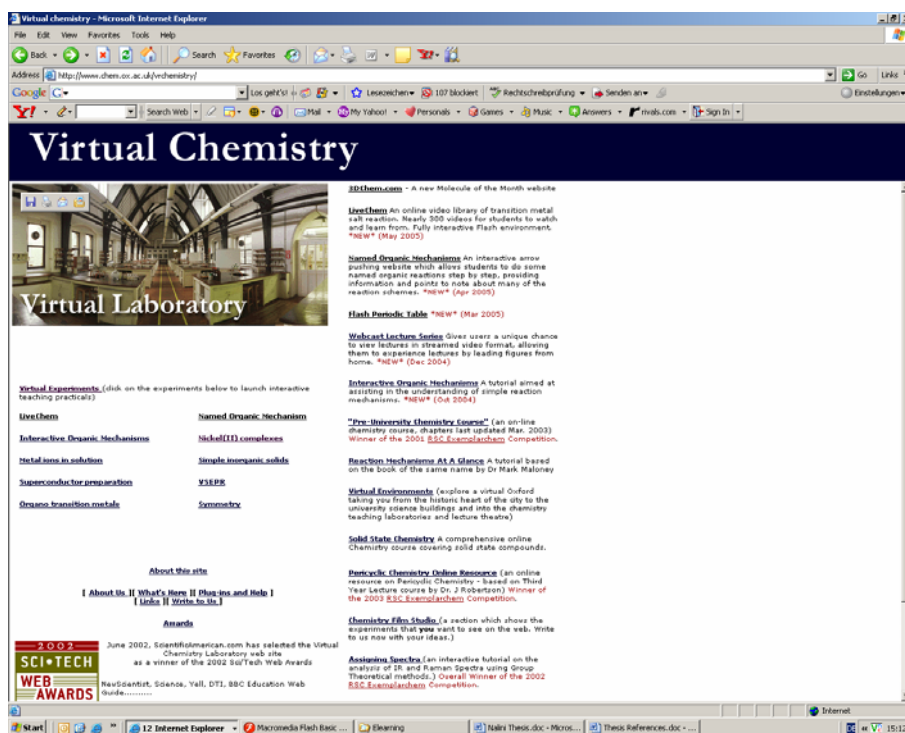


WWW Chemistry Guide

In this context, WWW Chemistry Guide, a web site designed for the specific needs of chemists, was created. Its mission consists in collecting and independently annotating all useful chemistry sites [109].



Virtual Chemistry



The Oxford VR Group is developing a three-dimensional simulated laboratory for the teaching of chemistry. This laboratory will be modelled using virtual reality techniques and it will contain interactive multimedia experiments.

Essentially, the student will be able to move around the lab in a web browser window and choose to take part in experiments that are distributed around this virtual lab.

Each experiment will make use of the latest multimedia technology. This will include: digitised video and animations of the experiment being carried out; animated three-dimensional simulations of chemical objects (including molecules); interactive sections where the student will be required to work out what is going on and answer questions; and links to other useful internet sites relating to that topic.

Live Chem

LiveChem - Online Reaction Video Library - Microsoft Internet Explorer

Address: http://www.chem.ox.ac.uk/vrchemistry/LiveChem/transitionmetals_content.html

LiveChem

Database is currently being updated.

LiveChem created, designed & maintained by Oliver Adcock final year MChem research student in the Department of Chemistry, University of Oxford Copyright 2005

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Chapter 2: e-Assessment

Introduction

In its broadest sense, e-assessment is the use of information technology for any assessment-related activity. This definition embraces a wide range of student activity ranging from the use of a word processor to on-screen testing. Due to its obvious similarity to e-learning, the term e-assessment is becoming widely used as a generic term to describe the use of computers within the assessment process.

E-assessment can be used to assess cognitive and practical abilities. Cognitive abilities are assessed using e-testing software; practical abilities are assessed using e-portfolios or simulation software.

An e-testing system comprises two components: (1) an assessment engine; and (2) an item bank. An assessment engine comprises the hardware and software required to create and deliver a test. Most e-testing engines run on standard hardware so the key characteristic is the software's functionality. There is a wide range of software packages. The software does not include the questions themselves; these are provided by an item bank. Once created, the engine uses the item bank to generate a test.

The creation of the item bank is more costly and time consuming than the installation and configuration of the assessment engine. There is currently no business model to support the creation of high quality item banks. Issues such as copyright and intellectual property rights remain unresolved.

This is an initiative to use modern technology to enhance the quality of the examination process for the benefit of candidates. It includes on-screen assessment, electronic marking of candidate scripts and electronic mark collection.

An assessment is a way of measuring what a student knows and can do. An alternate assessment is an assessment for students with disabilities who are unable to participate in the general assessments.

2.1 CAA – Online Assessment

2.1.1 What is CAA?

The acronym CAA [1] stands for **C**omputer **A**ided (or **A**ssisted) **A**ssessment and covers the use of computer-based technologies for testing and examination purposes. Other terms used in this area are ‘online assessment’ or ‘e-assessment’. CAA has been around for sometime but with the development of more Web-based teaching and learning software (including Virtual Learning Environments) it has become easier to use CAA as part of courses.

Computer-Assisted Assessment is a fast and efficient way to provide immediate feedback to the learner, and to save time on tutor marking. Computer Assisted Assessment is typically formative, in that it helps students to discover whether they have learned what the educator intended.

Computer Assisted assessment is a broad term for the use of computers in the assessment of student learning [2]. Various other forms exist, such as Computer-Aided Assessment, Computerized Assessment, Computer Based Assessment (CBA) and Computer-Based Testing. Online Computer Based

Assessment has existed for a long time in the form of Multiple Choice Questions (MCQ's) [3]. Computer Based Assessment commonly directly made via a computer, whereas Computer Assisted Assessment is used to manage or support the assessment process.

Commentators on assessment have identified 2 broad types of assessment, each with their own aims, assumptions and outcomes. These two types of assessment are formative and summative [4]. In his LTSN Briefing Paper on Assessment, Knight describes the 2 types of assessment as follows (Knight 2001):

Summative Assessment

- Used to make conclusions about achievement, and frequently leads to certification
- Usually high stakes assessment
- Learners may “conceal ignorance and suggest competence.”

Formative Assessment

- Used to “identify what learners need to do in order to improve their work.”
- Provides feedback
- “It is more helpful when learners are open about their limitations and don’t try to conceal ignorance or bury mistakes.”
- Can be used for diagnostic purposes

Online assessment can be used for both summative and formative assessment. In many ways the issues surrounding online assessment are very similar to those for traditional paper-based examinations. However, there are additional

considerations if one is using computer-based exams.

The most common form of online assessment is objective testing – this is where the student chooses from a set of pre-defined answers. A frequently used example of this is the multiple choice question (or MCQ) – see below for more information on objective testing.

2.1.2 Why to use Online Assessment

As previously stated, the reasons for using online assessment are the same as for any type of assessment (to check the progress of students against learning objectives, to provide a final grade or score etc). However, there are additional reasons why you may wish to provide assessment online:

- **Constant access to the assessment:** This is particularly useful for formative or diagnostic assessment. With the move to lifelong and distance learning, students may not be physically located on a campus, and the only way to circulate a test may be online.
- **Automatic marking:** Most online assessment tools offer options for automatic marking. This means that staff may save time and students can get instant feedback (see below)
- **Instant feedback:** Staff can build in feedback for correct/incorrect answers when designing the assessment. For formative assessment students can be given the correct answers, or pointers to further reading. For summative assessment students can be given an instant mark, or an idea of which areas that have not scored well on. Online assessment doesn't have to include

feedback, but this can enhance the formative learning experience.

- **Integration with other online resources:** With a move towards delivering more teaching online, online assessment is a logical step. Online assessment also allows integration with existing web-based materials such as audio/video. This allows for examinations using this material.

2.1.3 Issues to consider

Although there are a number of advantages to using online assessment, it is not a magic solution to the problems of marking and feedback. There are a number of issues which will need to be faced in the planning of assessment. Any of these issues may mean that online assessment would not be suitable for your purpose.

- **Assessment options:** The options available in online assessment packages are quite limited at present. It may be that the question types and output of answers will not be suitable for your purposes. The types of question and interface may not be suitable to the assessment of some skills, particularly practical skills.
- **Security:** Issues relating to security and plagiarism need to be considered, particularly relating to use of other packages at the same time as the assessment, spacing of computers, randomisation of questions, as well as security of the assessments for the test and the transfer of answers and data.
- **Automatic marking:** Automatic marking is not an option for all question

types, particularly the short answer or essay type question which relies on the strength of argument etc.

- **IT literacy levels:** Some students may not have IT skills in order to be able to use computers etc. This issue of whether this would be a disadvantage to the student will need to be addressed.

- **Question design:** As with all assessment, staff time will need to be spent on question design. This is especially the case with objective testing as staff may not be familiar with the issues around question design. Advice and support is available, and a good starting point is the CAA Centre's 'Designing Effective Objective Test Questions'.

2.1.4 The Blended Approach:

Online assessment is not a solution to all the issues surrounding assessment, and may be better seen as an addition to traditional assessment rather than a replacement. This mirrors changes in other areas of higher education towards mixing traditional and online teaching (or 'blended learning').

*"The power of these two approaches is
magnified when they are used in combination"*

Marc J.
Rosenberg

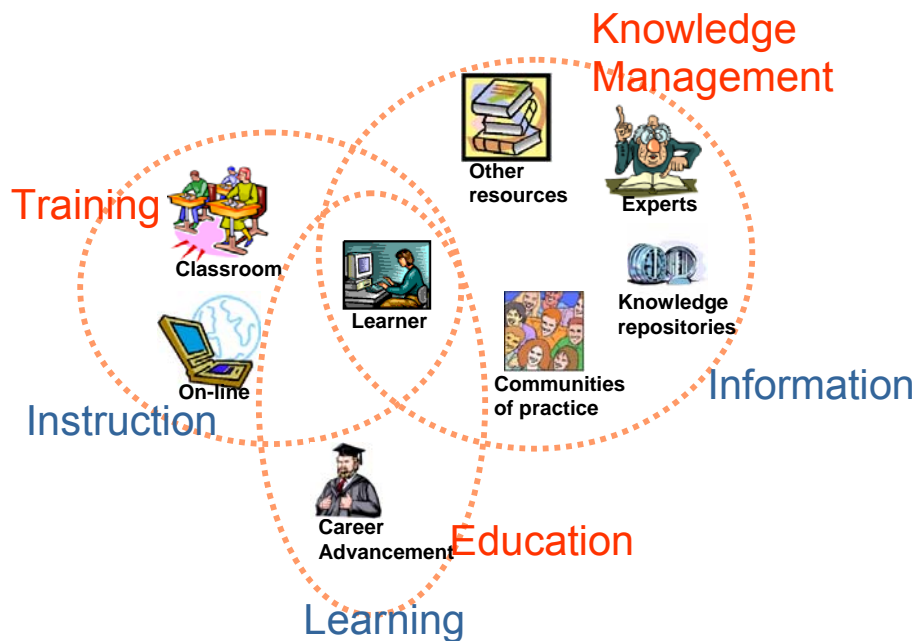


Figure: The Blended Approach

2.2 Use of e-Assessment

The term 'e-assessment' denotes any type of assessment that has an electronic component and incorporates one or more of e-testing, e-portfolios and e-marking. The following examples of e-assessment illustrate the potential scope and the range of its different uses. This list is not intended to be exhaustive.

- Assessments that are distributed, completed, marked automatically and administered electronically using local intranets/networks and individual workstations.
- Assessments that are distributed, completed, marked automatically and administered electronically using the internet.
- Assessments – comprising a combination of automatic marking and manual

marking that are delivered in either of the two ways described above.

- Electronic test delivery, with all marking completed manually on screen or on paper.
- A range of multimedia formats for submitting assessment.
- Electronic scanning of completed assessments for marking.
- Tests downloaded from the internet by the centre.
- Delivery of assessments' and submission of completed assessments by secure email.
- E-portfolios to store and manage candidates' evidence electronically.
- Assessments that are automatically marked and react adaptively to student performance.

