ONE CHEMISTRY - TWO MEANINGS. SCIENCE AND EDUCATION: COMPARATIVE ANALYSIS OF THE ROLES, PRESENTATION AND APPLICATIONS

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Abstract

The comparative analysis of different meanings of Chemistry is carried out, taking in account philosophical, didactic, psychological and socio-cultural aspects. The issue is discussed in terms of the concurrent existence of two different subsystems referred both to Science and Education which can be found in presentations of chemistry knowledge. The study overviews researcher's findings made in the field of Science Philosophy and Chemistry Didactics. Theoretical study based on profound concepts from Science and Chemistry philosophy as well on few empiric researches carried out by researcher in the field of Chemistry Didactics.
Keywords: *beautility, chemical object, chemistry education, modelling in science, visualization-based teaching*.

Introduction

What is Chemistry? Referred either to Craft, Art, Science or Philosophy? Why we need Chemistry? Only because we need products resulted from Chemistry activity? Or we could find from this activity something more: aesthetic and spiritual?

We live in the world where Technology and Science are among the forces defining the development of any country. Education gives people skills and knowledge, which make Technology and Science the tools to gain a progress and success. The time science created crisis seems to go away and just now the same science may resolve the most exciting challenges of our life. Chemistry is cornerstone of a scientific paradigm: it operates the body of exact sciences, explores the nature and concerning many humanitarian and social issues. Thus, questions how to explore (Science) and teach (Education) chemistry in all the aspects and what ways to choose for organizing a process of research and education are of great importance both for fundamental or applied researches and social, cultural and economic development of any country.

The other problem is how to distinguish two different meanings of one field of knowledge (Chemistry particularly): Science and Education (here cutting more general meaning of education to academic discipline). The scheme reflects the simplified interconnection between these divergent, but interdependent categories based on general basic invariant (object) and variable subject units, the latter having its own ramified system out of the focus of this analysis.

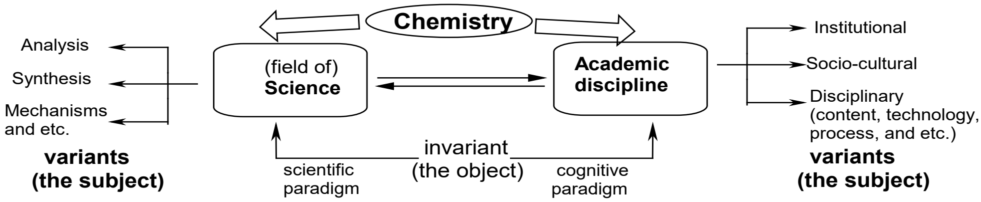

Figure 1. Interconnection between scientific and educational paradigms of Chemistry.

Research Methodology

The purpose of the study was to review previous findings in the field of Science Philosophy and Chemistry Didactics. Theoretical study based on profound concepts from Science and Chemistry philosophy as well on a few empiric researches carried out by the author in the field of Chemistry Didactics. Comparative analysis of the role, presentation and application of Chemistry knowledge was done based on the author's original articles devoted to theoretical principles of chemical philosophy and empiric researches in the field of Didactic Chemistry.

Population in empiric researches mentioned in the article included few groups of respondents. It covered almost all the ages starting from primary school pupils (Lakhvich, 2008) up to University students, and different lines of education. In all experiments two groups (experimental and control) were formed based on the results of pre-intervention test. The main reason of the sampling generalization was to form the bigger groups to validate the microstatistics under the circumstances of respondent lack. Pre-intervention test showed the statistical uniformity of both groups consisting of students from different age groups.

Visualization-based teaching has been implemented. The latter included models, animations, experiment, play-therapy, molecular docking and etc. Animations assisted different topics and the emphasis was made to form a visual-based acceptance of chemistry information, regarding the attractiveness and age-related accessibility of the models. In control groups students were supplied with regular didactic materials and accustomed educational techniques.

Research Results

In the beginning it is possible to start with a few attempts to understand the terms and find the common denominator for the two meanings of Chemistry knowledge.

