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Applications of Digital Simulation in the Field of Chemistry

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ABSTRACT

The development of digital technologies, computers now used as most powerful tool to learn and understand difficult concepts of chemistry in better way. In science education and research field computerised representation, descriptions and simulations are used to understand, explain and predict various complicated processes. These practises promote thinking and explaining abilities, that are of great aid for students and scientists. The applications of digital toolsare its flexibility in use that provide better opportunities to the students, teachers, research workers to interact, cooperate and collaborate more efficiently and effectively.

Key word: *digital technology, computers, simulations, education, research field.*

I. Introduction

Computers have opened up a new world with the internet, enabling information and activities to be easily accessible. Computer provide for a vast world of resources which is very helpful in education. Teachers can make use of internet to search for more information on various topics and therefore craft interactive activities for students. And the same can be used for students to dig deeper in their subjects and do their assignments & projects in an efficient way. The use of computers as teaching tools by the teacher is very beneficial teachers can construct PowerPoint presentations in order to provide their students with necessary information. Teachers can use different software programs to show geography, science, chemistry, and math, among other things, and help the students. The utilisation of technology, especially computer-based technology in teaching exists since its inception. Whether it is the use of overhead transparencies or power point presentations or browsers and graphics programs in website design, computer-mediated technology for instructional purposes, a mediated classroom designed as a virtual team an online/virtual classroom integrated learning management systems almost all modern educational institutes include at least some use of computer-based technology as far as role of computers in field of chemistry is concerned it can be used in various ways.

II. Applications of Computers to Chemical Problems

Studies of relationships between molecular structure and chemical properties (chromatographic retention, boiling points, aqueous solubility's) or biological activities (pharmaceutical effects or toxic effects); applications of computational methods including pattern recognition and neural networks and multivariate statistics to analytical data interpretation can be understood in a better way with the help of computers. Teachers and research scholars develop and use computer-assisted methods to investigate relationships that link molecular structures of organic compounds with their chemical properties or biological activities. Computer-assisted methods can be used to investigate relationships between molecular structure and chemical properties for large sets of organic compounds. This approach is data intensive and inductive because a large training set of compounds with known property values is the starting point for each study. Such studies involve

the following steps: a) graphical entry and storage of the structures to be used to develop the model along with their experimental property values, b) three-dimensional molecular modelling using either molecular mechanics or molecular orbital approaches, c) molecular structure descriptor generation, (d) analysis of the descriptors for utility, that is, feature selection, by interactive, user-guided methods or simulated annealing or genetic algorithm methods, and e) the development of quantitative predictive models using multivariate statistical methods.Examples of application areas where this methodology has been used include gas chromatography retention indices, high-performance liquid chromatography retention times, ion mobility spectrometry reduced mobility constants, henry's law constants, normal boiling points, aqueous solubility, supercritical carbon dioxide solubility, surface tensions, vapor pressures, and auto ignition temperatures.

Similar computer-assisted methods also can be used to investigate the area of quantitative structure-activity relationships. This area of study encompasses attempts to rationalize the connections between the molecular structures of organic compounds and their biological activities. Techniques drawn from chemical structure information handling, physical organic chemistry, pattern recognition, multivariate statistics, conformational analysis, molecular orbital theory, data analysis using computational neural networks, genetic algorithms, and other areas form this new approach to structure-activity studies the analysis of spectral data by computer assisted methods is another area of current interest. The data are from fibre optic sensorswhich have a number of polymeric coatings that alter the fluorescence spectra of analysts that are sensed. The raw data are a set of fluorescence time series, and the objective is to develop computational neural networks that can use these data to identify the analysed compounds.The computers techniques involved in these studies of molecular structure and chemical properties or biological activity have been combined into an interactive computer software system called adapt. The software is designed to support the computations necessary for these types of studies in a seamless system that makes the studies convenient to perform

Application of computers *as the chemistry coach* there is a well-organized site on internet that contains tutorials and quizzes for chemistry students. Subjects covered include: dimensional analysis, the theory of the atom, balancing equations, bonding, and stoichiometry.

