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The origin of misconceptions in inorganic chemistry and their correction by computer modelling

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The origin of misconceptions in inorganic chemistry and their correction by computer modelling

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Abstract. The paper goal was to analyse the typical mistakes in the learning of the university course of inorganic chemistry, determine the origin of misconceptions and estimate the effectiveness of the use of computer simulations to correct false chemical concepts. Ten problems that are the most typical for students were revealed. One of the leading causes of their occurrence is the failure of many students to form mental relationships between different levels of representation of chemical knowledge - microscopic, macroscopic and symbolic. Other reasons include an insufficient understanding of the material, the incompleteness of the knowledge of the microscopic basis of processes, and inability to work with different models, including misunderstanding of their purpose and constraints. NetLogo programming environment was used for students' self-administering tests to study gas laws. Scope for the usage of NetLogo models was estimated in correcting of incorrectly formed conceptions of the chemical knowledge. Independent work with NetLogo models facilitates the formation of stable relationships between multiple levels of representation of chemical information. It improves an understanding of the studied topic fundamentally, and this holds for all students practically independently of their grounding level in chemistry. The introduction of computer simulation into the practice of teaching chemical subjects shows promise. Still, it requires the solution of several scientific, methodological, logistical and organisational issues.

1. Introduction

Incorrect chemical concepts are observed fairly often among university students ([16], [28], [30]). Such a conclusion is based on the experience of teaching basic chemical disciplines at institutes of higher education and also follows from the analysis of the nature of students' wrong answers in examination papers. Two facts evidence the formation of misconceptions [11]. First, a large proportion of incorrect answers (for example, >50%) is observed among all responses obtained. Second, one misthought dominates among wrong answers (>60%), while other possible mistakes occur rarely.

The origin of chemical misconceptions should be analysed in dynamics when the level of assimilation of chemical knowledge at universities is compared with the results of students at secondary schools ([24], [35]). For example, the averaged data of monitoring of 24 secondary schools with 461 school students were described in [3]. A very significant difference was observed in the levels of assimilation of various topics of the school chemistry course. For instance, the proportion of correct answers to questions, which require an understanding of the nature of the periodic law and related regularities and rules, exceeded 80%. Determination of the type of chemical bonds or calculations of solubility and pH occurred with a 70% success.

At the same time, 14% of respondents did not even begin to perform tasks related to the writing of oxidation-reduction reactions. The number of correct answers to this topic did not exceed 25%. It is essential to note that responses to such questions require analytical and synthetic skills. Solving computational problems require skills of systematisation and algorithmisation. Up to 35% of respondents did not begin implementation of such tasks. The share of correct answers was less than 10%. In the course of study of chemical element properties, school students found difficulty in composing reaction equations by chemical transformation schemes. The share of correct answers did not exceed 2-3%; many students demonstrated an inability to compare, analyse, systematise and estimate the chemical properties of all classes of substances. Such a situation is typical not only for Ukraine. It is caused by a formal algorithmic approach which was introduced into an educational process to solving similar problems by teachers of chemistry ([7], [29]). Such an approach does not allow graduates to see various aspects of chemical phenomena at the macro- and microlevels. Still, it directs them to the use of symbolic designations.

All examples mentioned above point to the need to use educational technologies which help students to form the right chemical notations or correct misconceptions. As shown in many research ([10], [15], [28]), some chemical mistakes are persistent and severe to be corrected. Their presence among students is one of the critical problems in the teaching of chemical disciplines. Understanding the nature of errors will help to develop methods for their elimination.

The application of some learning resources based on the information and communication technologies (ICTs) shows promise in the formation of proper chemical concepts ([5], [8], [9], [12], [21], [22], [23]). Nevertheless, the use of ICT does not automatically improve the quality of knowledge. Students with different learning styles differently perceive some electronic learning resources (e-resources) for the teaching of chemistry ([9], [10], [14]). The effectiveness of the application of ICT requires compliance with the dominant styles of learning.