2.3 E-Assessment by design:

- Multiple Choice
- Yes/No
- True/False
- Fill in the Blank

Using multiple choice: Multiple-choice questions [5] (MCQs) are being increasingly used in higher education as a means of supplementing or even replacing current assessment practices. The growth in this method of assessment has been driven by wider changes in the higher education environment such as the growing numbers of students, reduced resources, modularisation and the increased availability of computer networks. MCQs are seen as a way of enhancing opportunities for rapid feedback to students as well

as a way of saving staff time in marking. Computer networks enable more flexibility in the delivery of MCQs (e.g. with delivery at times and places more in tune with student needs) and, with appropriate software, they automate and speed up marking and the collation of test results. Compared to paper-based MCQs, the use of online computer-assisted assessment (CAA) can significantly reduce the burden associated with testing large student cohorts [6]

MCQs require the selection of a correct answer from a set of alternatives, i.e. the recognition of the answer rather than the construction of a response. In addition, students have no role in setting the goals and standards for MCQ tests, nor are they usually in a position to clarify the test question or its purposes while taking the test (i.e. clarify goals and standards). It is difficult therefore to envisage how this method of testing addresses current concerns in the assessment research that students should be given a more active and participative role in assessment processes [7,8] or that assessment should develop in students the skills needed to self-regulate their own learning [9,10].

Multiple choice questions (MCQs) are the traditional 'choose one from a list' of possible answers.

Practice Multiple Choice Questions - Microsoft Internet Explorer

Address: <http://chemistry.basestate.edu/people/nicharibanks/organic/mc/mcquestions217.htm>

Google: multiple choice tests for chemistry

Organic Chemistry Practice Multiple Choice Question Set 6

1. What is the IUPAC name for the following compound?

$$\begin{array}{c} \text{CH}_3 \\ | \\ \text{CH}_3-\text{C}\equiv\text{C}-\text{CH}-\text{CH}=\text{CH}_2 \end{array}$$

(a) 4-vinyl-2-pentyne
(b) 4-methylhex-2-yn-5-ene
(c) 3-methylhex-4-yn-1-ene
(d) 3-methylhex-1-en-4-yne

2. What is the major product expected from the following reaction?

$$\text{CH}_3-\text{C}\equiv\text{C}-\text{H} \xrightarrow[\text{excess}]{\text{HCl (g)}}$$

(a) $\text{CH}_3-\text{C}(\text{Cl})=\text{CH}_2$ (b) $\text{CH}_3-\text{C}(\text{H})=\text{C}(\text{H})-\text{Cl}$ (c) $\text{CH}_3-\text{CH}_2-\text{C}(\text{Cl})_2-\text{H}$ (d) $\text{CH}_3-\text{C}(\text{Cl})_2-\text{CH}_3$

3. What is the major product expected from the following reaction?

$$\text{CH}_3-\text{C}\equiv\text{C}-\text{CH}_3 \xrightarrow[\text{low pressure, poisoned catalyst}]{\text{D}_2 \text{ one mole}}$$

(a) $\text{CH}_3-\text{C}(\text{D})=\text{C}(\text{D})-\text{CH}_3$ (b) $\text{CH}_3-\text{C}(\text{D})=\text{C}(\text{H})-\text{CH}_3$ (c) $\text{CH}_3-\text{C}(\text{D})_2-\text{C}(\text{D})_2-\text{CH}_3$ (d) $\text{CD}_3-\text{C}(\text{D})_2-\text{C}(\text{D})_2-\text{CD}_3$


4. What is the major product expected from the following reaction?


$$\text{CH}_3-\text{C}\equiv\text{C}-\text{H} \xrightarrow{\text{NaNH}_2}$$


Yes/No questions require a student to assess whether answer is yes or no.


Address: http://www.rc.nutgers.edu/~kroghes/Chem327507/Exam3_S2006.pdf


5. (12 pts total) Which of the molecules shown below can absorb microwave (far-infrared) radiation? Circle the correct answer (YES or NO) for each molecule.


A  YES ? NO

B  YES ? NO

C  YES ? NO

D  YES ? NO

E  YES ? NO

F  YES ? NO

True/False questions require a student to assess whether a statement is true or not.

2. (10 pts) True or False (put a circle around your answer).

(a) Linear molecules with a permanent dipole moment of zero may absorb in the infrared	T	F
(b) For a rigid rotor, the pure rotational absorption spectrum consists of a single line.	T	F
(c) The rotational zero-point energy is $2B$	T	F
(d) A heteronuclear diatomic may have a pure rotational spectrum	T	F
(e) A molecule with zero dipole moment cannot change its rotational state by absorption of a photon	T	F

Multiple response questions (MRQs) are similar to MCQs, but involve the selection of more than one answer from a list.

Close

Pick the major product(s) of the following reaction.

CC1=CCCCC1 $\xrightarrow[\text{peroxides}]{\text{HBr}}$

☐ a. CC1(Br)CCCCC1

☐ b. CC1=CCCCC1Br

☐ c. CC1(Br)CCCCC1

☐ d. CC1(Br)CCCCC1

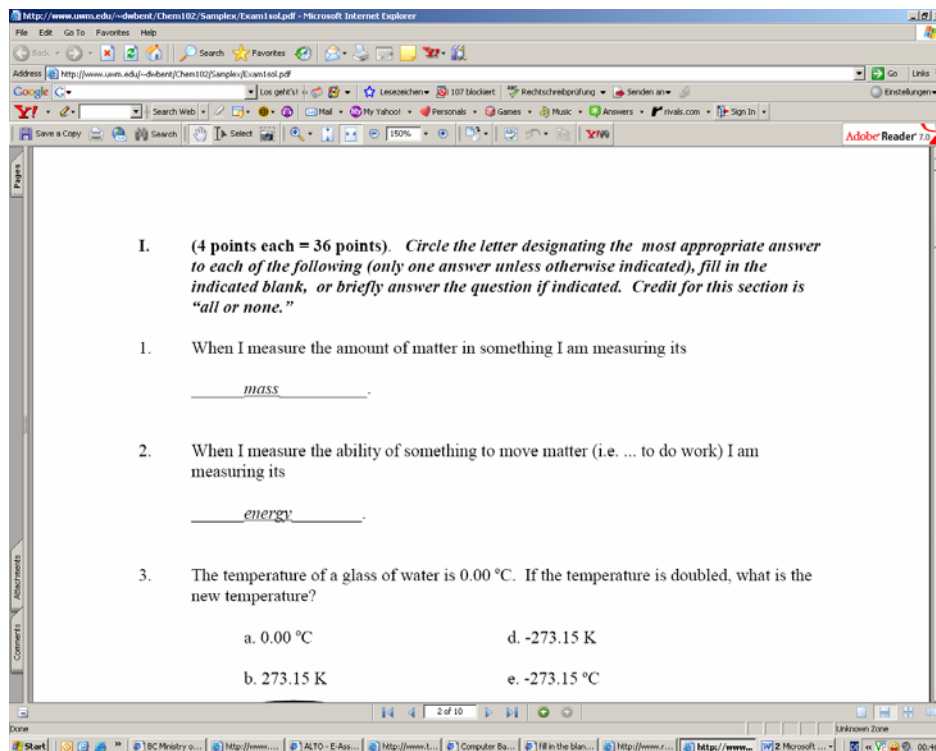
☐ e. CC1=CCCCC1Br

☐ f. CC1(Br)CCCCC1

☐ g. CC1=CCCCC1Br

Done

Fill in the Blanks question are solved by filling the appropriate answer at given blank space.



2.4 Advantages of e-Assessment

E-assessment is becoming widely used. It has many advantages over traditional (paper-based) assessment [11]. The advantages include:

- **Improved validity:** Well designed e-assessment can be more valid than traditional assessment. The use of text, sound and video can make questions clearer and more realistic than the narrative descriptions imposed by paper assessments. Research has shown that the reduced emphasis on language skills (through the increased use of multimedia) improves the performance of male candidates.

- **Increased reliability:** E-assessments can be more reliable than paper assessments. There is more year-on-year standardisation in the questions and less variance in marking standards. The reliability of traditional assessment has been a recurring problem to awarding bodies, centres and candidates.
- **Improved feedback:** Feedback is improved both in terms of its immediacy and level of detail. It is normally possible to provide instant feedback on candidate performance. Also, detailed analysis of candidate performance can usually be provided. This makes e-assessment particularly well suited to formative assessment when quick feedback can be used for remedial purposes.
- **More flexibility:** Traditional assessment is synchronous – question papers, exam rooms and candidates' attendance all have to be co-ordinated at specific times; e-assessment is asynchronous – candidates can undertake their assessment any-place-any-time. Once an appropriate infrastructure has been established, e-assessment is ideally suited to assessment-on-demand. This is particularly appropriate for diagnostic and formative assessment – and fits well with the flexible nature of e-learning.
- **Lower cost:** In the short to medium term, traditional assessment is less expensive to produce and use. But in the longer term, e-assessment is less expensive since it can be re-used from year to year (assuming that tests are drawn from an item bank). E-assessment is expensive to produce but, once created, is relatively inexpensive to operate and mark –

and has the potential to be re-used, year after year.

- **Increased motivation:** The use of multimedia makes e-assessment more engaging and more realistic than paper-based assessment. E-assessment also has the potential to be adaptive – that is, it can be modified in the light of previous responses to present more appropriate questions to candidates. The inherent privacy of this medium can reduce candidate's embarrassment and increase their confidence to attempt assessments.
- **More time to teach:** E-assessment should give teachers more time to teach and less time spent assessing and marking – whilst simultaneously providing more precise feedback on students' progress.
- **No alternative:** Awarding Bodies are coping with current demands for testing. The advent of the "learning society" will increase learning which, in turn, will increase the demand for assessment. The rigid nature of current assessment systems is inappropriate for this "any place, any time" learning.
- instant feedback to students
- immediate feedback to staff
- greater flexibility with respect to location and timing
- improved reliability (machine marking is much more reliable than human marking)
- allows rehearsal and revision
- can be linked to other computer-based or online materials
- allows evaluation of course's strengths and weaknesses

- enhanced question styles which incorporate interactivity and multimedia

2.5 Disadvantage of e-Assessment

There are also disadvantages.

- **E-assessments take time and money to produce:** E-assessment systems are expensive to establish and not suitable for every type of assessment (such as extended response questions). Traditional assessments are quick and simple to produce – but slow and expensive to use. E-assessment shifts the effort to the front of the process. They're time-consuming and expensive to create – and quick and simple to use. The pay-back for e-assessment is long term – but educational budgets are short/medium term.
- **E-assessment cannot be used for every type of assessment:** Although e-assessment can be used to assess most types of knowledge and understanding, it has limitations. For example, essay marking is currently not well done by a computer; e-assessment is (currently) not very good at measuring creative skills.
- **E-assessment requires more support:** Centres need to be 'tooled-up' for online assessment. The infrastructure for traditional assessment is already in place; the infrastructure for e-assessment is not. Depending on the specific e-assessment system in use, centres may require dedicated assessment centres and there is a requirement for on-going technical support throughout the assessment period.

- **E-assessment is new:** New things take time to be accepted – and new skills need to be developed to produce high quality e-assessments. Many teachers fear that e-assessment will de-skill their profession. Some teachers suspect the motives for introducing e-learning and e-assessment (“weapons of mass instruction”).
- **The main expense is not technical:** it is the cost of producing high quality assessment items.

