Eszterházy Károly University Doctoral School of Education Science

Thesis of doctoral (Ph.D.) dissertation

Modeling of the adsorption of air polluting materials, educational application of the simulations' outcomes and analysis of its effects

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1. Topic of the dissertation

The significance of environmental education is increasing in public education, mainly in the education of natural sciences. International and national surveys show that the attitude of students towards natural sciences decreases with the time spent in school. The popularity of physics and chemistry lags behind the other subjects, and by the end of the ninth and tenth grade, chemistry becomes a subject that is rather refused (*Fernengel, 2009*). The problem is not only that students' attitude decreases, but also that there is a fallback compared to other subjects (*Csapó*, 2000). Despite the fact that the curriculum has been extended over the recent years, the knowledge in the field of natural sciences cannot be implemented adequately in resolving everyday problems. In order to become more effective and efficient in teaching chemistry, it is important that we seek pedagogical-methodological novelties and up-to-date knowledge.

In my dissertation, I elaborate on one of the important areas of the chemistry curriculum, which is the teaching of particle's adsorption. The knowledge of high school students is not only incomplete, but also incorrect (*Tóth*, 2016). One of the problematic fields is to understand the characteristics of chemical particles and substantive aggregates, and to create the adequate approach to particles. In my dissertation I deal with a partial field which is tightly connected to molecules, adsorption and certain types of interactions between the particles, and also with environmental education through the modeling of molecules. Modern environmental education does not refuse environmental protection or the scientific approach of it. These are important parts of environmental education even today, but they are embedded in a more expansive system, which is the configuration of environmentally conscious behavior (*Nahalka, 1998*). Constructive pedagogy, also in the area of environmental education, sets out from the fact that children have the determining knowledge when entering the school system which will guide their learning of ecological learning, environmental protection and the setting up of their environmentally conscious behavior.

According to a European survey (*Teppo and Rennikmae, 2003*) the learning of natural science subjects would be less difficult if the emphasis was more on the investigation of the learning method of the students. We need to understand the basic principles of studying natural sciences, but mathematical and problem solving skills are also needed besides conceptual and visualization skills (*Vaarik, Taagepera és Tamm*, 2008). They point out that the students' knowledge is incorrect. Understanding is even more difficult because of the switches between the three levels of chemistry, which are the macro level (sensible reality), micro level (which are not sensible by human sense organs) and symbolic level (using the special chemical sign

system), and having to move between these levels is what makes understanding so challenging. They highlight that the main problem of students is how to understand the symbolic level, because they cannot imagine basic chemical bonds, the structure of particles, therefore the modeling process is also difficult for them.

Getting to know adsorption better can also contribute to forming the particle approach. That is the reason why we analyzed the adsorption on ice of some methane derivatives with the Monte Carlo simulation method. We are able to demonstrate the phenomena that are based on experience and are provable, authentic and scientific by using the computer-aided simulation method. This methodology is the opposite of all pseudo-scientific thinking that is based on assumption and its trustworthiness is doubtful. In my dissertation, I am going to show the outcomes of the computer simulation, and am also going to refer to how they can be applied, and with what benefits, in public education.

2. Scope of the research

In my research study, I explored the understanding process of adsorption, in which I processed the data of a pre-test done by ninth grade students at the beginning of the semester. The research questions can be divided into two groups. The first one is about the pre-test, in which students starting their ninth-grade school year were involved. The aim of this part is to reveal the knowledge of the sample population about the characteristics of particles at the beginning of the school year. Afterwards, using the outcomes in the field of adsorption, another round of test was administered to a control group to find out if the implementation of the newly applied information in the education process can make a change, and if it can, how significantly. Therefore, the application of the research hypotheses is different for the pre-test and for the post-test.

3. Strategy, methodology and applied research tools

The applied research strategy is *inductive*, i.e. I start from pedagogical reality, from empiricism, by analyzing data and then searching for the answers through generalization. I also used the *descriptive strategy* when describing the results of the test taken by the students at the beginning of the school term. Apart from these, the *correspondence analysis strategy* was also used to find out the relationship and the correlation between the different variables. I used the *experimental strategy*, too, as instead of describing the status quo, I reveal the effects of changing the independent variables. In the research, the students of the experimental group were taught about the results and the essence of adsorption including the new knowledge

material, while the students of the control group were taught in the conventional way, based on the core curriculum. By doing so, an intervention was made into the pedagogical process, according to the goal of the research, and the independent variables changed. The assessment tests provided the basis for the *revealing methodology*, in which personal data was also gathered at the beginning, for analysis and comparison. In the research, the *process methods* were statistical ones, in which I used Microsoft Excel and SPSS.