Chemical Objects as Integration Unit for Chemistry

Roles, applications and presentations are variable. The objects integrate both paradigms in one branch of knowledge. Taking into account all previous empiric findings and modeling about the structure of matter it's worthy to discuss three types of chemical objects: substance, molecule, and finally chemical presentations (or chemical models)

(Shummer, 1998; 2003). The latter category can't be neglected, because in most cases in educational process and in many cases in science we operate with presentations. Chemical formulas are the simplest example of chemical presentation that is quite different both from substance (possessing physical and chemical properties) and molecules (characterized with shapes, stereometry, distances between atoms, etc.). Formerly, we discussed the applicability of different formulas both in Education and Science (Lakhvich, 2006, 2007, 2010). They are neither substances nor molecules, integrating meanings from both. Inexperienced scholar could suppose the structural formula would be a simple pictogram reflecting geometry of the molecule. But obviously, the chemical bonds presented as lines (solid, dashed and wedged) barely reflect the real distances between atoms, mostly presenting the arrangement of atoms in space and strengthening the idea about prevalence off attraction on repulsion in chemical compound. The latter originates from molecule meaning. Chemical bonds in structural formula originate from substance meaning reflecting mostly the ability to take part in chemical reactions. The model of double bond is the great evidence for this. Obviously, it visualizes the chemical property of the substances to be saturated (the fact found in the experiment), the latter gave rise to double bond presentation model to visualize the substance "saturation" in terms of addition process. Instead of double bond we obtain two new bonds, and thus introduction of new atoms in compound being visualized in an adequate model.

Modeling and Visualization

Adequate modeling is a key technique for presentation of chemical objects both in science and education. The initial period of Science itself and Science Education was based on the experiment. The new Science paradigm is rather formal by nature and fundamental in Philosophy meaning. Still the tool for interconversion between the empiric and theoretical moieties seems can be associated with the problem of modelling, which is one of the most important in modern Science. Formerly, we postulated (Lakhvich, Kostareva, & Lehankova, 2009; Lakhvich, 2010) that adequate modelling and visualization in particular is to be the core element for the modern Educational model and paradigm for Science. A great number of publications, devoting to the problem, confirm dramatically its relevance. Still models were discussed in terms of object recognition and computational modeling. We consider the category of modelling is more comprehensive and can be discussed in various aspects, some of them are all-pervading philosophy principle (Harnad, 1987), psychological tool for cognition (Lakhvich, Kostareva, & Lehankova, 2009) and finally the model having for Science its own complex structure.

Models are appropriate not only for theoretical considerations but useful for practically oriented fields of Science. The typology of models has been developed regarding their hierarchy in dependence of their relative similarity (Trindle, 1984; Tomasi, 1986). Still it has been found (Tomasi, 1999) that for theoretical investigation the models can be classified in another way. The components of this subsystem are hierarchically dependent, and the most comprehensive definition refers to interpretative model. The interpretative model is absolutely appropriate for speculation of different scientific concepts; the adequacy of such a model ought to be judged with the aid of few criteria (generality, utility, self-constituency and etc.).

Structural formula is a good example of modeling of chemical objects and is widely used both in Education and Science. Molecular docking is another example of effective modeling. It predicts the preferred orientation of one molecule relative to another at their bonding to form a stable complex. Knowledge of the preferred orientation allows to forecast the strength of the association, or affinity to binding between two molecules. This modelling is widely used in Molecular Biology, Computational Chemistry and Drug Design (Scientific paradigm) and can be effectively introduced in Educational process (Educational paradigm).

Science Modeling vs Educational Application

Molecular docking has been developed actively for about three decades (Lengauer & Rarey, 1996; Kitchen, Decornez, Furr, & Bajorath, 2004). My own experience when working with Pharmacy students has demonstrated the relevance of the approach in educational process, in particular in context of introduction of inquiry technology which is aimed on using and learning content as a means to develop information-processing and problem-solving skills. Such approach is student centered, them being the participants of the projects.

Though inquiry can be done even in lectures, the best results are distinguished in lab or group work, and in particular within carrying out the student research. There are a lot of investigations done about the Student Research, including both fundamental works (Peters, 2012; Strayhorn, 2013) and focused on definite fields of knowledge, e.g. few investigations in the field of Biomedical and natural Sciences (Amgad, 2015; Ballamingie, 2013; Slack, 2016).

