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The Use of Molecular Simulation-Assisted Discovery Learning in Improving Science Process Skills

Andrian Saputra, Lisa Tania*, Mutiara Sari

Department of Chemical Education, Universitas Lampung, Indonesia

*Corresponding email: lisa.tania@fkip.unila.ac.id

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Abstract: ***The Use of Molecular Simulation-Assisted Discovery Learning in Improving Science Process Skills.*** ***Objectives:*** *This study aimed to describe the effectiveness of molecular simulation-assisted discovery learning (MSADL) in improving science process skills (SPS) on chemical equilibrium.* ***Methods:*** *This research used the matching-only pretest-postest control group design. The population in this study was all students of XI MIA at MAN 1 Bandar Lampung in 2019/2020. The sample was XI MIA 5 and XI MIA 6 obtained by purposive sampling. The data analysis technique used the t-test.* ***Findings:*** *The results showed the average n-gain of students' SPS using MSADL was 0.76 in high criteria, while the average n-gain of students' SPS using conventional learning was 0.54 in moderate criteria. The t-test results showed that the average n-gain of students' SPS using MSADL was higher than students' SPS using conventional learning.* ***Conclusion:*** *It can be concluded that MSADL is effective in improving students' SPS on chemical equilibrium.*

Keywords: discovery learning, science process skills, chemical equilibrium.

Abstrak: Penggunaan Model Pembelajaran Discovery Berbantuan Simulasi Molekul dalam Meningkatkan Keterampilan Proses Sains. ***Tujuan:*** *Penelitian ini bertujuan untuk mendeskripsikan efektivitas pembelajaran discovery berbantuan simulasi molekul (MSADL) dalam meningkatkan keterampilan proses sains (SPS) pada materi kesetimbangan kimia.* ***Metode:*** *Penelitian ini menggunakan the matching-only pretest-postest control grup design. Populasi dalam penelitian ini adalah siswa XI MIA MAN 1 Bandar Lampung Tahun 2019/2020 dengan XI MIA 5 dan XI MIA 6 sebagai sampel yang didapatkan dengan teknik purposif. Teknik analisis data yang digunakan adalah uji-t.* ***Temuan:*** *Hasil penelitian menunjukkan rata-rata n-gain SPS di kelas MSADL sebesar 0,76 berkriteria tinggi, sedangkan rata-rata n-gain SPS di kelas konvensional sebesar 0,54 berkriteria sedang. Hasil uji-t rata-rata n-gain SPS di kelas MSADL lebih tinggi dibandingkan kelas konvensional.* ***Kesimpulan:*** *MSADL efektif dalam meningkatkan SPS siswa pada materi kesetimbangan kimia.*

Kata kunci: *pembelajaran berbasis penemuan, keterampilan proses sains, kesetimbangan kimia.*

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INTRODUCTION

Natural science is a branch of science concerned with the description, prediction, and understanding of natural phenomena, based on empirical evidence from observation and experimentation. Mechanisms such as peer review and repeatability of findings are used to try to ensure the validity of scientific advances (Lagemaat, 2006). Chemistry is a part of natural science that involved with elements and compounds composed of atoms, molecules and ions: their composition, structure, properties, behavior and the changes they undergo during a reaction with other substances (Arifin, 2010). Chemistry content in the form of concepts, laws, and theories is basically the product of a series of processes using a scientific attitude. Thus, chemistry is not only a product of knowledge, but also a process.

Chemistry as a process or method of investigation includes ways of thinking, attitudes, and steps of scientific activity to obtain chemical products. Chemistry is not just how to work, see, and think, but as a way to know or discover (Nuh, 2014). Science process skills are the ability of students to apply scientific methods in understanding, developing, and discovering knowledge. Science process skills include the skills to formulate problems, make hypotheses, identify variables, collect data, make conclusions (Kheng, 2008). On the facts in the field, the learning process that has been applied in schools, teachers dominate in terms of explaining material which causes learning not to be student-centered, so that students become inactive and less capable in SPS (Yunita, Rosilawati, & Tania, 2015). Based on the results of observations in MAN 1 Bandar Lampung, teachers about chemistry lessons with the topic of chemical equilibrium teachers have linked the material with everyday life. According to the teacher, even though it has been linked to things that exist in everyday life, students are still passive in the learning process. From the observations, it was also found that practicum activities were only carried out on certain materials so that students were less trained in developing science process skills (SPS).