4. Sampling, the sample, population

I carried out a study at the beginning of September 2017 with the involvement of ninth grade students who attend the four and six-year program. The aim was to assess their knowledge of the adsorption process learned in chemistry classes in the previous two years. In this pre-test, one of the seven questions was about the characteristics in general and the reasons behind the different behaviors of particles. In this test, four and six-year program students were involved. The education of chemistry starts at the seventh grade, therefore there are students who arrived into a new school community in their ninth school year, meaning these students came from several primary schools, and there are also students who remained at the same institution, with the same teacher. The aim of my research was also to measure the knowledge of students who attend the eight-year program, but the colleagues did not accept the involvement from this type of schools. At the end of the school year, the students of the sample pool gave account of their knowledge by answering nine questions in the post-test.

5. Research hypotheses for the pre-test

1.) The relationship is significant between the number of the students' correct answers and their grades at the end of their eighth school year.

2.) There is no difference between the performance of male and female students.

3.) The relationship is not significant between students' performance coming from the countryside and the ones who are from the capital city.

4.) There is a difference between the performance of students who attend the four-year and the six-year program.

5.) The knowledge of ninth grade students about particles is incomplete, and they have misbeliefs about the topic.

6. Evaluation of the pre-test data

6.1. Hypothesis 1.

To test the first hypothesis, I analyzed the grades of the members in group *A* and group *B* individually and altogether. Then, I applied the statistical method to compare the four and six-year program students. The number of correct answers compared with the final grades can be seen in the Table 1.

	Number of all correct answers			
Final grades	**0**	**1**	**2**	**5**
Satisfactory	11	5	0	0
%	68,75	31,25		
Average	71	34	1	0
%	66,98	32,08	0,94	
Good	179	75	3	0
%	69,65	29,18	1,17	
Excellent	228	124	7	1
%	63,33	34,45	1,94	0,28
Total	**489**	**238**	**11**	**1**

Table 1: Final grades and the number of all correct answers

In group *A*, only 0, 1 or 2 out of the given seven questions were answered correctly, which is altogether a weak performance. The outcomes of the first hypothesis can be forecasted by now. There were only seven students in the sample (N=385) who answered all the seven questions correctly, four of them earned an excellent, two of them earned a good and one of them earned an average final grade. 250 students, i.e. 64.9% of all the students, were not able to give a single good answer. The outcome of the crosstab query is that χ^2 equals 3.547, the significance is 0.738 (DF - degree of freedom = 6), which means there is no significant relationship.

In group *B*, the number of correct answers was 0, 1, 2 and 5, and the five correct answers were given to the first five questions. In the sample (N=354) there were 239 students (67.5%) who did not get any of the answers correctly. The value of χ^2 is 4.679, the significance is 0.861 (DF=9), so the conclusion is the same as for group A.

It is true of the whole set of data that there is no significant relation between the final grades at the end of the eighth school year and the number of correct answers in the test (χ^2 equals 4.413, the significance is 0.882 and the degree of freedom is 9). It can be stated that there is no relation between the good final grades and the achieved points in the test, because

the ones who had good or excellent final grades were not able to answer more questions correctly than the ones with worse final grades. 489 from all the 739 students involved, which is 66.2%, were not able to answer even one question correctly. This result is thought-provoking because the seventh question can stand in itself, so it means that the students' knowledge is not only incomplete regarding the phenomenon studied in this research, but also when it comes to the general chemical and physical characteristics of particles, their polarity and their effects. Therefore, I ***refute the first hypothesis***.