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Chapter 3:

e-Assessment Tool for Virtual ChemLab

3.1 TUWEL: TU Wien eLearning

3.1.1 Introduction

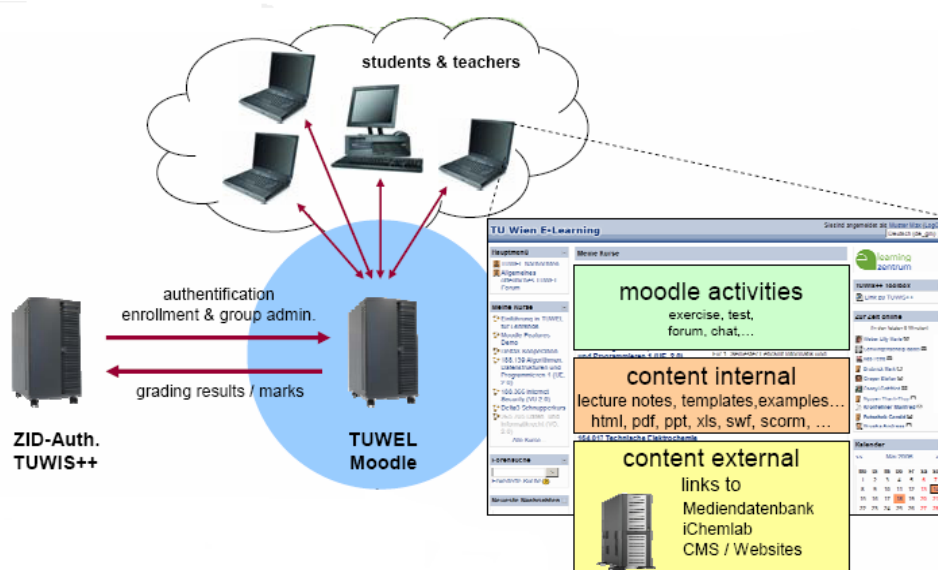


Figure: TUWEL structure

TUWEL stands for TU Wien E-Learning, which makes available the E-Learning centre of teaching and studying at TU Wien. TUWEL supplements the information system TUVIS++ [1] with functionality of the online course management of courses electronically supported to the settlement: Online tasks, chats, feedback cycles etc. The use of TUWEL in the apprenticeship eases the organization of the courses, above all in large listener's numbers. Simultaneously the manifold electronic communication tools enable a more

comprehensive and more individual care of the studying.

3.1.2 What is TUWEL?

TUWEL Online trained environment is based on the trained management system (LMS) Moodle. [2] MOODLE stands for: **M**odularly **O**bject- **O**riented **D**ynamic **L**earning **E**nvironment and serves in addition to organize internet based courses and to carry out electronically supported. Moodle is free software under GNU Public License and is available in more than 70 languages. It is used presently in 156 countries; over 11,500 Moodle installations with already over 1.6 million users in business.

Students		Staff*
Username	<i>immatriculation-Number</i> e.g. 0226703	<i>Lastname Firstname/Institute</i> e.g. Doe John/E000
Password	Your TU-Password (see also TU-Password FAQ)	

* If your lastname is unique, the lastname and code of the institute is not necessary. The syntax has to adhere to the White-Pages guidelines.

Alternative Login

Login for users with manually created accounts:

Username:

Password:

Login

Figure : TUWEL registration page

University has provided computer classrooms and about 400 places with connection to internet. Wireless LAN is established at the whole university.

Online evaluation for students on usability of technology in learning is mostly used for benchmarking.

In Austria, Moodle successfully is used for example BOKU - University of Natural Resources and Applied Life Sciences; Vienna, Johannes Kepler University; Linz, Klagenfurt University, Danube-university; Krems and many other.

3.1.3 Elearning partners

Students

Teachers



Institution

Interaction between students, teachers and institution is very important. TU Vienna E-Learning Center provides services and E-Learning Consulting Content Creation Support. LMS Moodle is connected with university information system.

- ❖ Moodle activities: exercise, test, forum, chat...
- ❖ Content internal: lecture notes, templates, examples..
- ❖ Content external: links to Mediendatebank, iChemlab,CMS/Websites
- ❖ Train the trainer program: 3 hours live introduction to teachers and the are

ready to start using moodle Experiences are that teachers are very cautious and reluctant to take early adopter role.

3.2 iChemEdu

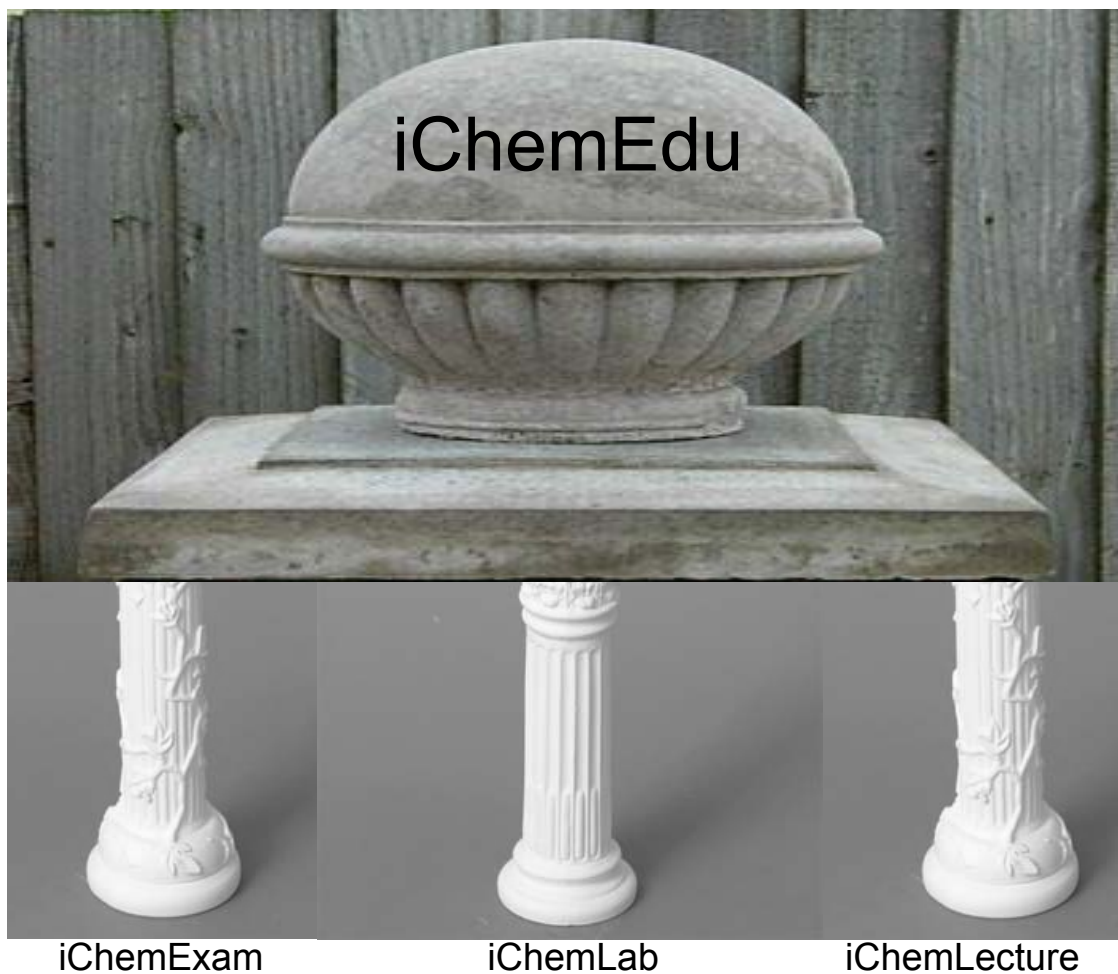
3.2.1 Introduction

iChemEdu an Internet based Information System for synthetic lab courses: Is e-Learning application created within “New Media in Teaching” supported by Austrian Ministry of Science. Synthetic lab courses play an important role in chemical education and within project internet based information system was created. Literature procedures often do not reflect available inventory. Expensive lab time is wasted by losing acquired knowledge.

This is computer assisted tools for teaching and learning Chemistry by designing protocols and tools for an Organic Chemistry practice Laboratory. The computer aid is articulated into three components which are the three pillars on which IChemEdu [4] rests. Each of the three components accomplishes a specific educational task. The most developed of them is IChemLab. The other two components are IChemLecture and IChemExam.

3.2.2 iChemEdu Concept:

iChemLab, iChemExam, iChemLecture. Program assures web preparation for electronic teaching, time and location independent preparation for students, didactically optimized programs, bi-directional interfaces to other data bases or modules. Program enables self-assessment and exams.

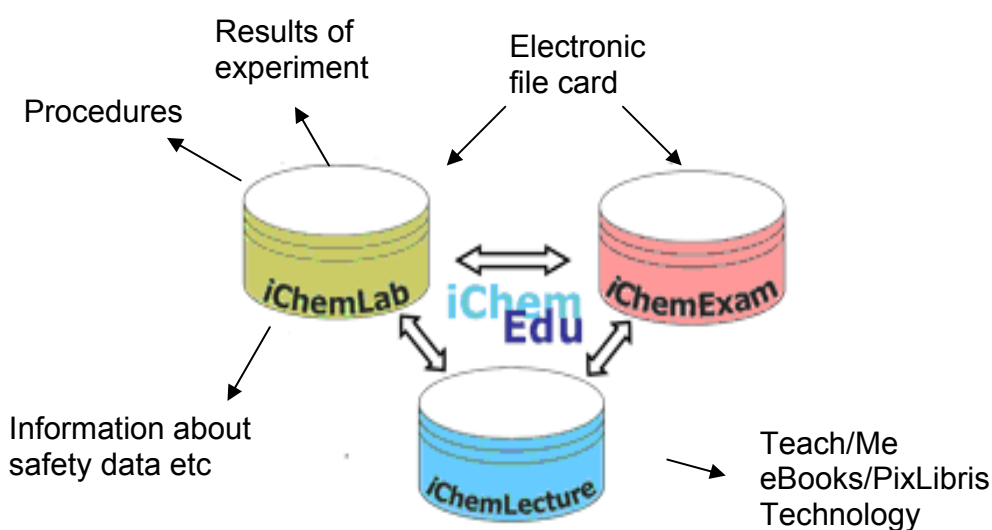


3.2.2.1 iChemLecture:

Is an "e-collection" of textbooks and contents for chemists converted from e.g. printed material by optical character recognition and full text indexing or generated by creating specific contents (e.g.: TeachMe products: <http://teachme.tuwien.ac.at>) with an appropriate author systems (e.g. Coimbra: <http://www.coimbra.at>).

The e-content pool of iChemEdu, IChemLecture, is an ensemble of texts and hypertexts assembled to illustrate the chemical concepts and technologies on

which the Laboratory is based. IChemLecture is made of several hypertexts specifically developed for ChemLab. However, it also includes several texts that have been turned into hypertexts by making use of a specific software developed by Springer Verlag to semiautomatically build into electronic copies of normal books the mark-up language specifications necessary to transform them into web hypertexts.



The 3 column model

iChemLab

3.2.2.2 iChemLab:

An Internet-based Information System for Synthetic Chemistry Laboratory Courses. This component guides the students to their personal paths to an Organic Laboratory practice. To this end several hundred practice Laboratory protocols have been restructured and organized in a way that the student has to interact with the computer to get instructions to proceed in the practice, to consult the relevant electronic data base and documentation, to store intermediate experimental information, to work out values and graphs necessary for the written

report, etc. All this is assisted by graphical interfaces so as to make the student intervention easy and focused on the chemical content of the experience that is being carried out.

3.2.2.3 iChemExam:

An internet based self-assessment tool within the iChemEdu concept. The third component IChemExam is a self evaluation tools that allows the student to challenge him/herself to discover the weak points of his/her preparation.

This is a self assessment area to check knowledge required performing the experiments. Besides the most common answering methods such a multiple choice selections and checks for numeric values, the Vienna group has developed new tools to answer and proof question via input of chemical structures. The supplied answer-structures are screened for correctness via a specially developed algorithm called SEICO [5] (Spherical Environment Integer Code). SEICO is able to discriminate almost all the most popular organic compounds by combining in a single integer code the information about the molecular geometry, the type of bonds, the stereo-chemical properties and other molecular features.

3.2.3 Aim of iChemEdu

The main scope of the project is to provide with a basic web environment tool, iChemLab, to practice on synthetic organic chemistry. Synthetic laboratory courses ("wet chemistry" [6]) play an important role in chemistry curricula.

Experimental procedures and theoretical backgrounds are mostly taken from printed literature, but have to be adapted to site specific general conditions. Due to frequently changing supervising staff information as well as knowledge about experienced practical problems get regularly lost, therefore iChemEdu aimed [7] at the development of an internet-based laboratory information and management system, iChemLab, (in connection with an e-content pool, iChemLecture, and an e-self-assessment tool, iChemExam) to preserve knowledge and to maintain data, thus to supply a sustainable solution.