In several works, students of different fields of study were shown to have different preferences in learning styles ([10], [11]). In particular, students of the natural field of study, including chemistry, demonstrate active and sensitive styles in information processing, prefer visual representations of instructional materials. Also, they adhere to a sequential style in learning, favouring in convergent thinking and analysis. Learning preferences are relatively stable because they represent a cognitive, psychological and emotional behaviour of a person and identify the ways of a person's interaction with the learning environment [10].

Therefore, identifying the learning styles for individual students and predominant profiles for student groups is an essential component of developing the best pedagogical approaches and ensuring high-quality teaching. Therefore, the formation of an optimal set of e-resources is a necessary stage of their practical application. To this end, it is required to develop appropriate pedagogical techniques and technologies which take into account the psychological aspect of the perception of ICT. The use of ICT in the educational process requires specific knowledge in the field of computer science from both teachers and students. Given the rapid development of information technology, such knowledge becomes crucial in the construction of psychological and pedagogical methods of teaching.

As is shown in previous research [9], computer modelling is now recognised as a method that is well received by most students, regardless of their learning preferences. Various researchers have proven the question of the effectiveness of computer modelling in the training of future chemists in the study of special disciplines. However, the software packages Mathcad, Gaussian, and other tools of quantum chemical modelling are both objects of study in special disciplines and learning tools. Accordingly, the approach to their application is very different from the traditional teaching of basic chemical disciplines. Students learn software tools and immediately use them to solve chemical problems.

In contrast, in the study of basic chemical disciplines, namely inorganic, analytical, physical and organic chemistry, simulation software packages are used either periodically or not at all. One of the main reasons is the lack of time that is not allocated by the curriculum for mastering the software product. Therefore, teachers are limited to showing demonstrations on the screen and conduct laboratory and practical classes in the traditional way. At the same time, the foundations of understanding chemical processes at the macro-, micro- and symbolic levels are laid in the study of these disciplines. Unless the links between these levels of understanding of chemical concepts are formed, the conceptual foundations of chemical knowledge will not be formed at the cognitive level in the future.

The first step in the development of methodological support of teaching chemical disciplines by ICT consists of the identification of concepts or topics that cause the most severe difficulties for students. Mistakes of a mass character help to identify the contradictions arising from the controversial nature of the studied material and/or contradictory students' perception. Such factors as a superficial, formal or one-sided understanding of some topics, vague ideas and terms, etc., can form the basis of chemical misconceptions.

Students often come from secondary schools with incorrectly formed chemical concepts. Still, the curricula of Ukrainian universities do not schedule a time to correct such mistakes [10]. At the beginning of the teaching, lecturers must conduct entrance control of students' knowledge. Then, they are trying to focus attention on most problematical issues. Still, they do this through the study of a new program or during instructional sessions. Students are encouraged to work without assistance using learner's guides and textbooks. Such an approach requires self-organisation and self-management skills. Such skills are often undeveloped for first-year students. Thus, it is essential to implement learning technologies that would envisage the stimulation and control of independent learning activities for young students.

The paper goal is to analyse the typical mistakes in the study of the university course of inorganic chemistry, determine their origin and test the effectiveness of computer simulations in correcting chemical misconceptions.

The NetLogo programming environment has been chosen as the one that best meets the principles of effective chemistry teaching using ICT. It provides several important features:

1) visualise the links between the microscopic level of data representation, the phenomena of the material world and symbolic forms of description, as well as to study situations that develop over time;
2) NetLogo has interface elements that allow students to adapt the work according to their characteristics, and allows teachers to manage the total cognitive load of students.

The previously formulated theoretical principles [9] and all the NetLogo possibilities mentioned above were used in the process of the training organisation.

2. Methodology

The experiment was conducted at the Faculty of Chemistry of Dnipro National University (Ukraine), and it continued for two academic years. All first-year students majoring in "Chemistry" for two years of admission participated in either the first or second phase of the experiment. In the first year of the experiment, the number of first-year students was 45 people, who were formally divided between two academic groups. In the second year of admission, 42 freshmen made up two academic groups. The purpose of the first phase of the experiment was to identify incorrectly formulated concepts of chemical knowledge. The purpose of the second phase was to correct incorrectly formed concepts by applying computer modelling in teaching. During both years of the experiment, one teacher provided course instruction, homework, and exams. Thus, the experiment was conducted under conditions of the same teaching style; the question of the influence of teaching style on learning outcomes was not investigated.