One of the chemical materials that involves SPS in increasing understanding of scientific concepts is chemical equilibrium. Changes in concentration, temperature, volume and pressure to a shift in chemical equilibrium will be difficult to understand if explained only through experimental results that can be observed in the laboratory or if only expressed symbolically by using a reaction equation, because it cannot show the actual dynamics occurring at the submicroscopic level. (Rahayu & Nasrudin, 2014). Therefore, an effort is needed to make these abstract chemical materials more concrete, namely through molecular simulations. In addition, a learning model that requires students to be active in the learning process is also needed. One learning model that suits this condition is discovery learning model assisted by molecular simulation.

According to Wilcox in learning by discovery, students are encouraged to learn largely through their own active engagement with concepts and principles, and teachers encourage students to have experiences and conduct experiments that allow them to discover principles for themselves. himself (Hosnan, 2014).

Molecular simulation is a simplification model to mimic and model molecular behavior so that it can be used to study the molecular system of a particular molecule that reflects the actual situation or state (Imaniastuti, 2011). One of the software that can be used to simulate molecules is Molecular Workbench. MW includes a set of computational engines that accurately simulate atomic motion, quantum waves, and atomic scale interactions based on fundamental equations and laws in physics. The Molecular Workbench significantly reduces the difficulty of learning and teaching abstract concepts (Xie & Tanker, 2006).

In a study conducted by Khoshoule, Ayub & Masrinejad (2014) examined the effects of using Molecular Workbench software on chemistry learning by high school students. The results of this study indicate that the Molecular Workbench Software helps students gain a better understanding of chemistry and helps them achieve better test scores compared to their schoolmates who were taught the conventional way. Lenczycki, Suto, Williams, & Strout (2014) also conducted a research entitled The Chemistry Between High School Students and Computer Science. The results of this study concluded that the Molecular Workbench Software provides an excellent platform for integrating computational models and particle simulations into high school classrooms.

Discovery learning model assisted by molecular simulation consists of 6 stages, namely stimulation, problem statement, data collection, data processing, verification, and generalization (Shah, 2004). Through molecular simulation assisted discovery learning models, SPS can be trained at all stages. At the stimulation stage until the data collection, students will be trained in observation skills where students can use all their sensory tools to observe phenomena, identify colors, and all the information needed for the analysis process at the next stage. At the data processing stage, students will be trained in communication skills, where students can process data from the experimental results of concentration factors and temperature factors in other forms such as tables or graphs, students are also given the opportunity to discuss with their groups to process the data that has been obtained. At the verification and generalization stages students will be trained in inference skills, where students can propose an explanation of the effect of the concentration and temperature factors obtained based on the results of their observations, students are also given the opportunity to analyze the causes and effects of these factors so that at the end of the lesson students can conclude the factors that affect the shift in the direction of chemical equilibrium. .

This is reinforced by the results of research (Rosalina, 2018), which was conducted at SMA Al-Kautsar Bandar Lampung, learning using animated media based on molecular simulations on mixed separation material can help visualize the movement of molecules so that learning is interesting and easy to understand. In addition, the results of research by Sukawati (2016) showed that the students of class XI MIPA SMAN 1 Bandar Lampung showed that the discovery learning model was effective in improving grouping and communicating skills on the buffer solution material. Based on the description above, this research was conducted with the title "The Effectiveness of Learning Discovery Assisted by Molecular Simulation in Improving Science Process Skills in Chemical Equilibrium Materials".

METHODS

The method used in this study is a quasi-experimental method with the research design of The Matching-Only Pretest-Postest Control Group Design (Fraenkel, Wallen, & Hyun, 2012). The population in this study were all students of class XI MIA MAN 1 Bandar Lampung in the 2019/2020 school year which were divided into 6 classes. The sample in this study was XI MIA 5 as the experimental class and XI MIA 6 as the control class. The sample selection technique used was purposive sampling technique. The instruments used in this study include students' worksheet learning model of discovery assisted by molecular simulations, grids of pretest and posttest questions, pretest and posttest rubrication questions, and pretest and posttest questions in the form of description questions to measure science process skills.

The data analysis carried out in this experiment is the quantitative data, including the calculation of student scores and the calculation of n-gain. According to Hake (1998), the n-gain classification are <g> e” 0.7; 0,3 d” <g> < 0,7; g <0,3 correspond to high, moderate, and low. Hypothesis testing in this study used the two-mean difference test before performing the two-average difference test, the normality test and the homogeneity test were performed first. The normality test in this study uses the help of the SPSS version 23 program with the Kolmogorov - Smirnov method. The test criteria used is to accept hypothesis if Sig > 0.05, which means that the research data comes from a normally distributed population and vice versa.