The system - although fully integrated in the student's everyday lab business - is still under development and improvement. In particular, currently extension of functions and adoption to new software technologies are in progress. Moreover, interfaces for a tighter connection to the TU Wien student's e-administration system TUWIS++ is in process of planning. Therefore a detailed description of such functionalities is postponed to a report at a later date.

3.3 eAT Virtual Chem Lab:

(eAssessment Tool for Virtual Chem Lab)

3.3.1 Used in iChemLab:

As we know that iChemLab is an Internet-based Information System for Synthetic Chemistry Laboratory Courses. eAT Virtual Chem Lab is going to be a study tool for technicians and students as well. The main purpose of the application is to provide a tool for the assemblage of the apparatus. One of the risky situations in a real laboratory environment is the assemblage of the experimental setup before starting a practice session.

Before starting any reaction, one should know how to mount an assembly in safe and correct way. For that purpose one should get proper knowledge and training of use and handling of equipments before starting any reaction. Unsafe and improper use of lab equipments can lead to the accidents.

In chemistry laboratory, this e- Assessment tool will be used to train the technicians and academic students for better understanding of Good Laboratory Practices (GLP), which ultimately will increase the safety norms.

3.3.2 Used in iChemExam

As we have discussed, iChemExam is a self evaluation tools that allows the student to challenge him/herself to discover the weak points of his/her preparation.

eAT Virtual Chem Lab students are allowed to check online, the level of knowledge and competence of apparatus and assembly mounting (Organic reactions should always be carried out in apparatus that is suitable for the task in hand) he/she has acquired. Where he can mount the assembly virtually and check whether it is correct or not. The number of possible connection option can be tried and tested by him/her. Once he/ she appears for this exam will not have to wait for examiners presence to evaluate it.

3.3.3 Development of aAT Virtual Chem Lab:

Chemistry is a laboratory Science and as such it requires that students participate in meaningful laboratory experiences. The fundamental purpose of these instructional laboratories is to (i) provide “practical experience” by

connecting the “theory” taught in the classroom with the “real world” of the laboratory, (ii) teach laboratory technique and (iii) teach the cognitive processes (or analytical skills) that form the foundation of chemistry and other laboratory sciences [8]. In actuality, however, a significant fraction of students go through these laboratories with little thought about what they should learn, but narrowly follow the written directions for an experiment to get the expected results (called “cook booking”). The reason for this are many, but certainly a prime factor behind this tendency to “cookbook” is the rigidity imposed upon instructional laboratories by severe time constraints, large numbers of students, costs, environmental consideration, and safety considerations[9,10].

The virtually unlimited (in terms of quantity, quality, space and time) domain of knowledge and relationships that can be dealt by virtual reality approaches embedded into semantic web technologies [11], has pushed us to link virtual environments to chemical safety, in particular in the context of the virtual assemblage of an apparatus and of the control of chemical processes. After all, safety in addition to being one of the main concerns and cost source for industry it is also an important educational issue in realizing practice hands-on laboratory at any level of education.

In this, virtual reality, with its intrinsic ability to simulate complex systems such as the interaction between human beings and machinery, enormously facilitates learning and training of personnel involved in risky operations. Designing learning environments for intrinsically hazardous situations and operations with complex equipments is crucial for chemical and chemistry related

industries since real-on-the-field training is often impossible in many cases (see Ref. [12] for a review) while virtual reality offers a risk free environment.

One of the risky situations in a real laboratory environment is the assemblage of the experimental setup before starting a practice session. Because of the potential danger of the related operations, this activity is conducted by a tutor who is also responsible for the final validation of the apparatus (the tutor certifies that the student is able to assemble the apparatus).

An attractive solution to address many of these issues is to develop realistic computed virtual laboratory. In our virtual reality approach the student has the possibility of activating a virtual session (in this respect the virtual session is used as a pre-laboratory) to practice in the building of the apparatus before attending the laboratory session.

Research group of SELE [13] tried to design such a tool for assemblage of apparatus. At the end of their research they came to the conclusion, the process of building a chemical apparatus (even relatively simple) is complex from the algorithmic point of view [11].

As a part of further development in our research group we set out to ask a question “whether we could develop a self assessment as well learning tool for reaction assemblage?”

3.3.4 A Realistic approach to software selection:

Selecting appropriate software was first major task. One of the key criteria for software selection should be its capability to allow teachers and students to handle it easily. Another is Web accessibility. With seven options to choose

from, one should be able to find software to fit ones goals, technology skills, and available equipment.

3.3.5 Java applet or Flash macromedia

3.3.5.1 Java Applet

A **Java applet** [14] is an applet delivered in the form of Java bytecode. Java applets can run in a Web browser using a Java Virtual Machine (JVM), or in Sun's AppletViewer, a stand-alone tool for testing applets. Java applets were introduced in the first version of the Java language in 1995. Java applets are usually written in the Java programming language but they can also be written in other languages that compile to Java bytecode such as Jython.

Applets are used to provide interactive features to web applications that cannot be provided by HTML. Since Java's bytecode is platform independent, Java applets can be executed by browsers for many platforms, including Windows, UNIX, Mac OS and Linux. There are open source tools like applet2app which can be used to convert an applet to a stand alone Java application/windows executable/ Linux executable. This has the advantage of running a Java applet in offline mode without the need for internet browser software.

3.3.5.2 Flash Macromedia:

Adobe Flash [15, 16], or simply **Flash**, refers to both the Adobe Flash Player, and to the Adobe Flash Professional multimedia authoring program. Adobe Flash Professional is used to create content for the Adobe Engagement Platform (such as web applications, games and movies, and content for mobile phones and

other embedded devices). The Flash Player, developed and distributed by Adobe Systems (which acquired Macromedia in a merger that was finalized in December 2005), is a client application available in most common web browsers. It features support for vector and raster graphics, a scripting language called ActionScript and bi-directional streaming of audio and video. There are also versions of the Flash Player for mobile phones and other non-PC devices.

Strictly speaking, Adobe Flash Professional is an integrated development environment (IDE) while Flash Player is a virtual machine used to run, or parse, the Flash files. But in contemporary colloquial terms "Flash" can refer to the authoring environment, the player, or the application files.

Since its introduction in 1996, Flash technology has become a popular method for adding animation and interactivity to web pages; several software products, systems, and devices are able to create or display Flash. Flash is commonly used to create animation, advertisements, various web-page components, to integrate video into web pages, and more recently, to develop rich Internet applications.

The Flash files, traditionally called "Flash movies" or "Flash games", have a .swf file extension and may be an object of a web page, strictly "played" in a standalone Flash Player, or incorporated into a Projector, a self-executing Flash movie with the .exe extension in Windows. Flash Video files have a .flv file extension and are utilized from within .swf files.

3.3.5.3 Advantages of Flash over Java applet

- Java applets and flash are two completely different things. Firstly, they require different plug-in to run in a browser. Flash requires the user to have the flash Player (or Shockwave player, depending), whereas to run an applet one need to have a java Runtime Environment (JRE) of some sort on your machine.
- Flash has its own scripting language, Action Script, which allows flash developers/designers to do some very advanced things from physics engines to server communication.
- Applets cannot be saved as images and I'd be interested to know how flash can be made to save as an image! Both require plug-ins/runtime environments to display, although flash has a very high plug-in penetration.
- The Java plug-in is close to 10 MB of size, whereas the Flash plugin is 400 KB.
- Java Applets do not run on Netscape 6.0 + browsers but Flash can. I mean even post the information back to the server.
- Java applets are comparatively slower than Flash players
- Flash runs on various platforms, including Win, Mac, Unix/Linux and others...
- As for Java on Windows, there is going to be a period where Java isn't available on new PCs. Even so, already there are problems for some CBT makers with Sun Java and MS Java incompatibilities and indeed problems between Java 1.3 and 1.4 .Regardless, many of the large corporate often have a (version of) Java as part of their standard desktop install.

- Macromedia Flash provides a powerful, intuitive drag-and-drop graphical authoring tool that is comfortable for both designers and developers. Designers are comfortable using the Macromedia Flash authoring tool design capabilities while developers can use to drag-and-drop interface components and ActionScript, the Macromedia Flash object-oriented scripting language.
- Macromedia Flash is platform independent (like Java) and widely supported. To use Flash Remoting, the client must have the Macromedia Flash 6 player installed. Currently, 98.4% of Internet users have the Macromedia Flash player installed, and there are Macromedia Flash 6 players available for Windows, Linux, Macintosh, and even PocketPC operating systems.
- Macromedia Flash allows your applications to have quick-loading, dynamic interfaces. Since Macromedia Flash is vector-based, Macromedia Flash binaries (SWF files) are very small and quick to load across even the slowest Internet connections. Additionally, Macromedia Flash supports dynamic loading of additional resources like images, sounds, video, and additional pieces of Macromedia Flash, so your application can load assets on demand.
- **Macromedia Flash MX is now a full-fledged application development environment which supports:**
 - XML
 - Socket connections

- Object-oriented ECMA compliant scripting language (ActionScript)
- Component architecture for GUI elements
- Styles to control look and feel
- Event broadcasting
- Object serialization
- Local data storage
- Remote method invocation through Flash Remoting
- Macromedia Flash MX exposes all of this functionality by combining an intuitive drag-and-drop authoring tool and a powerful with a well encapsulated ActionScript API. The Macromedia Flash authoring tool saves applications as FLA files, which it compiles into SWF files before streaming them to client browsers.

After studying these all points we come to the conclusion, Flash is the best software to design our virtual Lab.

3.3.6 Layout of eAT Virtual Chem. Lab:

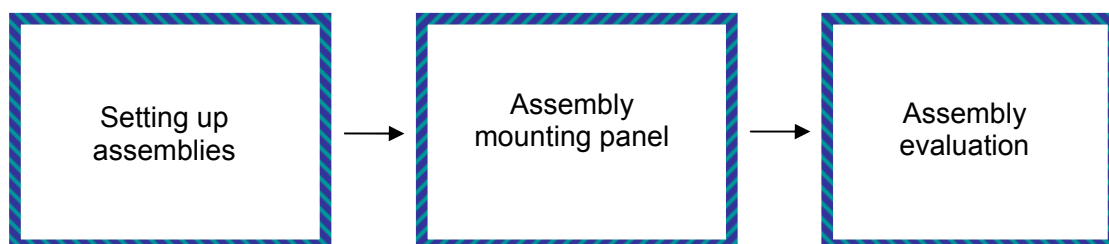


Figure: Block diagram

3.3.6.1 Setting up assemblies

The assembly set up is designed for examiner and program administrator. Assembly set is nothing but setting up question paper for exam. Here examiner has choice to set his own questions. He can constrain to use only specified set of apparatuses if he wants students to use only those apparatuses while mounting assembly. His role as an administrator is as follows to set up a test.

