MAIN DIRECTIONS IN TEACHING AND LEARNING CHEMISTRY BY USING THE COMPUTER

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Abstract:
The purpose of this paper is to present some aspects of the interdisciplinarity between chemistry and information technology in Romanian schools in this period.
Some of the didactic methods like: simulation, molding, experiment, evaluation, programmed instruction sometimes can be introduced in a chemistry class using the computer as a didactic tool.
In the paper we present aspects of our preoccupations regarding educational software used to simulate some laboratory experiments included in the curriculum for high schools and universities which can pollute the environment if we make them in the class.
We also illustrate how to use the Internet tools to get information about chemical substances, physical - chemical processes from data banks which can be used for statistical and graphical applications, or to work online on some free sites which allow an interactive process of teaching and/or learning chemistry.
We will either have in view the education of the students, the future chemistry teachers, to gain professional skills to integrate the educational software into didactic processes.

Keywords
Simulation, educational software, experiments, internet tools.

1. GENERAL CONSIDERATIONS

The connection between education and information technology is a part of the educational policy of our country at high school and university levels. The adoption of the political decision of starting such a reform has involved technical and social risks, but it has followed the orientation of the entire Romanian society in the assimilation of the EU standards and values. As far as this reform is concerned, the Ministry of Education and Research has taken the decision to implement the IES (The Informatic Educational System).The "SIVECO Romania" Company is the software integrator of the IES program and it has developed and coordinated the implementation of the EAHS platform (The Educational Assistant for High Schools) in one thousand twenty high schools of Romania.

Today, the main objective of the universities is to provide academic information to students consisting of projects, courses for professional improvement, documentation or distance learning. For that, the initial formation of the students has to train them to become users of the EAHS platform. The universities have difficulties with that because they are not integrated into this program and so they do not benefit from proper computers and software.

Chemistry, which operates with a huge number of experimental and theoretical data, should appeal to the facilities offered by computers in order to stock, access and process the required data. So, the chemist has to be at least a user himself.

In our opinion, to be able to use a computer is a proof of civilization and helps us to fit into the actual international context in which all kinds of communication skills are not possible without it.

2. RESULTS AND DISCUSSIONS

If a chemistry teacher whishes to make his lessons more attractive and understandable, he will definitely find many ways of using computer while teaching, such as: conversation, molding, simulation, lab experiment, discovery, programmed instruction and evaluation with traditional and/or alternative instruments.

In the following section, we shall present two examples of using certain software programmes on some chemical issues.

Model Science – ChemLab is an interactive simulation of a chemistry lab, ideal for lab run-throughs, demonstrations, pre-lab work, dangerous labs, pollutant experiments and labs which cannot be performed because of time limitations.

We would like to mention some of the experiments provided by the school curricula and which may pollute the environment and be performed with this software:
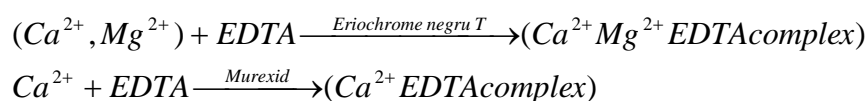
- ✓ Red Hg oxide decomposition at heat as method of obtaining O_2 and Hg (poisonous);
- ✓ Obtaining Cl_2 (toxic and corrosive) from reactions between $KClO_3$, MnO_2, $KMnO_4$ and HCl solution;
- ✓ Obtaining sulphur and nitrogen oxides (components of smog and producers of acid rains) from Cu with concentrated solutions of H_2SO_4 / HNO_3;
- ✓ Obtaining I_2 (harmful for the thyroid gland) from solid $K_2Cr_2O_7$ and KI at heat.

Among the many pre-programmed simulations of the ChemLab, we consider the hard water issue to be of a great practical interest, because it is not a part of the required chemistry content lists at a high school level. For example, in hard water the vegetables do not boil, soaps and detergents do not emulsify the impurities, and some little-soluble depositions are formed on pipes.