Student Research (SR) is often wrongly associated with lab studies. However, on the one hand, not every lab experiment is a study, on the other - similar to originally scientific research, SR is based on the same procedure and includes formulation of research problem, work with literature, design of experiments (formulating of the aim, conceptual framework and specific questions of research, choice of methodology and procedure), conducting the experiment itself, data collection followed by their verifying, analyzing and interpreting, summarizing and finally presenting the results (publishing and conference activity). Most of universities provide the equipment and resources for real scientific research, which is problematic for high and secondary school. But in all cases students are limited in time, being involved in different forms of academic activity. This makes the idea of the "real scientific research" illusive for most of students. To resolve the problem, an educator must organize SR in such a way to take in account all procedural, psychological and didactic aspects of educational process (Lakhvich, 2017):

- to use only few elements of research technology: the higher level of education, the closest research structure to scientific research;
- the experiments do not necessarily have to be absolutely innovative; the key point is a subjective novelty of the research for the students;
- the research primarily pursues educational and training rather than utilitarian objectives;
- mostly modeling, rather than useless transferring the real problem situation of scientific research in student research, with the exception of expensive equipment and materials;

- to take into account the psycho-physiological profile of students in particular age group.

We have proposed students (mostly from School of Pharmacy) the projects concerning primary investigation of bioactivity of organic substances as potential drugs. Molecular docking was the key element of the SR (Kitchen, 2004). SR included also the literary review and drug analysis (Journals, drug databases), the choice of the substrates (protein databases), the evaluation *in silico* the model, design of drug-candidates and the assessment of their activity *in silico*. The results obtained were valid and correlated with the data from previous researches, were presented in conferences and published. SR motivates students to study professionally oriented topics, trains their skill in the field of pharmaceutical chemistry and molecular biology, as well as helps us to find the candidates for entering the Master and PhD programs.

Aesthetics vs Applicability

Regarding the role of the Chemistry in scientific and educational context we should discuss its aesthetics and applicability. Formerly, we tried to apply the concept of Beautility to Chemistry meaning (Lakhvich, 2010).

Economics grab all the headlines, but beauty is just as important and even has serious financial ramifications. Beauty does serve a function. Beauty is more than skin deep. Beauty is powerful. Utility is beautiful and beauty has utility. Let's call it **'**Beautility**'** for short. Thus, beautility is a definition for objects that is both beautiful and useful, generally objects of special design (industrial, handmade, and finally in our case synthetic origin) which are meant to have utility while having a pleasing aesthetic. Like water and health care, Beautility is an essential civic utility that sustains our life form.

Earlier we postulated (Lakhvich, Kostareva, & Lehankova, 2009) a few additional criteria to judge models in a didactic framework. Models for the academic disciplines need to be adequate, effective, contemporary, exciting, and finally appropriate for successive usage. The similarity between real objects and models can almost be neglected in this context. To create an effective molecular model, we need to accept the influence of many features and conditions, which include both the nature of real objects and didactical (for the academic disciplines) aspects.

Postulating the model/visualisation is to be exciting, we strengthen the idea about aesthetic potential of chemistry knowledge. "Chemistry, the art, craft, business, and now science of substances and their transformations, is today paralleled at every step by hard-won microscopic knowledge of molecules and their reactions" (Hoffmann, 2003). Chemistry is also human labour, and/or matter of their activity. For those it gives both feeling of inspiration and sense of achievement as the feeling of spiritual gratification. Their products (both mental and tangible) originate perception of other people and thus granting the essence of what Chemistry induced. Aesthetics is commonly known as the study of sensory or sensory-emotional values, sometimes called judgments of sentiment and taste. It may be defined narrowly as the theory of beauty, or more broadly as that together with the philosophy and "critical reflection on art, culture and nature" (Encyclopedia of Aesthetics, 2003, p. 24). Aesthetics studies new ways of seeing and of perceiving the world. Thus, Aesthetics is cornerstone of a spiritual paradigm: it operates the body of fine arts and Philosophy, reflects the nature and concerning many humanitarian and social issues. References to Chemistry and Aesthetics reflect the symmetry and their interpenetration: scientific (empiric, objective and utilized) and sensual (spiritual, subjective and ephemeral), forming the symmetry of the World, and the latter looks very aesthetic.