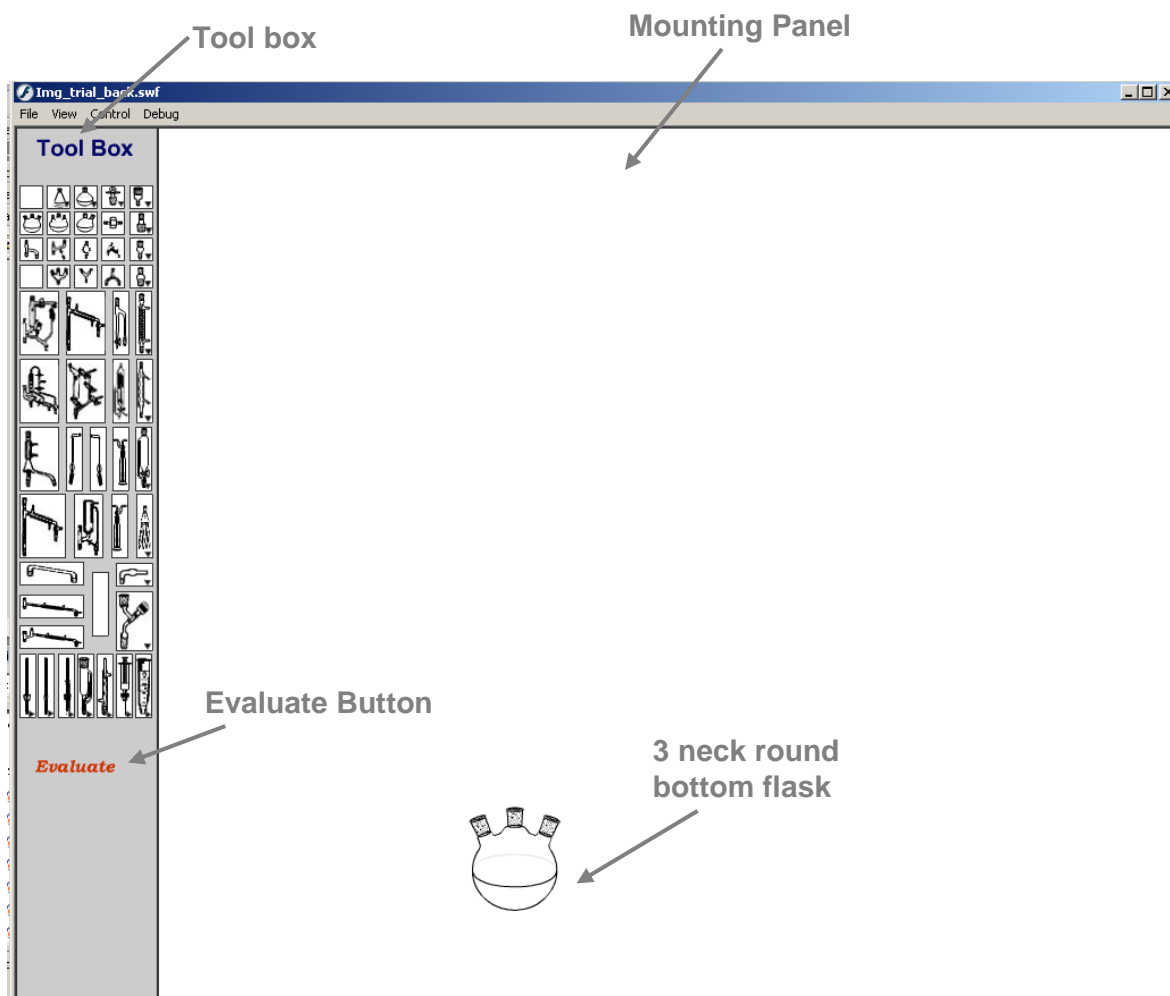
- First Input the list of assemblies.
- Provide the set of apparatus for required assembly.
- Can restrict student to mount an assembly using available/provided set of apparatus.
- Can give choice to a student to select his own set of apparatus for mounting mentioned assembly.
- Set the right possible answer(s) for mentioned assembly. For setting the right answer/s he has to follow specific connection string criteria which I will discuss further.

3.3.6.2 Assembly Mounting panel

This is the area of our virtual laboratory where students are going to practice and test their knowledge of apparatus assemblage. The actual mounting of apparatus will be done here.

Assembly Mounting panel is further classified in two different panels.

- Tool Box
- Mounting panel / Design panel



3.3.6.2.1 Tool Box

The toolbox contains all apparatuses (in form of buttons) needed to mount any assembly. For example, there are 1/2/3 necks round bottom flasks, reflux condenser, dropping funnel, stopper, connectors, which are used constantly in Laboratory.

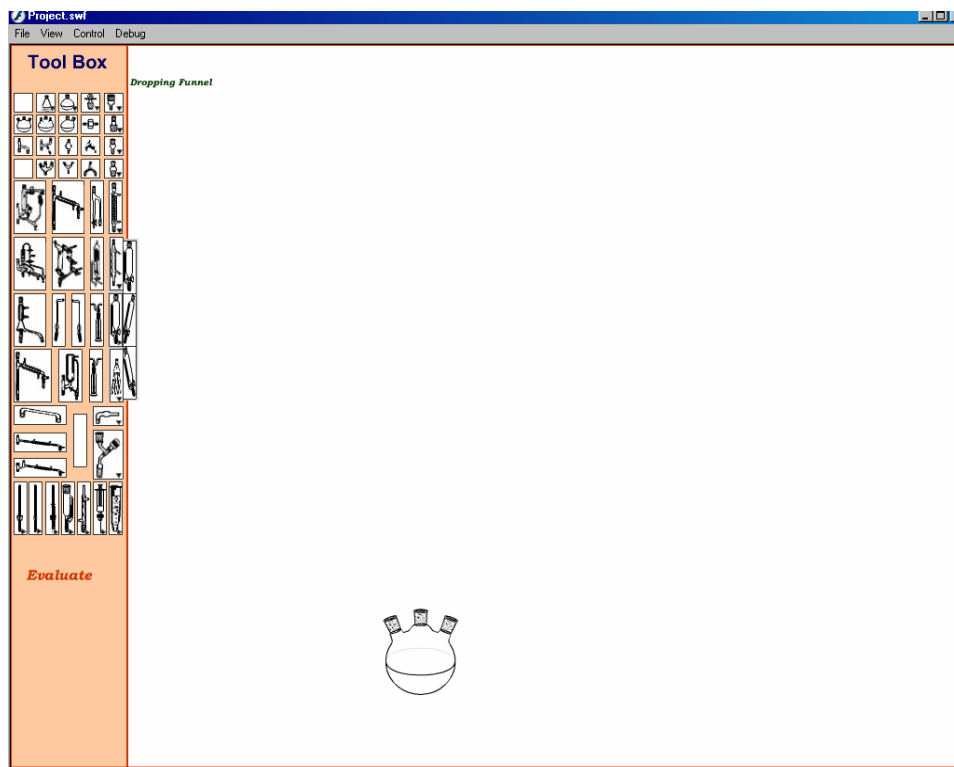
Few apparatuses are only connected vertically. Specific required button from this category can be selected by mouse click. The other type of buttons pops up with three different buttons by scrolling mouse over it; required button can be selected out of these three buttons. When mouse is scrolled over any button it's

name is been displayed, which will help to identity apparatus as well to learn the name. Even programmatically it is possible to make certain set of buttons enabled (available to use) if examiner wants to restrict to use only this set of apparatuses.

3.3.6.2.2 Mounting Panel

This is the main working area of our virtual laboratory, where students are going to design an assembly. One has to select required apparatus by clicking on that apparatus in tool box and has to connect it to the assembly. For connecting the apparatuses to each other the program finds their x and y coordinates using the self invented formulas with respect to the x and y coordinates of the mouse click on mounting panel. Further we will discuss these formulas in detail.

➤ Design of Mounting panel



Here you can see a three neck round bottom (RB) flask. It is by default available to start an assembly. What should be the starting apparatus will be decided by examiner while setting the assembly. It will be always placed at default location which is predefined. Even if students want to make a choice of a starting apparatus can be programmed in future.

➤ **Connecting apparatuses**

Is it possible to connect one apparatus to another? It was a major question in front of me when I started designing actual program. To answer this question I had to answer few more questions.

1. Are we going to use CGI (computer generated images) [17]? Where will I get all apparatuses from?

Using CGI could be one of the best choices but our main aim of designing this program was to generate assembly and evaluate it. As we didn't want to spend more time on generating all required apparatuses we decided to use images which are available to use. One of the choices to get apparatuses is from books or chemical apparatus catalogue. I had to drop this idea as I did not want to use scanned images, which could have lead to difficulty in getting clear image, transparent image and resizable image and same format for all.

2. Are they all available by any single source?

I am very thankful to Sigma Aldrich (<http://www.sigmaaldrich.com/catalog/>) for making their glassware catalogue available online. 40% of the apparatuses I could get it from this catalogue. 40 % of rest of the apparatuses I took from Chemdraw glassware (clipware) templates. The rest 20% I have designed using Photoshop and Corel draw.

3. All apparatuses gathered from all available sources will be in same and standard size?

No, all apparatus images gathered from different sources were available in different sizes. Few of them while resizing lost details and were blurred. I played around almost all images to resize them in standard format but it didn't work, as they were taken from different sources. After researching a lot I came to the conclusion that only a connecting point that is the neck of apparatus should be of same and standard size. According I redesigned all images in Photoshop and CorelDraw. I followed the following procedure step by step.

- Copied an image to Photoshop
- Erased unwanted part like connecting points (necks)
- Redrawn the image to make it clear and sharp
- Copied this sharpened image in CorelDraw to make image available in transparent format
- Recopied and pasted image to the Microsoft PowerPoint. Made it transparent with transparent tool
- Copied and pasted this image to flash to resize at required size.
- Added necks of standard and specific size to this image and grouped them.

4. Are these all apparatuses are symmetrical?

Hardly few apparatus like RB flasks, stopper, reducers, and expanders are symmetrical the rest all are unsymmetrical.

5. Is it possible to find the centre connection point?

It will be wrong if I say it's not possible to find CCP (central connecting point) of each apparatus. It's rather impossible to get the CCP of all apparatuses applying same logic or same formula as we know that all are not symmetrical.

6. How to calculate x and y coordinates of connecting apparatuses based on available values of x and y coordinate of lower connecting apparatus? Is there any formula available to calculate x and y coordinate?

To get Y of apparatus at 0 degree:

Yapp : Y of the apparatus we want to connect

YL : Y of lower level apparatus

Ht_app: Height of apparatus to be connected

ht_inlet: height of inlet of lower level apparatus. (Const Value 14.3)

$$Y_{app} = Y_L - Ht_{app} + ht_{inlet}$$

To get X of apparatus at 0 degree:

Xapp: x coordinate of the apparatus we want to connect

XL: x coordinate of lower level apparatus

cent_app: Distance from the centre of the connecting apparatus

To calculate this distance we have to mark the centre point of the outlet of apparatus.

Then subtract the x (**xb**) of the marking from the x (**xa**) of the apparatus at current location.

$$cent_{app} = xb - xa$$

cent_Lapp: Distance from the centre of the lower apparatus

To calculate this distance we have to mark the centre point of the inlet of apparatus.

Then subtract the x (**xb**) of the marking from the x (**xa**) of the apparatus at current location.

$$\text{cent_Lapp} = \text{xb} - \text{xa}$$

$$X_{app} = XL + \text{cent_Lapp} - \text{cent_app}$$

To get Y of apparatus at 20 degree:

Yapp: y coordinate of the apparatus we want to connect

YL: y coordinate of lower level apparatus

Ht_app: Height of apparatus to be connected

Yline: Y of line drawn to get the common distance

cmnNkOutlet: $\text{cmnNkOutlet} = \text{Yapp} + \text{Ht_app} - \text{Yline}$

cmnNkInlet: $\text{cmnNkInlet} = \text{Yline} - \text{Yapp}$

$$Y_{app} = YL - \text{Ht_app} + \text{cmnNkOutlet} + \text{cmnNkInlet}$$

To get X of apparatus:

Xapp: x coordinate of the apparatus we want to connect

XL: x coordinate of lower level apparatus

Wd_app: Width of apparatus to be connected

PRdist_Inlet: To draw a line on inlet to get the common distance from

right.

$$\mathbf{PRdist_Inlet = Xapp + Wd_app - Xline}$$

PLdist_Outlet: To draw a line on outlet to get the common distance from left.

Xline: x coordinate of line drawn to get the common distance

$$\mathbf{PLdist_Outlet = Xline - Xapp}$$

$$\mathbf{Xapp = XL - PRdist_Inlet - PLdist_Outlet}$$

To get Y of apparatus at -20 degree:

Yapp: y coordinate of the apparatus we want to connect

YL: y coordinate of lower level apparatus

Ht_app: Height of apparatus to be connected

Yline: y coordinate of line drawn to get the common distance

PcmnNkOutlet:
$$\mathbf{PcmnNkOutlet = Yapp + Ht_app - Yline}$$

PcmnNkInlet:
$$\mathbf{PcmnNkInlet = Yline - Yapp}$$

$$\mathbf{Yapp = YL - Ht_app + PcmnNkOutlet + PcmnNkInlet}$$

To get X of apparatus at -20 degree:

Xapp: x coordinate of the apparatus we want to connect

XL: x coordinate of lower level apparatus

Ldist_Inlet: To draw a line on inlet to get the common distance from left.

$$\mathbf{Ldist_Inlet = Xline - Xapp}$$

Ldist_Outlet: To draw a line on outlet to get the common distance from left.