In order to determine the hardness of a water sample, we should follow three steps:

Theory – a hard water solution means a solution containing appreciable amounts of calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions, but may include other components, such as solids, organic compounds, dissolved gases, or other negative and positive ions. In the presence of the HCO_3^- ions, a pH>7, and at heat, massive carbonate scale formations occur.

To determine the hardness of a water sample, the chemist may use the EDTA (ethylendiaminetetraacetic acid) titration. The EDTA anion reacts quickly with any bivalent metal in order to form a soluble metal EDTA complex. But these salts are colorless and require an indicator to show when the reaction ends.

$$(Ca^{2+}, Mg^{2+}) + EDTA \xrightarrow{\quad Eriochrome\ negru\ T \quad} (Ca^{2+}Mg^{2+}EDTAcomplex)$$

$$Ca^{2+} + EDTA \xrightarrow{\quad Murexid \quad} (Ca^{2+}EDTAcomplex)$$

Procedures (calcium hardness determination) – fill a 50 mL burette with 0.01 M EDTA solution; add 50 mL of an unknown hard water solution into a 100 mL beaker; add 4 mL of 1 M sodium hydroxide solution; add 100 mg of Murexid indicator; place the beaker on a stirrer and titrate.

Report – Initially, the solution in the beaker is orange. If the sample is hard water, the color of the solution turns to purple on the endpoint.

The report paper can contain some items for self evaluation:

I_1. How do you explain the necessity to use the "Calgon" in the washing machine to prolong its functioning?

I_2. In a hard water sample that also contains FeS, we add HCl. What danger is there?

For the high school level, we can use the **CHIME** software for interactive learning of the structural properties of amino acids. The pupils can also obtain information on the amino acids binding to form the peptide chain. This software can be found and used freely at the web address http://www.chime.tv

For the university level or for special high school classes (or even for very clever pupils in ordinary classes), we can use computers and internet tools in order to reveal the structural properties of the proteins. The most well known bank that contains structural data for proteins is the Protein Data Bank of Brookhaven National Laboratory (PDB). It can be accessed freely using the internet; its web address is http://www.rcsb.org. This bank of data also allows downloading files, which contain a 2D or 3D visualization of the entire protein or of its domains. In order to achieve such a visualization we may use two types of software:

The **RasMol**, which is a software that allows users a 3D visualization and the animation of the biological macromolecules. It is easy to use when looking at the macromolecular structure and its relation to the biological function. It also allows us to see infrared spectra with animated molecular vibrations. We can download freely the RasMol from its web site at the address http://www.umass.edu/microbio/rasmol/;

The **MolScript**, which is a software that enables users to create schematic and detailed graphics of molecular 3D structures. Its web address is http://www.avatar.se/molscript.

The steps used in order to obtain structural information and data files from PDB are the following:

- Accessing the web page of PDB – http://www.rcsb.org;
- If we do not know the identifier for the protein we choose "search" and type the name of the protein. In this case, we will obtain a list containing all the files for the requested protein and we will choose the file that we need;
- If we know the protein identifier, we type it in the corresponding space;
- On the screen, we will obtain the page for this protein. If we need structural information, we choose it from the left side of the page "Download/Display File" and then we choose "Display the structure file" and the format "Complete with coordinates". If we only want the visualization of the protein or of its domains, we must choose "View structure".

From the PDB file we can also obtain other pieces of information: the geometry of the structure and geometrical parameters, information about the sequence details, the structure factors and the opportunity to access other sites with similar information.

3. CONCLUSION

The aforementioned aspects reveal the interdisciplinarity between chemistry, biology and information technology, which are naturally shown with the help of the didactic software and the Internet.

Simulation and molding are the bases of all computer applications used in the study of theoretical and experimental chemistry.

The teachers should give up the simplest methods in favor of the more complex ones, which use the computer as a didactic tool.

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