Chemistry resource centre, the teacher resource site, offers more than chemistry demonstration ideas this is an interactive site, modelling the ideal gas laws. Students and researchers can control the number of particles, velocity of the particles, the pressure in the container, and the size of the container to see correlations between different variables and the volume.

The pressure chamber, this simulation demonstrates gas laws such as: constant volume, constant temperature, and the ideal gas law. Three experimental procedures with excellent instructions are provided.

III. Application of Simulation in Chemistry

The computer can also work as a simulator to allow students to explore phenomena. Some applications are too expensive or too impractical for the classroom, but we can use computers to simulate them. Computer simulations and animations are usually excellent tools for chemistry education. Animations can help in presenting complicated concepts or theories by showing step-wise sequences of images, diagrams or numbers. On the other hand, simulations imitate the system. Upon changing or putting certain values or parameters the computer reflects change in the output. Some variable or random elements are present in simulations. Simulations provide students to get a hands-on experience in cases when real systems are difficult to setup, thus providing best alternative way to explore science.
Tutorial and multimedia software engage students in meaningful interactive dialogue and creatively employ graphics, sound, and simulations to promote acquisition of facts and skills, promote concept learning, and enhance understanding.

Simulation software should provide opportunities to explore concepts and models which are not readily accessible in the laboratory, e.g., those that require:

A. Expensive or unavailable materials or equipment
B. Levels of skills not yet achieved by the students
C. More time than is possible or appropriate in a real-time classroom,
D. Hazardous material and procedure.

Some examples of simulation technique: Simulation means different things to different people. Science can be seen as a simulation of nature in a broader sense. As we all know, newton simulated the motion of objects by using simple formulas, and the properties of most gases are simulated by the ideal gas law. However, these simulations are around for such an extended time that we have a tendency to settle for them as a truth, as a result of validation of these models or simulations by a lot of individuals. Simulation can be concluded as a good model for exploration or learning. A simulation for teaching general chemistry is mostly supported by some theories within the domain of this level. Certainly, the main plus point of these simulations is a life like visual effect to teach these theories.

A system could be created based on few theories. For example, van der Waals equation can be used for real gases to illustrate how real gases differ from the ideal gas. These equations are used to simulate a system in a java applet for the user to appreciate the difference. From this simulation, a user is asked to find out conditions in which the ideal gas law gives results within a set error limit.

A java applet is composed for the purpose of simulating the properties of gases. A user can pick any of the several gases to examine at a particular time. The temperature and volume are two independent variables that can be altered, and the pressures calculated by the two models are presented.

IV. Chemical Reaction Simulations

Chemical reactions are indeed the backbone of chemistry, and we mostly focus on the rate laws on this topic as we intend that the students develop the skills required to find the variations of reactants or products in the system. There are many types of chemical reactions, and their modelling depends on the reactants, the products, and the rate constants. Every reaction modelling is unique in nature, and it can be of several types. Reaction modelling makes it more attractive than the ones using words, equations, tables, and graphs. We have also written a simulation to show the variation of reactants and products using random rate constants and order of reactions. The object of this type simulation is for the user to figure out the order and the rate constants. Some aids were built in. For example, by pressing certain keys, the user can plot diagrams to figure out the order of the reactions. Evaluation of the rate constant is easy.

Properties of gases

Properties of gases are integrated in general chemistry. Avogadro's law, Boyle's law, Charles's law, and Dalton's law (the laws of gases) and the ideal gas law have always been in Nernst equation the effects of temperature and concentrations in a voltaic cell is simulated. The user can alter the concentration and temperature to find cell potential calculated by the Nernst equation.

Atomic orbital plots electron density of an atomic orbital on a plane quite same as the java applet that plots electron densities of the hydrogen molecule as previously shown.