6.2. Hypothesis 2.

	Number of all correct answers				**N**
	0	**1**	**2**	**5**	
Boys	232	119	6	0	**357**
%	**65,0**	33,3	1,7	0	
Girls	257	119	5	1	**382**
%	**67,3**	31,1	1,3	0,3	

Table 2: Number of all correct answers made by boys and girls

Table 2 shows that 65.0% of the boys and 67.3% of the girls did not answer correctly at all, while the ratio for giving only one good answer is 33.3% for the boys and 31.1% for the girls. Given these numbers (χ^2 is 1.525; significance is 0.677; DF=3) it can be stated that there is no notable difference between the performance of boys and girls. So, the ***second hypothesis is true***, meaning there is no significant difference between the performance of boys and girls.

6.3. Hypothesis 3.

	Number of all correct answers				**N**
	0	**1**	**2**	**5**	
Budapest	276	160	11	1	**448**
	61,6	35,7	2,5	0,2	
Countryside	213	78	0	0	**291**
	73,2	26,8	0	0	

Table 3: Number and percentage of all correct answers given by students living in Budapest or in the countryside

I analyzed separately the performance of students living in the capital city and in the countryside (Table 3). Comparing the relative frequencies, the students from Budapest (N=448) answered correctly 0, 1, 2 or 5 questions, while the students from the countryside (N=291) gave correct answers to 0 or 1 questions. The rate of students who did not answer correctly to any of the questions is 61.6% among the students from Budapest and 73.2% among the ones from the countryside. The standard deviation for students from Budapest is 0.581; the variance is 0.338;

while these numbers for the students from the countryside are 0.444 (standard deviation) and 0.197 (variance). The outcome of the crosstab query (χ^2 equals 15.724 and the significance is 0.001; DF=3) supports that the difference is substantive between the two groups.

According to these, ***the third hypothesis is not proven to be true***, because the difference is significant between the performance of the students from Budapest and those from the countryside. The performance of the students from Budapest was proven to be higher.

6.4. Hypothesis 4.

	Number of all correct answers				**N**
	0	**1**	**2**	**5**	
Six-year program	159	92	4	1	**256**
%	**62,1**	**35,9**	1,6	0,4	
Four-year program	330	146	7	0	**483**
%	**68,32**	**30,23**	1,45	0	

Table 4: Number of all correct answers for the two different programs

The number of students who attend the six-year program (N=256) and the four-year program (N=483) is illustrated in Table 4. Since the numbers of respondents from the two groups are considerably different, I added the percentage of the students in each study program under the number of all correct answers. The performance of the four-year program students shows smaller standard deviation (0.501) and the variance is also smaller (0.251) than the six-year program students (0.594 and 0.353). Based on the relative frequency, a larger part of students attending the four-year program were not able to answer any questions, moreover, fewer of them replied correctly to one or two questions. By the crosstab query (χ^2 equals 4.571; DF=3, significance 0.206) we can state that **the fourth hypothesis is true**, so the difference is significant between students who attend the four or the six-year program, and the students of the six-year program performed better.

6.5. Hypothesis 5.

The analysis of the fifth hypothesis will be made according to the answers to the seventh question in the pre-test. This question was about a compound gas, in which one of the three listed gases can be separated from the others with the help of active coal. Students had to choose the correct reason for this phenomenon from the four alternatives in this multiple-choice test. The gas compound for group *A* contained ammonia, oxygen and nitrogen, while it contained carbon monoxide, sulphur dioxide and carbon-dioxide for group *B*. The listed items were the

following: the different size, the difference in speed of movement, the different polarity of the particles and its reaction with coal. This question could have been answered correctly without the knowledge of adsorption, because it is part of the curriculum in primary school. Sadly, both groups performed poorly in this task. The chemical reaction, an incorrect answer, was chosen in most cases in both groups, which can imply the students' incorrect knowledge or misbelief. Summarizing the previous answers, it can be stated that the students' knowledge about chemical particles is quite incomplete, they have many misbeliefs and remarkable contradictions can be seen regarding their answers in many cases. ***The fifth hypothesis was proven to be true***.

7. Research hypotheses for the post-test

1.) There is no difference between genders in the achieved points and in their performance.

2.) There is no difference in the performance of the students involved in the four and the six-year programs.

3.) A significant difference can be seen in applying the adsorption outcomes in the experimental group, compared with the control group.