Xline: x coordinate of line drawn to get the common distance

$$\text{Ldist_Outlet} = \text{Xline} - \text{Xapp}$$

$$\text{Xapp} = \text{XL} - \text{Ldist_Outlet} + \text{Ldist_Inlet}$$

7. Whether apparatus will be connected by drags and drop method or will be simply connect smartly on single click.

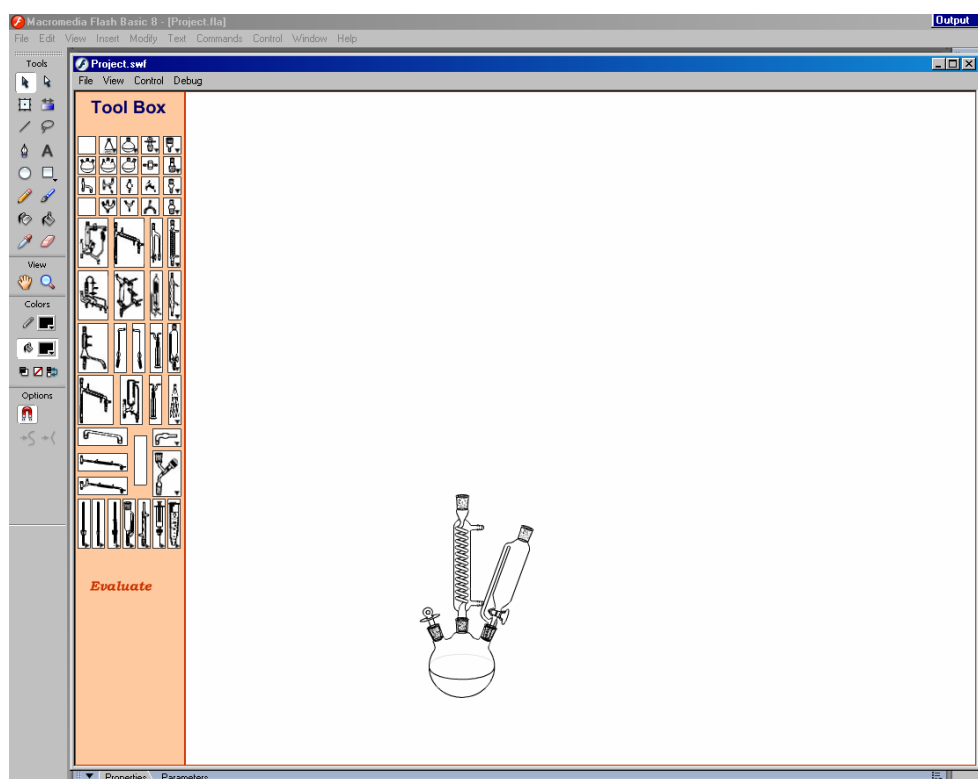


Figure: Apparatus example

Instead of drags and drop method program will calculate the x and y coordinates of connecting apparatus using above explained formulas. In this case user has to select the apparatus from tool box and click once on the inlet (neck) of the apparatus to which it wants to be connected.

Complete assembly is shown above. As we discussed earlier there will be default starting apparatus. Other apparatuses are connected on top of it. One has to start with selecting next required apparatus from tool box.

In above example 3 necks RB flask was a starting apparatus. Then stopper, reflux condenser and dropping funnel are connected at left neck, middle neck and right neck respectively.

3.3.6.3 Evaluation

- **"Evaluation"** is the systematic determination of merit, worth, and significance of something or someone. Evaluation often is used to characterize and apprise subjects of interest in a wide range of human enterprises, including the Arts, business, computer science, engineering, foundations and non-profit organizations, government, health care, and other human services.
- Evaluation is the process of determining significance or worth, usually by careful appraisal and study.
- Evaluation is the analysis and comparison of actual progress vs. prior plans, oriented toward improving plans for future implementation. It is part of a continuing management process consisting of planning,

implementation, and evaluation; ideally with each following the other in a continuous cycle until successful completion of the activity.

- Evaluation is the process of determining the worth or value of something. This involves assigning values to the thing or person being evaluated.
- Evaluation is about using monitoring and other information you collect to make judgements about your project. It is also about using the information to make changes and improvements.
- Evaluation aims to answer agreed questions and to make a judgement against specific criteria. Like other research, for a good evaluation, data must be collected and analysed systematically, and its interpretation considered carefully. Assessing 'value' - or the worth of something - and then taking action makes evaluation distinctive. The results of an evaluation are intended to be used.
- Evaluation is also known as “assessment”. Evaluation is that part of a project where you stand back and take stock.

Answers “How *well* did we do?”

Answers “How *much* did we do?”

Monitor “what you are doing?”

Measure “what you have done?”

Find out “what was effective and what was not?”

It is essential that the procedures used for the assessment of students' achievement in chemistry should correspond to the knowledge, abilities and skills that are to be developed through their degree programme. Evidence, on which

the assessment of student achievement is based, should include: Formal examinations, including a significant proportion of 'unseen' examinations and Laboratory reports.

These are different kinds of evaluations:

- Internal evaluation
- External evaluation
- Preliminary evaluation
- Formative evaluation
- Summative evaluation

3.3.6.4 Assessment in Chemistry and the role in exam:

The development of student's higher- order cognitive skills (HOCS) in the context not only of the specific content and processes of the science disciplines but also of the interrelationships of science, technology and society has become one of the most important goals of chemistry and science education [19-21]. However, although the teaching, learning and assessment of these skills are advocated by many, they are rarely actually perused in college chemistry teaching. A shift from dominant lower-order cognitive skills (LOCS) to the HOCS orientation in chemistry teaching requires a drastic change not only in teaching and learning, but also in assessment strategies consonant with this. Since very few exams that push beyond tasks of information retrieval, relabelling or recognition or focus beyond basic skills in the subject matter are currently used, the implementation of assessment methods that attempt to capture more complex aspects of learning is clearly in order [19, 22].

It is well established that in self-regulated learning (the fusion of “skill” and “will”), students manage their learning not only by use of cognitive, meta-cognitive and volitional control strategies, but also by use of motivational strategies [23]. This requires them to take more responsibility for their learning by assuming an active role in the learning process, including self-assessment of their own progress.

Teachers in higher education are increasingly aware that assessment is a (if not the) major driver for students in higher education. Students apply the ‘assessment’ test. If a concept, skill or knowledge chunk is deemed to be assessable in a way that contributes to the ultimate goal (of degree, diploma etc), then a high priority is accorded in the learning strategy [18] of the student. Given this prevailing culture, we can adopt either of two strategies: to change this culture of assessment driven learning or to use it as an opportunity to improve learning. Another possibility might be to remove assessment entirely but the arguments for assessment are powerful, embodying ideas of guiding student improvement and progression, diagnosis of faults, providing feedback to teachers and informing employers [24].

Over the last decade and more, there have been many laudable and, to a large extent, successful programmes that have introduced context-based learning [25], problem solving approaches and holistic perspectives. Nevertheless, even with such approaches, assessment remains a major learning driver for many students. So accepting that there is a strong argument for the retention of assessment, and that changing the culture of assessment-motivated learning would be difficult if not impossible to achieve, a critical consideration of

the quality of assessment should be a feature of every study programme.

"The World Wide Web is becoming increasingly attractive as a mechanism for the delivery of assessment." With an increasing use of online technologies for course delivery, it is only natural that we are exploring ways to assess students online. Formative or summative, requiring multiple choice responses or full-text answers, completed in a controlled lab environment or from their home – there are many possibilities for online assessment today and no doubt more that are yet to be devised.

Despite the widespread use of computers in teaching and learning, their uses for assessment have only been limited. There is a tendency to associate computer-based assessment with automated multiple-choice questions, possibly because it was one of the earliest uses of computer technologies. Computer-based assessment not only automates routine tasks like marking multiple-choice questions, but can enrich student's learning experiences (Brown, Race and Bull, 1999). Another popular use of online technologies is for the electronic submission of written assignments which can streamline administrative processes. As issues of security, access and equity are resolved summative online testing are increasing in the hope that it will help manage large volumes of marking and administration generate efficiencies that can ease academic workloads.

3.3.6.5 Graph Theory and Chemical Structures:

The present algorithm provides an efficient and easy handle to examine the terminal as well as core vertices of given chemical graphs. The sequential identification of vertices of subgraphs facilitates the formation of connectional

tables. This can be used for the computation of characteristic matrices and topological indices. Also, it finds application in storing, sorting and retrieving of chemical structures and databases. As this typically demarcates the core and terminal vertices in graphs, it can be put an easy use in comparing two or more structures or parts thereof for any given purpose.

➤ **Morgan's algorithm**

- Provides canonical numbering for the nodes in a graph that doesn't depend on any original numbering
- Works by taking more of the graph into account at each iteration
- essence of "relaxation" technique is iteratively updating a value by looking at its immediate neighbours
- It is not infallible
- some graphs are known where the algorithm cannot distinguish nodes that are not symmetrically equivalent
- There are many variations on it and several theoretical papers analysing it mathematically.

➤ **Canonicalisation [26]**

- Algorithms are applied to graphs not chemical structures
- Issues such as aromaticity, tautomerism and stereochemistry need to be addressed before canonical numbering of the graph
- Daylight's canonicalisation algorithm for SMILES perceives aromatic rings (using its own definition of aromaticity) as first step

- SMILES denotes a molecular structure as a graph with optional chiral indications. This is essentially the two-dimensional picture chemists draw to describe a molecule. SMILES describing only the labeled molecular graph (i.e. atoms and bonds, but no chiral or isotopic information) are known as generic SMILES. There are usually a large number of valid generic SMILES which represent a given structure. A canonicalization algorithm exists to generate one special generic SMILES among all valid possibilities; this special one is known as the "unique SMILES". SMILES written with isotopic and chiral specifications are collectively known as "isomeric SMILES". A unique isomeric SMILES is known as an "absolute SMILES".

3.3.6.6 SMILES

SMILES [27, 28] (*Simplified Molecular Input Line Entry System*) is a chemical notation language specifically designed for computer use by chemists. This sort of line notations are popular method for representing chemical formulas. It is the most widely used chemical line notations. It denotes a molecular structure as a graph that is essentially the two dimensional valence-oriented picture chemists draw to describe a molecule (chemical structure) to one unique notation.

Integrating data involving chemical structures is simplified when unique identifiers (UIDs) can be associated with chemical structures. For example, these identifiers can be used as database keys. One common approach is to use the Unique SMILES notation introduced in [29]. The Unique SMILES views a

chemical structure as a graph with atoms as nodes and bonds as edges and uses a depth first traversal of the graph to generate the SMILES strings. The algorithm establishes a node ordering by using certain symmetry properties of the graphs. In this paper, we present certain molecular graphs for which the algorithm fails to generate UIDs. Indeed, we show that different graphs in the same symmetry class employed by the Unique SMILES algorithm have different Unique SMILES IDs.

SMILES is now the most widely used chemical line notation, though others have been proposed [30, 38] SMILES has become popular because its rule base is very small and it is not encumbered by the need to generate a unique form.^{2,3} In fact, the rules which govern derivation of a formula for an organic molecule are easily mastered by a synthetic chemist. SMILES is best regarded as a language which encodes a connection table representation [30]. Therefore the key to SMILES is that it has its roots in graph theoretical concepts. But its algorithmic definition derives from computer languages and thus permits enhancements which can be expressed as syntactic expressions.

Examples of SMILES notation[39]:

➤ Atoms

C	methane	(CH4)
P	phosphine	(PH3)
N	ammonia	(NH3)
S	hydrogen sulfide	(H2S)

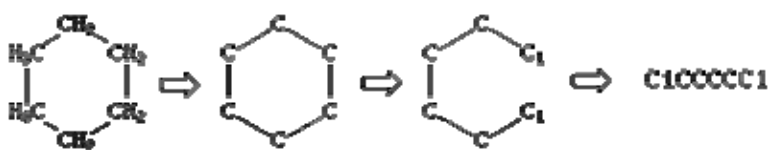
➤ Bonds

CC	ethane	(CH ₃ CH ₃)
C=O	formaldehyde	(CH ₂ O)
C=C	ethene	(CH ₂ =CH ₂)
O=C=O	carbon dioxide	(CO ₂)
COC	dimethyl ether	(CH ₃ OCH ₃)
C#N	hydrogen cyanide	(HCN)
CCO	ethanol	(CH ₃ CH ₂ OH)
[H][H]	molecular hydrogen	(H ₂)

➤ Branches

CCN(CC)CC	CC(C)C(=O)O	C=CC(CCC)C(C(C)C)CCC
Triethylamine	Isobutyric acid	3-propyl-4-isopropyl-1-heptene

➤ Cyclic structures



3.3.6.7 AACS (Apparatus Assembly connection String)

Inspired from the SMILES concept we have invented a similar type of line notation for chemical assemblies, named as AACS. Which generates an abbreviated string which demonstrates the apparatus connecting sequence from left to right.