Contribution: What We Have Done to Explore the Potential of Chemistry Visualization

We explored the problem of Chemistry modelling and visualization in different contexts. Based on the original concept (Lakhvich, 2009) of disciplinary didactic principles (DDC: structural adequacy principle, functionality principle, and mechanistic simplification) we elaborated the new didactic system for design of Organic Chemistry course. It consists of original epistemology, didactics, and mathematical evaluation of the adequacy of course design. Reactions were quantitatively assessed (Lakhvich & Vjunic, 2013) in context of their relevance to DDC. The latter includes formal division of reactions to simple stages, stage classification, and finally, matrix and graph analysis of reaction-stage database. Reactions are classified according to 4 criteria: Addition-Elimination, Nucleohilic-Elecrophilic, Carbon-Heteroatom associated processes, Single-multiple bonds. E.g. in acetal formation the hemiacetal protonation stage is classified as $\mathbf{A_{EH1}}$ process which means Electrofilic (**E**) Addition (**A**) to Heteroatom (**H**) with a single (**1**) bond. Based on graph theory and the approach (Tõldsepp, 2003) the continuity and compatibility of content units (stages of reactions) have been also assessed.

We also explored the effectiveness of different visualization and modelling techniques, in particular Condensed Visualization Technology (CVT). The empirical studies showed the utility of the didactic system proposed both for University and School students (Lakhvich, 2006; Lakhvich, Traunikava, & Efimava 2007; Lakhvich & Traunikava, 2009, Lakhvich, 2017). Within the experiments we judged the adequacy of CVT approach for Chemistry course design. That approach was indicated to be more effective for teaching Chemistry in didactic, methodological, cognitive aspects, particularly useful for short-period learning.

The special attention of our study was centred on the problem of the acceptability of CVT approach in general (grade 8-10) and pre-university (grade 11-12) school. On the basis of empiric data obtained (Lakhvich, Traunikava, & Efimava, 2007) we consider 8-10 grade school students are psychologically capable to perceive such level of formalization. The latter, to our mind, facilitates to the formation of so-called Chemistry type of mentality and force the possible reactivity of hit site of the molecule on students' attention.

Appealing results justified the acceptability of visualization type presentation of chemistry information for primary school (Lakhvich, Lehankova, & Traunikava, 2008; Lakhvich & Lehankova, 2009). Thus, we obtained 6-7- year pupils are able to resolve correctly problems in the field of Organic Chemistry, including tests on variety addition and substitution reactions (e.g. addition of methyl lithium to methylcyclohexanone) in the case we presented aesthetically and psychologically adopted technology. Grounded on the results we postulated the need of propaedeutic introduction of the chemistry language semantic subunits in primary school as the reflection of aesthetic potential of molecular representation. The main reason for such approach ought to be the realization of illustrative and imaginary thinking familiar to children of this age groups. The other reason was to facilitate the learning of Chemistry on the basis of the semantic system presented in propaedeutic introduction of molecular representation. Surely, the approach requires the adequate visualization techniques including excited samples (graphic and computer) and psychologically adaptive system of successive information presentation (CVT Technology).

The other contribution was made in the framework of the project aimed to facilitate the process of teaching hearing impaired students (Lakhvich, Kostarava, & Lehankova, 2009). The investigation included different forms of visualization-based educational techniques. The latter included various models, animations, chemistry experiment, play-therapy and etc.