8. Evaluation of the post-test data

There were two definitions in the tests: students had to define adsorption and surface tension. Students also had to give examples for materials used as adsorbents and for an everyday adsorption process in other two tasks. Furthermore, students were asked to analyze two illustrations. In the first one, they had to describe briefly the visible difference, while in the other one they had to choose the correct type of chemical bond from the listed three types. After these, there were three more multiple choice questions.

8.1. Hypothesis 1.

I compared the achieved points at the group level and then at individual level, too, based on the nine tasks. One point could be achieved for any task solved correctly, and these are independent items. In group *A*, the boys were only able to solve seven tasks at the most, whereas two girls were able to solve 8 tasks, and one girl achieved the total of 9 points. The boys were able to answer correctly (2.75) fewer times than the girls (3.05), and the standard deviation is higher for the girls (1.847, while for the boys 1.724). The result of the χ^2 test (12.213; DF=9, significance: 0.202) shows that there is no difference between genders and performance in group *A*. In group *B*, two of the boys were able to solve eight tasks correctly, while four of the girls achieved the same result, and one girl answered all the questions correctly. The average

for the boys (2.95) is below the girls' average (3.13), but the standard deviation is higher for boys (1.791, girls: 1.697). It can be stated from the data (χ^2 is 18.247, significance is 0.032; DF=9) that there is a significant difference between gender and the total number of points achieved. The performance of the girls is slightly better than the boys'.

Although in the whole sample there is no significant difference between the genders and the total number of points achieved (χ^2 equals 11.343; DF=9, p= 0.253 and the correlation is 0.069), girls achieved slightly higher scores in group *B*. We can conclude that ***the first hypothesis was found to be true***.

8.2. Hypothesis 2.

I also compared the scores of the students in the four and the six-year program by question. The first question was the definition of adsorption. Exact and exhaustive definition was provided by 37 students from the four-year program students (N=406) and by 45 students from the six-year program (N=238, 12.7%). Based on the results of the χ^2-test (12.953; DF=1 and p=0.001), we can say that there is a significant difference between the two programs, because members of the six-year program scored higher.

The second task was more difficult because fewer students (10.2%) were able to give the exact definition of surface tension. This could mean that defining surface tension was not part of the core curriculum. The difference can still be identified based on the value of the χ^2-test (4.195; p=0.041), which means that students who attend the six-year program performed better.

The third question was to name three substances which are used as adsorbents. It is very important to show several adsorbents when teaching the phenomenon of adsorption. It is also indispensable to support the understanding process by including everyday examples. 73 students (11.3%) gave the correct answer to the third question, and the student from the six-year program performed better again. Therefore, we can state (χ^2 is 14.964; p=0.001) that there is a difference between the results of the four and the six-year program students.

The fourth question was to give two examples from the students' own experience which are based on adsorption. The majority of the students answered this question, but there were many students who answered only with one example (61 in group *A* and 71 in group *B*). 151 students answered with two valid items. 23.4% of the students did this task correctly. In this case no significant difference can be identified between the performances of the students studying in the two different school programs. It turned out that students knew several everyday

examples. We can also see that approaching the subject matter in different ways and supporting it with everyday examples greatly increases the efficiency of the educational process.

In the fifth question, students were asked to show the different behaviors of the two molecules on the surface of ice, based on an illustration. There were 164 correct answers, but the proportion of students from the six-year program (31.9%) is higher than those in the four-year program (21.7%), so a significant difference can be identified in their performance (value of the χ^2 is 8.318; p=0.004). Regarding the total sample size, only 25.5% of the students were able to answer correctly. Since this question did not require a solid knowledge of chemistry, it can indicate reading comprehension problems.

The next four were multiple choice questions. In the sixth one, the task was to choose the cause of the difference shown in the previous illustration from three options. This could be answered correctly even without having seen the illustration before, by using the knowledge of interactions between particles and the polarity of molecules. The number of correct answers can be seen in the Table 5. 59.2% of all the students replied correctly.

Correct answers	Four-year program	Six--year program
Group A	60,4%	56,2%
Group B	59,8%	59,3%

Table 5: Percentages of correct answers in the two groups

Outcomes show that there is no significant difference between the performance of students who attend the four and the six-year program (χ^2 is 0.399 and p=0.527).