In the first year, 45 first-year students completed the basic course of inorganic chemistry. The course consisted of 16 topics and delivered in the first semester of the school year. On completion, the examination (initial test of the two-years experiment) was conducted. The examination paper was aimed at the assessment of student knowledge for each of the 16 topics. It also focused on the determination of typical chemical misconceptions and the origin of their formation.

The test papers corresponded to the subject and the complexity of the delivered material. Approximately 70% of all tasks consisted of tests of a closed type with the choice of one of four/five answer variants. Open-type tests covered about 7% of the tasks; they implied free responses to theoretical questions. 12% of the tasks included calculating problems. Another 12% were devoted to the equations of reduction-oxidation processes and hydrolysis reactions which should be completed, indicating interaction products and ascribing reaction coefficients. One point was assigned for a correct answer and 0 points to wrong answers. The proportion of students who completed each task was calculated and then averaged for each topic.

The nature of incorrect responses, namely the distribution of false answers among possible options, was analysed to identify the typical misconceptions of the students. A misconception was supposed to arise when two conditions are fulfilled. First, a task is characterised by a large number (≥50%) of incorrect answers, and second, one incorrect variant dominates (≥60%) over all other wrong answers.

One year later, the next phase of the experiment was performed with the participation of 42 first-year students of the next admission. It was focused on the correction of chemical misconceptions by computer simulation followed by the estimation of the effectiveness of the method used.

This phase consisted of three stages. At the first stage, an incoming writing test with 20 tasks was conducted at the beginning of the study of the topic “Gas Laws”. The average score for each student at all second phase exams was calculated by a two-point system similar to that used a year ago. The results of the incoming test allowed a lecturer to determine the level of knowledge of each student and identify the most difficult tasks. The tasks were designed to promote mental transitions. As is known, the chemical material can be usually presented on different representation levels. They are microscopic (micro), macroscopic (macro) and symbolic (mathematical or math) levels. Test questions and answers assumed different options of mental transitions. The analysis of the results allowed one to reveal weak unformed links and determine which transformations are the most difficult to perform.

At the second stage of the experiment, students started to learn the topic “Gas Laws”. At first, they listened to an overview lecture. They then were offered to use the programmable modelling environment NetLogo [27]. The authors of NetLogo created some models related to various sections of chemistry. They united them in the course entitled “Connected Chemistry”. Dozens of the developed models are available for free use on the project website [4]. Loss of links between microscopic and macroscopic representation levels is often observed in the course of gas laws study [20]. This finding serves as an argument in support of the selection of the gas laws topic.

The second phase of the experiment was designed to fit it into the existing discipline curriculum. This approach significantly limited the time reserved for various forms of classes, as well as the number of computer models that were used in the learning process. In case of a successful introduction of computer modelling in teaching basic chemical disciplines, correction of the curriculum will be necessary for future development.

The students were offered to complete their homework modelling tasks independently in the NetLogo environment. Each task was based on the use of eight ready-made free models related to the topic “Gas Laws”. Since a high level of load characterises the curriculum of inorganic chemistry course, only the first three of the eight models were reviewed by a lecturer during an 80 min practical class. Each student worked on a separate computer with installed NetLogo, and the lecturer used the projector. Manuals were developed for all models to support independent students’ work methodologically.

Four hours of independent work were planned to fulfil all tasks within the next two weeks. The time gap between listening to the overview lecture, training in a classroom and getting a homework task ranged from one to two days for different groups. Such an approach was used because it did not require the reorganisation of the educational process.

Upon completion of the work, students handed in their papers with calculations, charts and answers. The results of homework were scored on a point scale with a maximum of 24 points for the entirely correct solution of all tasks for eight models. These results were used to analyse possible correlations between the quality of independent work and progress in the study of gas laws.

Then they underwent final testing with 28 questions on the topic “Gas Laws.” Twenty issues were virtually identical to those in the incoming test. Additional eight problems were included to assess more accurately the problem areas identified by the incoming control. The results of the final examination using a two-point system were compared with the input testing. Progress in learning was evaluated using the answers to the 20 questions contained in both tests.