The structure of polonium builds the simple cubic unit cell of polonium by steps. This structure is very simple, but also very rare. The existence of this structure was suggested from a powder x-ray diffraction, but so far, no other metal has this type of structure.

The a to b conversion simulates the type of chemical reactions

$$A \underset{k_b}{\overset{k_f}{\longleftrightarrow}} B$$

With a forward and a backward reaction rate constant, k_r and k_b. In this version, any value even the negative ones are accepted for these rate constants.

Titrationand simulation a titration experiment graphically. The pH is calculated after the titrant is dropped into the beaker from a burette by the user upon pressing a key. The simulation works for a titration of a strong acid by a strong base, a weak acid by a weak base or a weak acid by a strong base. In order to evaluate the pH at equivalent points for laboratory reports, some students come back to this program at higher years.

pH of solution when a strong acid added to water can be determined using experiment simulation of mixing of acid to water in absence of buffer. Dropin pH due to formation of $H_3O^+Cl^-$

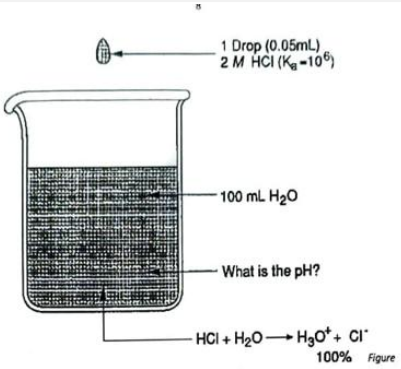


Fig: Experiment to show how pH changes on addition of acid (the azimuth project- petri net, n.d.) (chieh&sze, computer animations and simulations in general chemistry)

Computer simulations can be utilised for education, prediction of natural phenomena and problem solving. There are many internets site gives simulations made up using forms on the chemistry, and in particular computational chemistry and molecular modelling, is well suited for learning over the internet using the world wide web augmented by other internet.

Computational and theoretical polymer science

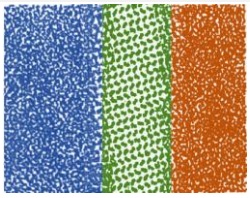
The primary aim of the journal of computational and theoretical polymer science is the publication of high-quality manuscripts dealing with analytical theory, computational methods, and simulations of polymeric systems. Representative areas include the following: - molecular mechanics and quantum mechanical calculations - polymerization reactions - distribution functions, fluctuations, correlation functions - electronic structure - molecular dynamics of polymer chains.

Computers And Chemical Engineering

Computer & chemical engineering is primarily a journal of record for new developments in the application of computing and systems technology to chemical engineering problems

Computers and chemistry

Some approaches that are particularly appropriate for teaching computational chemistry as well as other areas of chemistry.



Ice Liquid water

Fig: Ice melting simulation

What do we see in this picture? The image is a 'snapshot' from a 500 ps molecular dynamics named simulation that shows how the structure of water changes when ice melts. The red spheres represent liquid water molecules, blue spheres represent ice, and green spheres represent water in the interfacial region. The image shows researchers that water molecules form clusters when they melt (the clusters can be seen in the interfacial region). Many topics in chemistry require learners to understand structures in three dimensions, changes over time, and causality. Molecular animations can be powerful tools for learning these dynamic and three-dimensional chemistry concepts. However, a problem with the use of animations for teaching molecular structure and dynamics is that merely viewing visualization may lead to learning at a lower level than would draw or building a molecular structure

V. Conclusion

In this study, the application of computer simulation has been considered as great aid in contemporary chemistry education and research work over several fields such as organic chemistry, biochemistry, physical chemistry and work related to research. several simulations were used by students and researchers to solve many problems in chemistry. It provides a better platform to represent, explain and understanding complicated phenomenon of chemistry. Digital aid has a powerful application in research and development field by solving many problems within less time frame.

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