Animations assisted different topics of general course and the emphasis was made to form a visual-based acceptance of chemistry information, regarding the attractiveness and age-related accessibility of the models proposed. Thus, the concept of valency was visualized in form of 4-handed (for Carbon), 3-handed (for Nitrogen), 2-handed (for Oxygen) and finally 1-handed (for Hydrogen and Halogens) mannikins. They were allowed to form chemical bonds and structure taking into account their valence/hand-capacity. Discussing topics from organic chemistry the isomerism of organic compounds was visualized in the same manner, in addition various animals were proposed as the imaginary models of chemical elements. The initial introduction of visualized social and/or domestic patterns followed by the interchange of the latter for geometrical figures grouped in proper manner and finally to structural formulae. The special attention was made to use of condensed visualization technology elaborated earlier and accessed for regular pre-university and university students. The approach had been pursued in the framework of game-learning therapy. The latter included students cast, which played elements forming chemical bonds. The game enhanced the usage of additional sensors accessible for deaf students (visual, tactile and kinaesthetic). The positive motivation facilitated the study process. The study showed great motivation of HI students to carry out experiments in school laboratory. The latter obviously correlates with the fact that impairing hearing has little effect on the ability to work in the laboratory. Moreover, circumstances are favourable for such students to realise their potential in science. We used the potential of the chemical experiments both in individual and collective forms. The latter was supplemented with graphic presentations, 3D-animations, molecular modelling and play therapy activity. We consider the schematic type of presentation when being aesthetic and adequate should facilitate the teaching process regarding the psychological aspects of "commix"-type of mentality familiar to recent generation "commix".

Modelling as it was mentioned above was also applied in the construction of inquiry technology educations, in particular for SR-learning both at the University and High school (Lakhvich, 2017). To simulate the SR activity, we guided docking modeling projects of potential drugs. It was done mostly because of the cheap equipment we needed for student research and were inspired by the work of the colleague who studied some biochemical issues with the aid of molecular docking. In some cases, we used species synthesized and tested on TB activity previously. In other cases, *in silico* researches were based on the analysis of data about bioactivity of the different groups of substances (cardiac glycosides, capsaicinomimetics, thymidilate synthase inhibitors, terpenoids, and etc.) When organized properly, docking modelling gives really new knowledge. But only in the case we use the proper scientific approach. E.g. in the case of TB drug research, we based on the previous experimental data (some substances have been synthesized, and then biologically assayed in vitro), followed by the elaboration of the model of interaction (we needed to propose the protein fragment for simulation *in silico*). Then we compared the results of *in silico* computations and tests *ex vitro* (on TB strands) and then generated mentally the new structures with fragments of definite shape and orientation to bond more effectively with receptor. Just a normal scientific research based on proper scientific paradigm! Our experience has proved that modelling was attractive and interesting for students. They really were involved both in experiment (it was available and productive) and in the process of acquisition of knowledge. They found out a lot about the subject of their professional interest and shared their knowledge with mates.

Finally, we prepared textbooks and handbooks (Lakhvich & Traunikava, 2013; Lakhvich et al, 2010; Lakhvich et al, 2017; Ryneiskaya et al., 2018, and etc.) based on the technology and our understanding of what is to be aesthetic to facilitate teaching process.

Sometimes we hear from our colleagues working in the field of Science and Science Education about the uselessness of models and simulations. They propose only to train skills to teach some operations which will be used in future professionally. I dare say it's a college approach to prepare blue-collar workers for a primitive industry.

Conclusions

Chemistry can be regarded as cornerstone of two interfering paradigms: scientific and spiritual. Aesthetic analysis of Chemistry meaning includes the cultural image of chemistry as well as chemistry's contribution to the image of the world and the chemists' behaviour to arrange-explore-produce their labs, instruments, materials, texts, research objects and, finally results according to the aesthetic criteria. Visualization and modelling of chemical information, which are of major priority for chemists, who more than any other scientists communicate with each other through images and symbolic units, comprise a special issue for consideration.

Empiric results from our previous studies confirmed that the idea adequate and aesthetically designed visualization promote motivation to do Science as well as to teach/learn Chemistry. It facilitates the understanding/encoding of "encrypted Chemistry meaning". The aesthetic nature of Chemistry gives rise to its new paradigm promoting a new attitude to Chemistry knowledge. Applicability of Chemistry knowledge is tightly connected with its aesthetic nature which can be regarded as the main spiritual motif for the development of the technology. And otherwise aesthetically designed products, including Chemistry objects and Chemists' activity seems to be useful and pragmatically aimed to satisfy the expectation of modern people "cultural and humanitarian-tendency" appetites of our time. And the best way to find the way from chemistry objects to sensual perception of a man is to visualize aesthetically encrypted Chemistry information. It can be done both in Science and Education.

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