The critical question for assessing the importance of the work is to compare the results of the input and final testing at the second phase of the experiment. The experiment can be considered successful if a statistically significant difference is detected between these results in favour of the final test. The SPSS statistical package was applied, and the t-criterion method for pair samples was used for the comparative analysis of the results of the input and final control.

3. Results and discussion

3.1. The effectiveness of material learning

Table 1 contains titles of topics and the numbers of examination tasks and questions. The results of input testing are also illustrated: The average percentage of correct answers and the quantity of the most complex tasks with the maximal amount (>60%) of mistakes are given for each topic. The average proportions of correct answers ranged from 31% to 79% for various issues that prove the conformity of the tests with the requirements for the complexity index.

Table 1. Topics of inorganic chemistry course.

Topic	Number of exam tasks (questions)	Correct answers, %	Number of tasks with >60% mistakes
1. Basic concepts and laws of chemistry	3(63)	64.9	1
2. Equivalent mass	2(30)	70.4	0
3. Classification of inorganic compounds	6(42)	79.0	0
4. Atomic structure	4(55)	56.2	1
5. Periodic law	3(64)	51.5	0
6. Chemical bonds	3(50)	44.7	1
7. Thermodynamics	3(16)	44.6	1
8. Kinetics	5(15)	64.6	1
9. Equilibrium	4(34)	52.5	1
10. Solutions	3(43)	31.4	2
11. Electrolytic dissociation	3(22)	31.2	2
12. Electrolytes	2(19)	51.7	0
13. Solubility product constant	3(41)	53.3	1
14. Hydrolysis	1(52)	34.6	1
15. Reduction-oxidation reactions	3(96)	37.2	2
16. Structure and properties of compounds	6(33)	33.7	5

The level of solvability exceeds 50% only for 9 of 16 topics. Two topics, namely, “Classification of inorganic compounds” (topic 3 in figure 1 and table 1) and “Equivalent mass” (question 2) can be considered as assimilated on a high level. The average solvability for them is 79% and 70% respectively and is almost independent of task type. All other topics contain at least one or more tasks which are difficult for students, even if the average solvability for them is high enough. For example, the percentage of correct answers exceeds 60% for topics 1, 8 and 13 in figure 1. However, the level of solvability of challenging tasks in these topics varies within 0-35% (figure 1).

3.2. Typical mistakes in the most complex tasks

Based on the results of the input testing, standard mistakes were identified and briefly described for the most complicated topics (average correct answers <50%) and individual tasks with the lowest solvability metrics (table 2).

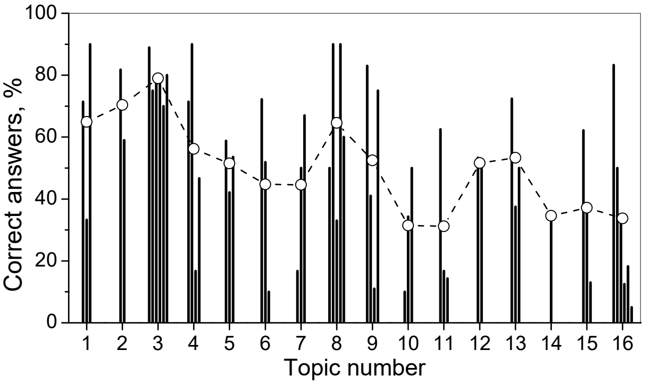


Figure 1. Percentage of correct answers by topics. Separate columns illustrate the results of the performance of individual tasks. The dashed curve represents the average results for each topic.

Table 2. Typical mistakes in the most complicated topics.