This was the major task of development to generate such a string out of apparatus connecting data. Although we have achieved our task of making a line notation for the assembly connections we had to concentrate on putting more efforts on making it unique line notation irrespective with the connecting sequence and positions of apparatuses.

Our main focus was to apply a graph theory, as discussed above to generate a unique AACs. However apparatus connection is not similar to molecule (chemical structure). Apparatus connection doesn't follow any standard path like molecules therefore trying to generate graph and trees failed with AACs.

3.3.6.8 Generating AACs:

To carry out a simple distillation, the apparatus set up is used as shown in above figure. The apparatus consists of a round-bottomed distillation flask, a still head, and a condenser equipped with a receiver adapter attached to the preweighed receiving flask. Assume that apparatus is adequately supported with clamps.

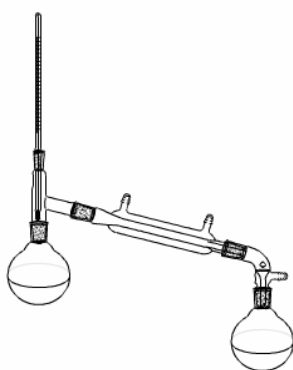


Figure: Apparatus for simple distillation.

For above given example the AACCS will be **N1(DA(TM N1))**, Where

N1: Single neck round- bottomed flask

DA: Distillation Adapter

TM: Thermometer

For generating AACCS we have followed third rule of SMILES; Branches are specified by enclosing them in **parentheses**, and can be nested or stacked. In all cases, the implicit connection to a parenthesized expression (a "branch") is to the left.

3.3.6.9 Unique AACCS:

In last three years I have been interacted with more than 20 chemists at our department. I have been observing them while assembling apparatus. With all my observations I came to the conclusion, all chemists have their own practice to deal with reaction and assembly. Some chemists work only with few and available apparatus, at the same time few of them have tendency to use specific apparatus for particular assembly. I neither noticed any common practice among all nor seen them all following SOP (Standard Operating Procedure). Every chemist has his own style and aspect to deal with apparatus. For example one of my colleague always connects reflux condenser only at middle neck (inlet) of three neck round bottomed flask, where as it doesn't make any difference for others.

Even some assemblies can be mounted in number of possible ways. Here is one example in which air sensitive solid is added with solid addition tube. Below I have drawn two assemblies and both of them are correct. This apparatus has

only two possibilities as overhead stirrer is restricted to connect to middle neck only for frequent stirring, else there would have been more possibilities.

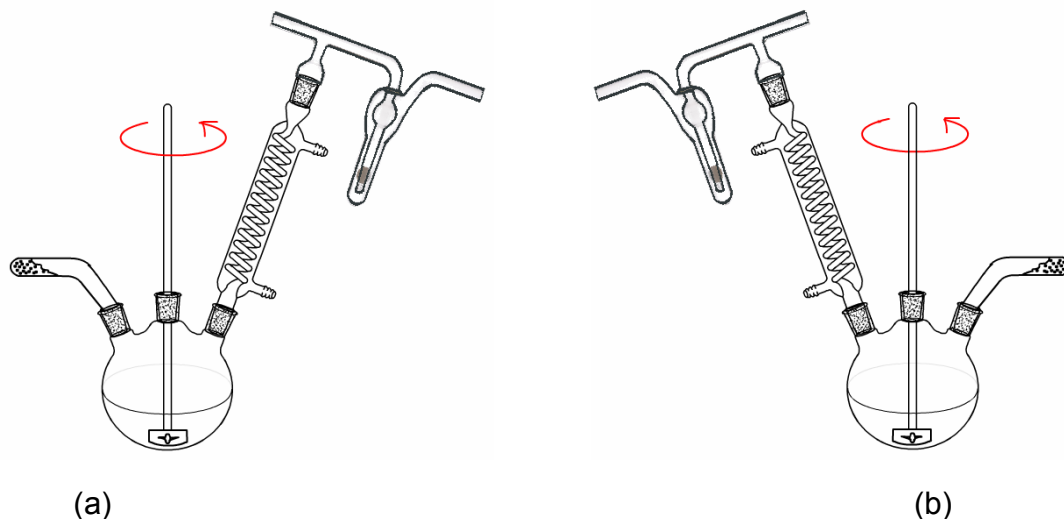


Figure: Reaction flask fitted with solid addition tube, overhead stirrer and condenser.

AACS for (a) RB(ST SR RF(BB))

AACS for (b) RB(RF(BB) SR RF)

Where RB: 3 Nk RB flask

ST: Stirrer

RF: Reflux condenser

BB: Bubbler

As we know in case of computer assessed program correct answers has to be stored and the given answer is being compared with it. If it matches then student receive points for it. As this possible correct answer has to be stored in database we can not store number of right possibilities. There are few assemblies, can be connected in 10 to 20 combinations. In this case we can not enter all these answers in database to check against. We have to find one or

minimum correct possibilities. For this reason we need to make AACCS unique irrespective of its order of connection.

3.3.7 Algorithm and functions

3.3.7.1 Functions:

➤ **Sequence of function calling:**

```
on(release){
    _root.setBtn_val (181);
}
this.createEmptyMovieClip("RBFIsk_mc", 40);
RBFIsk_mc.loadMovie("flsk_3N_1.swf");
onMouseDown = function(){
    this.set_Param();
    this.IdMovie(mvName){
        this.storeName(indx,mvName_var);
        this.getLowerApp(){
            this.lowAppParameter(){
                this.changeSize();
            };
        };
        this.chkHitFlag();
        this.set_rotation();
        this.createEmptyMovieClip(mvName_var,btCkCnt);
```

```

        this[mvName_var].loadMovie(imgName + ".swf");

        this.setHitFlag();

        this.set_ValForSmile();

    };

    exit_IdMovie=function();

};

```

```

EvaluateBtn.onPress=generate_SmileString(){
    setFlag();
    pushSS1(){
        recPushSS1(){
            pushSS1()
        };
    };
    sortSS1(){
        repeatArrange(){
            getX();
            compX(xSmall, xComp);
            arrgString();
        };
    };
    finalSmileString();
};

```

➤ Role of each function

```

on(release){
    _root.setBtn_val(181)
}

```

This Release function is a built in function of action script and is called on click event of each apparatus button and passes a value of button. In

above example conical flask button is clicked and its number 181 is passed.

createEmptyMovieClip("RBFIsk_mc")

This is also a built in function: Which creates an empty movie clip and the movie clip value can be assigned to it with loadMovie function. Name of the movie is passed as a value to the function.

RBFIsk_mc.loadMovie("flsk_3N_1.swf")

This is again a built in function of Action Script. Using this function first by default apparatus is getting uploaded on mounting panel in form of a movieClip. MovieClip name is passed to the function as value with .swf extension. In this case .swf file has to be saved in root directory of application.

onMouseDown()

This is a built in function of Action Script, which is invoked on mouseDown event. Inside this function it calls these functions: *set_Param()*, *IdMovie()*, *storeName()*, *getLowerApp()*, *chkHitFlag()*, *set_rotation()*, *createEmptyMovieClip()*, *loadMovie()*, *setHitFlag()*, *set_ValForSmile()*

set_Param()

This is a user defined function and used to set all parameters with respect to the apparatus value passed in *setBtn_val()* function. These initialised parameters will be used calculating x and y coordinates of connecting apparatus.

IdMovie(mvName)

This is a user defined function and used to load the next connecting apparatus (movieClip) after following some checks and events for that particular apparatus.

storeName(indx,mvName_var)

This is a user defined function and is called to store the name of each connected apparatus in connection sequence in an array. This stored information will be further used while sorting connection string.

getLowerApp()

This is a user defined function and called to find the name and parameters of lower apparatus to which the selected apparatus is expected to connect. It further calls these two functions: *lowAppParameter()*, *changeSize()*

lowAppParameter()

This is a user defined function. It is used to set all required parameters of lower apparatus based on lower apparatus found in *getLowerApp()* function.

changeSize()

This is a user defined function. It is used to change the parameters of connection apparatus and lower apparatus if the apparatus is getting connected with lower connecting point.

chkHitFlag()

This is a user defined function. It is specially called to check whether the apparatus is already connected at clicked location. If yes it displays the status message else it connects at the clicked location.

set_rotation()

This is a user defined function. It is called to select the appropriate movieClip (.swf file) based on value of app_rotation variable, which stores one of these values 0, 20 or -20. Few apparatus can be connected in three different angels. Depend on app_rotation value it calls particular apparatus from root directory. For example app_rotation is 0, 20, -20 then imgname_1.swf, imgname_2.swf, imgname_3.swf called respectively. Here imgname is a name of .swf file given to the apparatus.

createEmptyMovieClip(mvName_var, btCkCnt)

This is a user defined function. After traversing through all function it has movie name to be loaded and it's all required parameters to calculate x and y coordinates of that apparatus. It creates a empty movieClip to load an apparatus.

[mvName_var].loadMovie(imgName + ".swf")

This is a user defined function. It loads the movie with the movie name passed in above function. Here actual apparatus is getting connected at calculated location of x and y.

setHitFlag()

This is user defined function. It is used to set the flag to true to denote that at particular connecting point some other apparatus is connected. This flag further gets checked in *chkHitFlag()* function while connection next apparatus.

ValForSmile()

This is a user defined function. It is called after loading apparatus and stores the name of the lower apparatus in abbreviated form in an array, which further will be used to make a connection string as smile string.

exit_IdMovie=function()

This is a built in function of action script. If it doesn't satisfy all conditions to load an apparatus then this function is called to unload that apparatus and display the message that apparatus can not be connected.

EvaluateBtn.onPress=generate_SmileString()

This is a user defined function. It gets called on press event of Evaluate button. This function generates a connection string called as a smile string with respect to the apparatus connecting sequence. For generating a connection string it takes elements of array stored in *ValForSmile()* function.

pushSS1() and recPushSS1()

These two functions are user defined functions. These are used to

regenerate an apparatus connection string in certain format. These two functions are called within each other till it reaches to the end condition. The regenerated connection string is again stored in array and further it is sorted.

sortSS1()

This is user define function. It is used to sort the connection string. With the help of *repeatArrange()*, *getX()*, *compX(xSmall, xComp)*, *arrgString()* and *finalSmileString()*. It is used to sort the connection string and arranges it in from left to right connecting order. Further it is used to make string unique.

uniqueString()

This is user defined function. This function checks and applies all rules of chemical apparatus assembly and generates a unique connection string respect with the connection order and use of similar apparatus. This is the final and major function of this program. It helps evaluation process easy.

3.3.7.2 Algorithm

What is an algorithm?

A set of ordered steps for solving a problem, such as a mathematical formula or the instructions in a program. The terms algorithm and logic are synonymous. Both refer to a sequence of steps to solve a problem.