In the seventh question, students in both group *A* and *B* were asked to identify the type of possible chemical bond between the fluorine atom and water molecules. The listed options were: covalent (A), hydrogen bond (B) and dispersion bond (C). The position of the two molecules compared to each other was presented in an illustration, and the correct answer was B. The six-year program students (70.2%) performed better than the four-year program students (65.8%), but the difference is not significant (the value of χ^2 is 1.325 and p=0.250).

I also looked into the percentage of the incorrect answers, which was 32.7%. The answer option A, namely the covalent bond was chosen the fewest number of times (Table 6). This information should be highlighted because the covalent bond is a primary chemical bond while the other two in the list are secondary. This means that, in the sample, most of the students got to know well the difference between primary and secondary chemical bonds by the end of the

school year, and they know that one of the secondary bonds should provide the connection in this case.

	Answer A	Answer C	Did not reply
Four-year program	14,3%	17%	3%
Six-year program	14,3%	12,6%	3%
Total in the sample	14,3%	15,4%	3%

Table 6: Percentage of incorrect answers in the whole sample

Regarding the eighth question, students were asked about the effect of the increasing temperature on the adsorption process (in group *A*) and the increase of pressure (in group *B*). 44.6% of the four-year program students knew the right answer, while 50.4% of the six-year program students chose the right one, which equals 46.7% of all the students. These factors should also be taught thoroughly when teaching about adsorption. Based on the answers of the students, it can be said that the difference between the four and the six-year program students is not significant (χ^2 is 2.055 and p=0.152).

The last question was the same as a task in the pre-test. The question was to choose the right answer out of four options as for the reason for the outcome of adsorption on active coal. In this question, the four-year program students (43.3%) performed better than the six-year program students (35.3%), and there is a difference between the results (the value of χ^2 is 4.045 and p=0.044). However, only 40.4% of all the students were able to choose the correct answer in this case. This is considered weak performance because the test was taken at the end of the school year, when material aggregation and the structure of particles (polarity, speed, size and reaction ability, which are part of this question) should all be part of students' knowledge, since they were dealt with in several topics during the school year. This question was the only one in which the students from the four-year program scored higher than the six-year program students.

The best result by students from the four-year program was eight questions answered correctly, while two students from the six-year program got all the nine answers right (Figure 1). The average number of points in the four-year program (2.82) is lower than the average of the students in the six-year program (3.22), although standard deviation and variance are higher for the latter. Comparing the overall test scores, I got the result that the six-year program students did better than the four-year program students. Also, the difference is significant between the two samples' performance (χ^2 equals 20.099 and DF=9, p=0.017).

To sum up, it can be stated that ***the second hypothesis was found to be false***, meaning that the difference is significant between the four and the six-year program students' performance, with the result of the six-year program students performing better.