No	Task content	Description of typical mistakes/difficulties
1.	Formulation of laws	Loss of essential components in the wording of concepts leads to misconceptions
4.	Isotopes; Ionic state	Confusing the concepts (neutrons, protons, electrons, and mass numbers); Lack of understanding of atomic radius change when electron joining; Problems with symbolic notations of ion electronic configuration
5.	The periodicity of element properties	Confusing the concepts (electronegativity, ionisation energy, electron affinity) and directions of property changes
6.	Bond type – substance correspondence; MO and VB theory	Misunderstanding of the polarity concept and failure to distinguish covalent, polar and nonpolar bonds; Inability to apply the molecular orbital method and complete orbital diagrams
7.	Calculation of ΔH and ΔS	~50% of errors in calculations by the corollary from Hess's law
8.	Reaction rate and Vant-Hoff equation	Incomprehension of pressure-concentration relations in gases and errors in mathematical calculations
9.	Pressure and temperature effect; Equilibrium constant	Misunderstanding of the concept of activation energy because of a lack of understanding of temperature effects at a microscopic level; Failures in calculating the equilibrium constant and predicting the impact of pressure on equilibrium
10.	Calculation of concentrations	Failure in estimates of the concentrations of solutions and transitions between different units; Lack of understanding of the colligative properties
11.	Dissolution of acid in the water, dissociation constant, pH	Failures in the calculations of pH for acid and alkaline media, dissociation constant, and accounting for changes in reaction conditions
12.	Strong and weak electrolytes	Problems with the classification of compounds which properties were not taught in class
13.	Solubility and sediment formation	Incomprehension of pressure and temperature effects and problems with mathematical calculations
14.	Finish the hydrolysis reaction; pH, hydrolysis constant	Misunderstanding of electrolyte nature leads to failures in the identification of strong/weak electrolytes, and electrolysis stages and products; Many errors in mathematical calculations
15.	Determine the redox reaction type; finish the reaction and identify reaction products	Failures in the identification of reaction types and determination of products by standard electrode potentials
16.	Oxyacids of Cl and I, H_2O_2, O_3, acids and peroxyacids of S; S, Se, Te base compounds	Incorrect characterisation of the strength of acids and redox properties; Unsatisfactory explanation of the properties of H_2SO_4, H_2SeO_4, H_2TeO_4

3.3. The origin of misconceptions

The experimental results obtained denote inadequate students' knowledge of the material. It consists in the incompleteness of understanding of the microscopic basis of processes, and inability to work with different models, including misunderstanding of their objectives and constraints. The following items within the inorganic chemistry course were identified as the most challenging issues for students.

1. Students are not well aware of the structure of atoms at the microlevel and cannot characterise the properties of an element following the structure of its atom. They do not entirely understand processes when the electrons are lost/connected, and cannot often represent the electronic configuration of an excited atom. Thus, it is difficult for students to make transitions between concepts at the micro and symbolic levels.
2. Many mistakes are made in characterising the change in the energy properties of atoms that indicates an inadequate understanding of the concepts of ionisation energy and electron affinity.
3. They have insufficient practical skills in establishing the type of chemical bonds in real substances. They cannot often compare the geometry of molecules.
4. Plotting electron arrangement by the molecular orbital method is difficult.
5. Students merely memorise the macroscopic influence of changes of pressure, temperature and volume on the processes in chemical systems. Still, they do not understand the microscopic nature of these changes.
6. Additional difficulties arise from inexperience in mathematical calculations.
7. Students are challenging to imagine the colligative properties and the nature of the formation of solutions. Half of them do not understand what the solubility is and how the pressure affects this value.
8. Students do not understand the microscopic essence of the processes of dissociation and solvation. The misunderstanding causes problems with writing the reactions of hydrolysis. They cannot distinguish between strong and weak electrolytes, especially for unknown substances. They are mistaken when calculating pH, pOH, and dissociation constants in solutions. The problems mentioned above are caused by insufficient understanding of chemical concepts and unformed structures of chemical knowledge.
9. Inadequate skills are found for calculating the concentrations of solutions and transitions between different units. It is difficult for students to calculate the equivalent concentration of a substance with due regard for the reaction in which it participates.
10. The ability to predict reaction products using the values of standard electrode potentials is unformed.