Example:

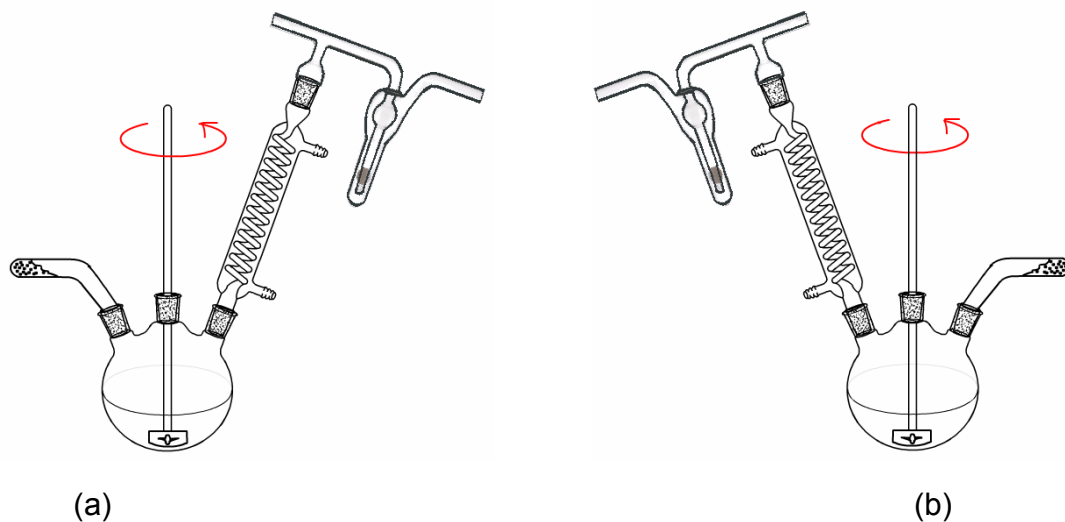


Figure: Reaction flask fitted with solid addition tube, overhead stirrer and condenser.

In this apparatus assembly the addition reagent is air sensitive and has to be added periodically while reaction, so solid addition tube is used here.

(a)

1. Declare and initialize all required parameters (variables)
2. Create empty movieClip with the name RBFIsk_mc.
3. Set all required arrays and require flags for first apparatus.
4. Load movie that is flask_3N_1.swf with respect to RBFIsk_mc. At this point user can see first apparatus placed on panel.
5. User selects first apparatus as Addition tube and its button value is passed to the function setBtn_val() where this passed value is stored in variable BtnValue, which further will be used.

6. User clicks mouse on first neck of the three neck round bottomed flask.
Here `set_Param()` function is called. This function keeps checking, if the button value matches with the clicked apparatus button number. If it matches then it sets all parameters of addition tube apparatus else it checks this with another button value.
7. If `btnFlag` is true then `ldMovie(mvName)` function is called, where `mvName` stores the name of addition tube.
8. `mnName` value is added to `LAppName_arr` array for further use.
9. `storeName()` function is called to maintain a record of connected apparatus so name of addition tube will be added in an array.
10. `getLowerApp()` function is called. Comparing the x and y coordinates of clicked mouse position with x and y coordinates of already connected (available) apparatus it finds the name and location of lower apparatus. Here in this case it finds RB as a lower apparatus.
11. `getLowerApp ()` function calls `lowAppParameter ()` function inside and set or initialises all required parameters of RB as a lower apparatus.
12. Calls `chkHitFlag()` to check at the connecting point which is just clicked by user whether any other apparatus is already connected or not? If not this apparatus is allowed to connect.
13. `set_rotation()` function is called to check at which angle the addition tube has to be connected? According to this rotation value is set to -20 degree.
14. As rotation value is -20, `addTube_2.swf` file is called from root directory to connect.

15. Calls setHitFlag() function is called to mark that first point of RB is connected with addition tube.
16. Calculates the x and y coordinates of new connection addition tube.
17. Empty movie clip is created for addition tube.
18. addTube.swf is loaded, means it is connected to the first end of the RB.
19. set_ValForSmile() function is called to maintain the apparatus connecting sequence and information.
20. User selects next apparatus as stirrer and its button value is passed to the function setBtn_val() where this passed value is stored in variable BtnValue, which further will be used.
21. User clicks mouse on middle neck of RB. Here set_Param() function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all parameters of stirrer apparatus else it checks this with another button value.
22. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according stirrer and connection position on RB.
23. User selects next apparatus as a reflux condenser and its button value is passed to the function setBtn_val() where this passed value is stored in variable BtnValue, which further will be used.
24. User clicks mouse on right neck of RB. Here set_Param() function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all

parameters of stirrer apparatus else it checks this with another button value.

25. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according reflux condenser and connection position on RB.

26. User selects next apparatus as a bubbler and its button value is passed to the function `setBtn_val()` where this passed value is stored in variable `BtnValue`, which further will be used.

27. User clicks mouse on top of RF. Here `set_Param()` function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all parameters of stirrer apparatus else it checks this with another button value.

28. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according bubbler and connection position on RF.

29. At the end of all connection we have connection string like this

Apparatus	RB	AT	SR	RF	BB
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RB	RB	RF
-----------------	---	----	----	----	----

30. User clicks evaluate button to evaluate the apparatus

31. `generate_SmileString ()` is called. It rearranges the connection string. If apparatuses are not connected sequentially from left to right it rearranges it from left to right. Consider if the connection sequence is as below instead of above sequence.

Apparatus	RB	SR	RF	BB	AR
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RB	RB	RF
-----------------	---	----	----	----	----

Then it rearranges it from left to right and display like below

Apparatus	RB	AT	SR	RF	BB
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RB	RB	RF
-----------------	---	----	----	----	----

32. simplifies the connection string

Apparatus	1	RB	AT	1	RB	SR	1	RB	RF	1	RF	BB	1
Lower Apparatus	1	N	RB	1	N	RB	1	N	RB	1	RB	RF	1

33. It further simplifies

Apparatus	1	RB	(AT)	1	RB	(SR)	1	RB	(RF)	1	RF	(BB)	1
-----------	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---

34. It further simplifies

Apparatus	1	RB	(AT)	1	RB	(SR)	1	RB	(RF	(BB))	1
-----------	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	----	---	---	---

35. It further simplifies

RB (AT SR RF (BB))

Connection string: RB (AT SR RF (BB))

(b)

1. Declare an initialize all required parameters (variables)
2. Creates empty movieClip with the name RBFIsk_mc.
3. Sets all required arrays and requires flags for first apparatus.
4. Loads movie that is flask_3N_1.swf with respect to RBFIsk_mc. At this point user can see first apparatus placed on panel.
5. User selects first apparatus as Reflux condensor and its button value is passed to the function setBtn_val() where this passed value is stored in variable BtnValue, which further will be used.
6. User clicks mouse on first neck of the three neck round bottomed flask. Here set_Param() function is called. This function keeps checking, if the button value matches with the clicked apparatus button number. If it matches then it sets all parameters of addition tube apparatus else it checks this with another button value.
7. If btnFlag is true then IdMovie(mvName) function is called, where mvName stores the name of addition tube.
8. mnName value is added to LAppName_arr array for further use.
9. storeName() function is called to maintain a record of connected apparatus so name of addition tube will be added in an array.
10. getLowerApp() function is called. Comparing the x and y coordinates of clicked mouse position with x and y coordinates of already connected (available) apparatus it finds the name and location of lower apparatus. Here in this case it finds RB as a lower apparatus.

11. getLowerApp () function calls lowAppParameter () function inside and set or initialises all required parameters of RB as a lower apparatus.
12. Calls chkHitFlag() to check at the connecting point which is just clicked by user whether any other apparatus is already connected or not? If not this apparatus is allowed to connect.
13. set_rotation() function is called to check at which angel the addition tube has to be connected? According to this rotation value is set to -20 degree.
14. As rotation value is -20, reflux_2.swf file is called from root directory to connect.
15. Calls setHitFlag() function is called to mark that first point of RB is connected with addition tube.
16. Calculates the x and y coordinates of new connection addition tube.
17. Empty movie clip is created for addition tube.
18. reflux.swf is loaded, means it is connected to the first end of the RB.
19. set_ValForSmile() function is called to maintain the apparatus connecting sequence and information.
20. User selects next apparatus as a bubbler and its button value is passed to the function setBtn_val() where this passed value is stored in variable BtnValue, which further will be used.
21. User clicks mouse on top of RF. Here set_Param() function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all parameters of stirrer apparatus else it checks this with another button value.

22. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according bubbler and connection position on RF.
23. User selects next apparatus as stirrer and its button value is passed to the function `setBtn_val()` where this passed value is stored in variable `BtnValue`, which further will be used.
24. User clicks mouse on middle neck of RB. Here `set_Param()` function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all parameters of stirrer apparatus else it checks this with another button value.
25. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according stirrer and connection position on RB.
26. User selects next apparatus as a Addition tube and its button value is passed to the function `setBtn_val()` where this passed value is stored in variable `BtnValue`, which further will be used.
27. User clicks mouse on right neck of RB. Here `set_Param()` function is called. This function keeps checking, if the button value is matches with the clicked apparatus button number. If it matches then it sets all parameters of stirrer apparatus else it checks this with another button value.
28. Repeat steps from 7 to 19 only respective parameters like rotation value, movie names are according addition tube and connection position on RB.
29. At the end of all connection we have connection string like this

Apparatus	RB	RF	BB	SR	AT
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RF	RB	RB
-----------------	---	----	----	----	----

30. User clicks evaluate button to evaluate the apparatus

generate_SmileString () is called. It rearranges the connection string. If apparatuses are not connected sequentially from left to right it rearranges it from left to right.

Apparatus	RB	RF	BB	SR	AT
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RF	RB	RB
-----------------	---	----	----	----	----

31. simplifies the connection string

Apparatus	1	RB	RF	1	RF	BB	1	RB	SR	1	RB	AT	1
Lower Apparatus	1	N	RB	1	RB	RF	1	N	RB	1	N	RB	1

33. It further simplifies

Apparatus	1	RB	(RF)	1	RF	(BB)	1	RB	(SR)	1	RB	(AT)	1
-----------	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---

34. It further simplifies

Apparatus	1	RB	(RF	(BB))	1	RB	(SR)	1	RB	(AT)	1
-----------	---	----	---	----	---	----	---	---	---	----	---	----	---	---	----	---	----	---	---

35. It further simplifies

Connection string : RB ((BB) SR AT)

RB	(RF	(BB)	SR	AT)
----	---	----	---	----	---	----	----	---

Here we see (a) and (b) both are correct but we get two different answers i.e. (a) RB (AT SR RF (BB))

(b) RB ((BB) SR AT)

To solve above mentioned problem we have to make a string unique irrespective with the connection sequence.

The has to be checked against few rules like if there are Addition tube and Reflux condenser connected to the RB flask then rearrange the connection and irrespective with the position of addition tube just make it sure that addition tube is connected at left neck of RB and reflux condenser and it's further connection is connected to the right neck of the apparatus. Then example (b) is solved in this way

Apparatus	RB	RF	BB	SR	AT
-----------	----	----	----	----	----

Lower Apparatus	N	RB	RF	RB	RB
-----------------	---	----	----	----	----

32. User clicks evaluate button to evaluate the apparatus

generate_SmileString () is called. It rearranges the connection string. If apparatuses are not connected sequentially from left to right it rearranges it from left to right.

Connection is passed through uniqueString() function, which checks it against set rules and rearranges.

Apparatus	RB	AT	SR	RF	BB	
Lower Apparatus		N	RB	RB	RB	RF

33. simplifies the connection string

Apparatus	1	RB	AT	1	RB	SR	1	RB	RF	1	RF	BB	1
Lower Apparatus	1	N	RB	1	N	RB	1	N	RB	1	RB	RF	1

34. It further simplifies

Apparatus	1	RB	(AT)	1	RB	(SR)	1	RB	(RF)	1	RF	(BB)	1
-----------	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	---

35. It further simplifies

Apparatus	1	RB	(AT)	1	RB	(SR)	1	RB	(RF	(BB))	1
-----------	---	----	---	----	---	---	----	---	----	---	---	----	---	----	---	----	---	---	---

36. It further simplifies

RB	(AT	SR	RF	(BB))
----	---	----	----	----	---	----	---	---

Connection string is: RB (AT SR RF (BB))

The concept of unique string is proven as we have same answer in both cases.

(a) RB (AT SR RF (BB))

(b) RB (AT SR RF (BB))

3.3.7.3 Conclusion

eAT Virtual Chem Lab has been included in iChemLab, which is accessible via TUWEL. With the success of simplified evaluation process of the eAssessment tool, It is possible to conduct and evaluate chemistry laboratory exams online.

In future when SOPs will be in practice, this tool will be used as a standard protocol to educate the students and technicians. We believe that the use of this tool will not only improve the assembly knowledge of the students but also will help to great extent for improving safe laboratory practices in chemistry laboratory.

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