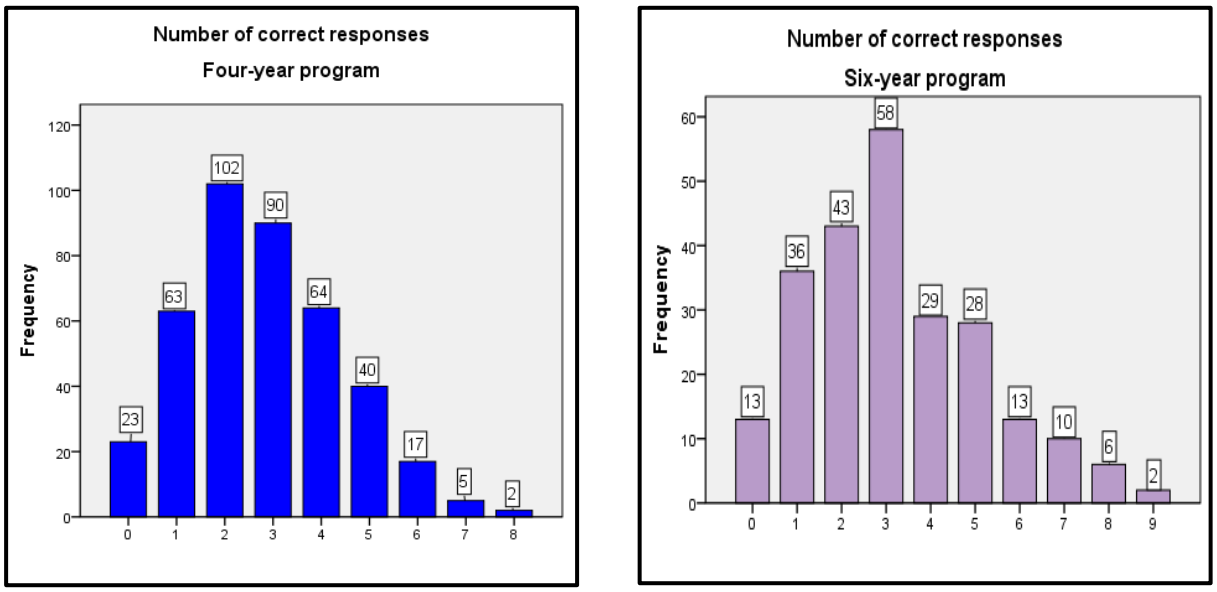

Figure 1: Number of all correct answers among four-year (and six-year) program students (total sample)

8.3. Hypothesis 3.

In the research, students from four high school classes (two from four and two from six-year program) were included in the experimental group (N=117), while the other students, who were asked to solve the pre-test, were part of the control group (N=527). In the experimental group, I also demonstrated the results gained through the Monte Carlo simulation method and we analyzed these in the chemistry classes. The most important question of the research is to find out if the application of the computer aided simulation method made a significant difference in learning the subject matter.

Comparison by type of task

	Type of the task	Experimental group	Control group	
		correct answers (%)		χ^2
1.	Concept of adsorption	30,8	8,7	41,858
2.	Concept of specific surface	33,3	5,1	82,836
3.	Listing three applied adsorbents	27,4	7,8	36,486
4.	Two everyday adsorption processes	53,0	16,9	69,527

Table 7: Distribution of the correct answers in the experimental and control group (questions 1-4)

Based on the first four questions, it can be stated that the students in the experimental group achieved higher performance than the control group, and the difference is significant (p=0.001). The biggest difference appears in the definition of the concept of specific surface. The previous analysis also showed that this concept was not emphasized enough in all the classes involved in the research, so the difference is understandable. I also looked into the analyses of the results of the simulation and the choices about the interaction of particles (Table 8).

	Type of the task	Experimental group	Control group	
		correct answers (%)		χ^2
5.	**Graph analysis**	53,0	19,4	57,072
6.	**Reason of the visible difference**	60,7	58,8	**0,137**
7.	**Type of the bond between molecules**	73,5	66,0	**2,431**
8.	**Temperature and pressure dependence of adsorption**	62,4	43,3	14,074
9.	**Adsorption on active coal**	46,2	39,1	**1,985**

Table 8: Distribution of the correct answers in the experimental and control group (questions 5-9)

The fifth question, the graph analysis showed a significant difference (χ^2 is 57.072 and p=0.001), and the experimental group's members achieved outstandingly better results. The sixth and seventh questions are related to each other. The task was to give the reason for the different behaviors of the two molecules, then to choose the interaction between particles based on another graph. Both questions can be answered if having general knowledge in chemistry, so the result is satisfying because there is no significant difference between the experimental and the control group in this question. This should be pointed out because the bond types between particles are part of basic knowledge when studying chemistry. So it can be said that this part of the curriculum was emphasized enough in all of classes involved in the research.

When it comes to the eighth question, the experimental group performed better than the control group again, and the difference is significant (the value of χ^2 is 14.074 and p=0.001). The difference in the answers about the dependence of adsorption on temperature and pressure is interesting because this topic is part of basic knowledge in chemistry, too. Correct answers were given in all of the classes, which means that the modifying factors were part of education,

but many of the students were not able to connect this with their general knowledge of chemistry. However, the percentage of the correct answers is low, especially in the case of the control group, which indicates that the average knowledge about particles and the students' chemistry perspective are not well established by the end of the school year.

Regarding the last question, the results were more similar between the experimental and the control group. The difference is not significant (χ^2 is 1.985 and p=0.159), but the experimental group's result is slightly higher. The correct answer about the differences of adsorption was the different polarity of the molecules. The high amount of correct answers (260) indicates that there is a remarkable development in their knowledge. Compared with the pre-test, in which 30.3% of the students knew the correct answer, this percentage increased to 40.4% in the post-test. Despite this favorable change, the overall result is not satisfying because the majority of the students gave incorrect answers, which indicates misbeliefs and serious incompleteness in their knowledge.