The above-listed problems are very typical and often caused by the inability of many students to link multiple levels of chemical knowledge representation mentally ([6], [26], [31], [34]). For example, they often use and merely memorise mathematical equations only, but do not understand the nature of phenomena at either atomic or macroscopic levels. In the first case, the problem lies in the unformed links between the microscopic and symbolic levels of knowledge. It is illustrated by the problematic issues 1, 4, 9 and 10 from the list shown above (table 2). In the second case, the unformed connection is between the macroscopic and symbolic levels (issues 6 and 8). Also, in many cases (items 2, 3, 5 and 7), students are not able to understand the relationship between different macroscopic effects, which are based on the same microscopic processes. In other words, they cannot make a transition from macro to micro-level or in the opposite direction.

3.4. Correction of wrong chemical concepts using computer simulation

Answering the questions of the entrance tests, the students experienced astonishment, misunderstanding and cognitive discomfort. Almost all respondents could not link the behaviour of gas particles in a closed volume with the influence of pressure and temperature. There was a lack of knowledge of the microscopic nature of the process. Unformed links between the macroscopic and microscopic representations of a considered phenomenon negatively affect subsequent students' understanding of the influence of changes in parameters (pressure, temperature and volume) on the course of various processes ([1], [13], [25], [31]).

Problem situations, which are desirable to resolve further by ICT tools, were specified with the use of the developed methodology and the data obtained at the first stage of the experiment. The questions in homework asked students to change specific parameters of a NetLogo computer model and record the results in the form of graphs on the screen. Students plotted dependencies, changed the number of particles, temperature and volume, and independently deduced mathematical equations. Having obtained their equations, then they used them for forecasting. From the dependencies derived empirically, they deduce the equation of ideal gas state already in the form accepted by science. Some tasks included the independent creation of new models. NetLogo allows students to draw a container of any shape, set valves, visualise the direction of particle movement with arrows showing their speed in colour, etc.

Various aspects of the effectiveness of the application of NetLogo models were discussed in some papers ([17], [18], [19], [32]). The use of the NetLogo environment visualises the links between the macro- and microlevels of representations. It also connects real-world phenomena and symbolic forms of their description and simulates model situations that develop in time. Using NetLogo models, students can observe the macroscopic events of the real world, and also try to predict their changes resulting from the interaction of many microscopic objects. Integration of different levels of chemical knowledge contributes to their better understanding ([2], [33]). Perhaps, it is the key advantage of such models.

The NetLogo environment has interface elements that enable students to adapt their work according to the characteristics of their learning style. As a result, lecturers can organise step-by-step work. For example, one can accelerate/slow down the show or repeat it several times to manage the cognitive load of students. It is also possible to make changes to the model parameters and observe what changes occur. All these options clearly illustrate the relationships between different levels of representations and help to make transitions between them etc.

3.5. The effectiveness of computer simulation

Particular test tasks were designed for studying the effectiveness of using computer simulation to correct the typical problems encountered by students. In total, N=31 persons participated in both input (A1) and final (A2) testing. These students were divided into three groups according to the results of NetLogo modelling. In groups 1, 2 and 3, students correctly performed <50%, 50-75% and ≥75% of NetLogo tasks respectively. One may expect that the homework assignment rating generally correlates with the overall student rating; that is, usually, the best students demonstrate better homework results. The results of A2 and A1 testing by these groups are shown in table 3. The difference A2-A1 is significant if $p<0.05$.

Table 3. Difference between the average points scored in A2 and A1 testing for three students' groups which demonstrated different levels of homework performance.

Group	Test	N	Mean	Std. Deviation	Std. Error Mean	t	df	Sig. (2-tailed) p
1. (≤50%)	A1	7	0.3743	0.08344	0.03154			
	A2	7	0.5514	0.05581	0.02109			
	A2-A1		0.17714	0.10750	0.04063	-4.360	6	0.005
2. (50-75%)	A1	10	0.4120	0.14093	0.04457			
	A2	10	0.5890	0.11060	0.03497			
	A2-A1		0.17700	0.14758	0.04667	-3.793	9	0.004
3. (≥75%)	A1	14	0.5621	0.11383	0.03042			
	A2	14	0.6864	0.09361	0.02502			
	A2-A1		0.12429	0.12513	0.03344	-3.716	13	0.003

The results can be summarised as follows.

1) For all groups, the difference between the results of A2 and A1 tests is positive, i.e. the received score has increased, and statistically significant ($p<0.05$). If only the best students could overcome the mark of 0.5 in the input test, the mean scores of all three groups exceeded 0.55 in the final examination.

2) The average mark expectedly increases in going from group 1 to group 3, both in A1 and A2 testing.

3) The increment of points is practically identical for groups 1 and 2 and is only slightly lower for group 3. In other words, the use of computer simulation significantly improves the results of testing, and the value of the effect does not practically depend on the initial level of students' knowledge.

The design of the tests compels students to make mental transitions between multiple levels of representations of the chemical material. For example, the skills of finding the correspondence between the real-world phenomena and microscopic processes behind them are necessary to solve tasks which include macroscopic and microscopic representations. Another job involves macro-math and math-macro representations when one needs the ability to describe the events of the real world at a symbolic level. Finally, the most complicated problems include transitions between all three representation levels, such as math-macro-micro or micro-macro-math.

Different test questions/answers included different transition options; the analysis of the results allowed one to determine which transitions and links are the most difficult. The results of such a study are shown in coordinates the increment of points scored in A2 compared to A1 tests vs the scored points in A1 (figure 2a) or A2 (figure 2b) tests. The results of a majority of tasks form a reasonably compact general group on the graph marked with shading. The average points obtained for different tasks vary between 0.2 and 0.9 and 0.5 and 1 in the initial and final test, respectively.

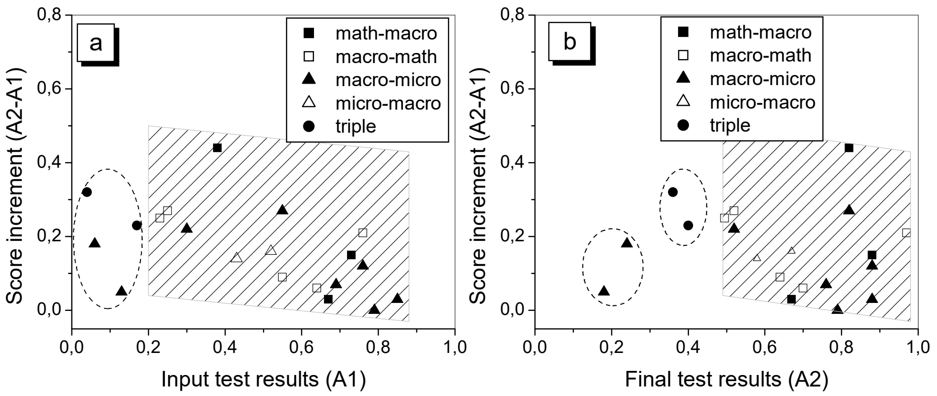
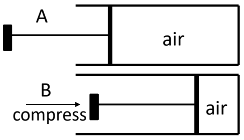


Figure 2. Results of individual task performance in the input (a) and final (b) tests: the score increments (A2-A1) vs the scored points.

The most significant difficulty in the input tests was expectedly caused by the tasks with the most complex triple transitions (figure 2a). Students scored only 0.04-0.17 points, 3-10 times less than the average 0.48 points for the input testing. Two tasks with binary micro-macro transitions shown in table 4 also dropped out of the general group (shaded area) in the initial examination (figure 2a). They differ by lower rates of correct solutions (<15%).

Table 4. Most complicated tasks with binary transitions by the results of final testing

No	Task	Options of answers
8	Basketball ball pumped with air. Assume that the size of the ball does not change, and the temperature remains constant. How does the average number of collisions of particles with the walls of the inflated ball change?	An average number of collisions: (1)Increases (2)Decreases (3)Does not change
19	 There is a hermetic cylinder with a piston (Fig. A). This piston is pressed in Fig. B. The air is not added and does not come out of the cylinder. The question concerns the states A and B relative to the air inside the cylinder.	Average particle velocity is: (1)Same in A and B (2)Higher in A (3) Higher in B

Training with NetLogo modelling contributed to the improvement of knowledge. The results of the final test shifted to the right along the OX axis for most of the tasks (figure 2b). The most considerable progress (on average 71% of correct answers in the final test) was achieved for macro-math and math-macro binary transitions. The tasks with macro-micro and micro-macro bridges demonstrated somewhat worse but, in general, sufficient progress (63% of correct answers). Some tasks with macro-micro transitions, illustrated in table 4, turned out to be difficult-to-correct that influenced the average result for binary tasks of this type. In other words, the proposed training option turned out less effective for macro-micro and micro-macro transitions than for binary transitions with symbolic representations.