Comparing the overall performance of the experimental and the control groups, there is a significant difference (the value of χ^2 is129.581; DF=9, p=0.001), which can be seen in Figure 2. This means that significantly better results can be achieved if the new outcomes connected to adsorption are applied in education.

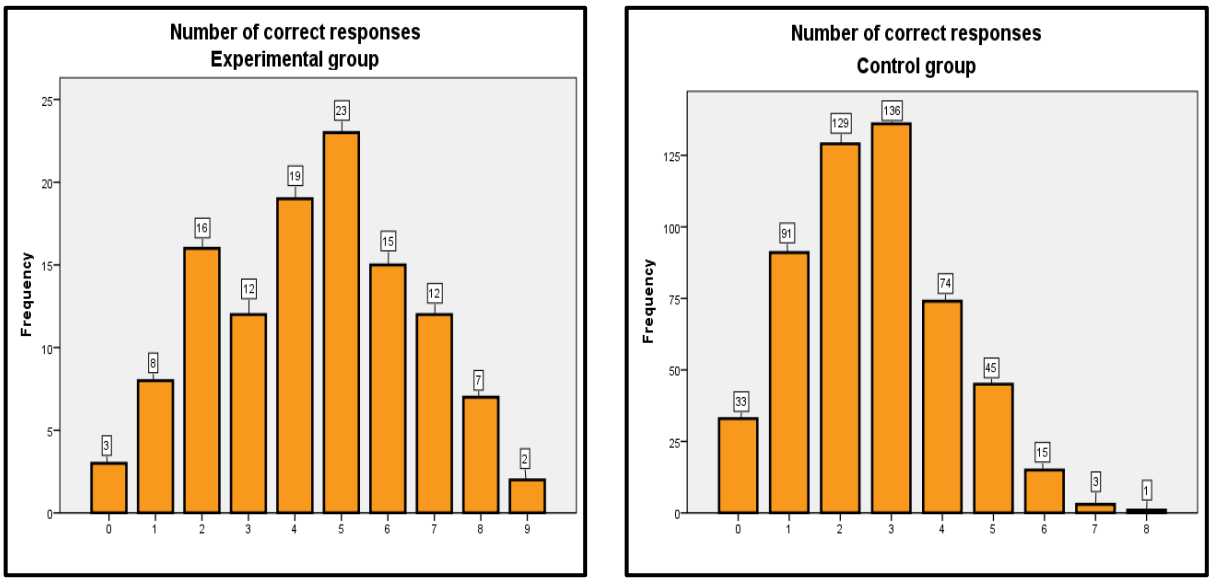

Figure 2: Overall number of points achieved by the experimental and the control group

According to the two-sample t-test it, can be stated that there is a significant difference between the curriculum expanded with the new adsorption outcomes and the traditional

curriculum (t=10.473 and p=0.001). The results of the experimental group are better than those of the control group.

The third hypothesis was proven to be true.

9. Additional research directions and opportunities

The result shows that applying the outcomes of adsorption research in education can make a significant difference because the experimental group achieved higher points in the test than the control group. This indicates that it would also be favorable to integrate the adsorption of other compounds into the teaching process, because that could lead to an even better result. We can broaden the scope of compounds and adsorbents that are used in everyday life and can be involved in adsorption processes. The application of other simulations could be taken into consideration to facilitate the understanding of other parts of the curriculum. In the assessment of how students can define concepts, the word association method could be used more widely, which is becoming more common in the assessment of science knowledge. By using this method, incomplete knowledge and misbeliefs can be identified not only in the field of adsorption, but in connection with any subject matter that forms the basis of moving on in the curriculum. Also, the research can be expanded to involve year ten students, and based on certain concepts, even students attending optional extra classes. By doing so, not only would we be able to assess and analyze the students' mind maps in themselves, but also the changes and adjustments caused by the application of computer assisted simulations. In the future, I am going to seek opportunities to further expand and continue this research by using my former results in this area.

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