The scored increment, namely the difference between the results of the final and initial tests, can be considered as a measure of the efficiency of NetLogo modelling. Figure 3 illustrates the average increments in points for tasks with different types of transitions. The most significant increase (~0.27 compared to the average value of 0.16) was found for lessons with the most complex triple transitions. Therefore, the use of NetLogo modelling allows one to improve efficiently the understanding of issues requiring the formation of the most complex links between multiple levels of chemical knowledge representation. However, since the triple tasks were solved very poorly in the input test (figure 2a), the proportion of correct answers remained quite limited (<40%) in the final examination.

The approach used ensured a transition from the global, undifferentiated images of chemical reality to the operations with its elements, properties and relationships more and more divided into parts. Such experience leads to an increase in the ability of students to link mentally different levels of material representation, improving their professional training.

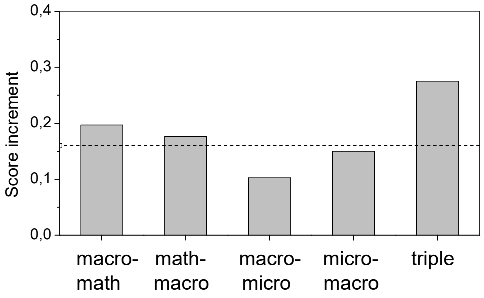


Figure 3. Score increments in the final test compared to the initial examinations for tasks of different types. The dotted line illustrates the increase averaged over all tasks

However, the question arises as to how to combine the use of computer simulation and traditional teaching of inorganic chemistry? Traditionally, ICT tools are used occasionally to teach some selected topics of inorganic chemistry. For example, multimedia presentations are top-rated in delivering lectures or practical classes. Multimedia support is easy to integrate into a traditional curriculum. Such technology requires only the availability of projection equipment and lecturer's computer. It does not require any organisational changes in the work of students in conventional chemical laboratories. A certain level of readiness for all participants of the educational process is necessary for the use of computer simulation methods inorganic chemistry teaching. From the lecturer's side, it needs the solution of some scientific, methodological, logistical and organisational issues.

4. Conclusions

Unformed conceptual structures of chemical knowledge and inability to make transitions between multiple levels of representation of chemical information are the most critical problems of learning inorganic chemistry. Students often cannot explain the causes of the phenomenon at the molecular level; they just memorise information but do not understand it deeply. As a result, they cannot solve tasks that require conceptual reasoning and cannot operate with chemical knowledge at different levels. Independent work of students with models in the NetLogo environment facilitates the formation of stable links between different levels of representation of chemical information.

At the input testing, students showed practically equivalent results in solving problems with binary transitions. The use of computer simulations during the training process better strengthens the links between macro and math levels, while the impact on the macro-micro transitions was the weakest compared to other variants. Complex triple transitions are the most difficult tasks for understanding. Still, the use of computer simulation demonstrates the best progress in correcting misconceptions caused by complex triplicate representations.

The reported study does not solve all the problems that arise during the teaching of a cycle of chemical disciplines. The introduction of computer simulation into the practice of teaching chemical subjects requires the solution of several methodological, logistical and organisational issues. If simulation software packages with similar NetLogo features are available, the experience of using them can be extended to the whole course of inorganic chemistry. In particular, the integration of the contents of the courses "Introduction to the speciality" and "Inorganic chemistry" may be desirable for the formation of first-year students' readiness to use computer simulation methods. The following topics show promise for further research:

- the introduction of appropriate changes to the curriculum, and
- the development of the content modules, forms of training and control, which involve the use of computer simulation in the block of fundamental training of chemistry students.

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