The homogeneity test of this study uses the help of the SPSS version 23 program. The test criterion used is to accept hypothesis if Sig > 0.05, which means that the two research classes studied have homogeneous variances and vice versa. The two-average equation test was carried out to determine whether the initial ability between the experimental class and the control was equal or not. The test criterion used is to accept H_0 if the value is sig. > 0.05 and vice versa. The two mean difference test is used to determine how effective the treatment of the sample is by looking at the n-gain value of science process skills. The test criteria used are accept hypothesis if the sig (2-tailed) value> 0.05.

■ RESULTS AND DISCUSSION

Based on the research that has been done, the obtained data are in the form of the pretest average of science processing skills, the two mean equation test results, the n-gain average, and the two mean difference test results. The average of pretest score on students' SPS is presented in Figure 1.

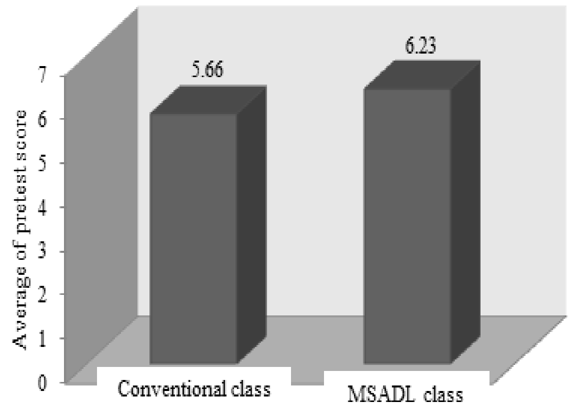

Figure 1. Average value of students' SPS in pretest

In Figure 1, it can be seen that the average pretest score for each class is not much different, this shows that the students' initial PPP skills in the class using molecular simulation assisted discovery learning and the class using conventional learning are relatively the same.

The data from the pretest results are used to test the two-mean equation, based on the results of the analysis using SPSS version 23, the data obtained are not normal and homogeneous, then the two-average equation test uses the Mann-Whitney test. The value of significance or sig. (2-tailed) obtained from the Mann Whitney test of 0.255. This indicates that the sig. (2-tailed) value obtained is greater than 0.05. Based on the test criteria, accept H0, which is the pretest average value of students 'SPS class using discovery learning model assisted by molecular simulation is the same as the pretest average value of class using conventional learning, so that the students' initial SPS ability is significant in the class using the model. Molecular simulation-assisted discovery learning and classrooms using conventional learning are the same. The average n-gain value of students' SPS is presented in Figure 2.

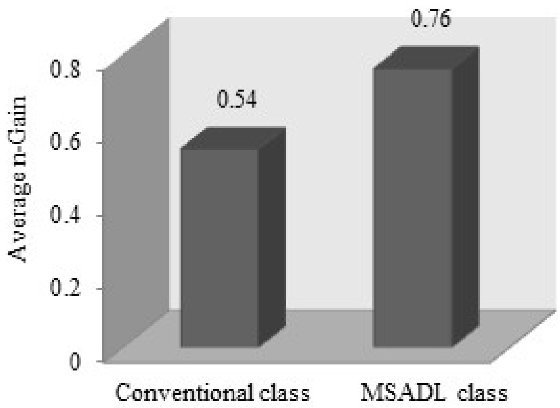

Figure 2. The average n-gain of students' SPS

In Figure 2 it can be seen that the average n-gain value of the experimental class (discovery learning assisted by molecular simulation) is 0.76 with high criteria, while in the control class (conventional learning) it is 0.54 with moderate criteria. This shows that the average n-gain value of the experimental class is higher than the control class, so it can be concluded that the increase in student SPS in the experimental class is higher than the control class.

The results of the difference test for the two mean science process skills are presented in Table 1.

Table 1. Independent sample T-test Result

Class	**n-gain average**	**N**	**sig. (*2-tailed*)**
MSADL	0.7642	30	0.000
Conventional	0.5462	30	

In Table 1 it can be seen that the value of significance or sig. (2-tailed) which is 0,000. The value obtained is less than 0.05. Based on the test criteria, accept H_1, that is, the average n-gain of SPS applied to molecular simulation-assisted discovery learning is higher than the average n-gain of student SPS with conventional learning. Based on this, it can be concluded that the discovery learning model assisted by molecular simulations is effective in improving PPP in chemical equilibrium material.

The results of the average percentage of student activity in the class using discovery learning assisted by molecular simulations are presented in Figure 3.

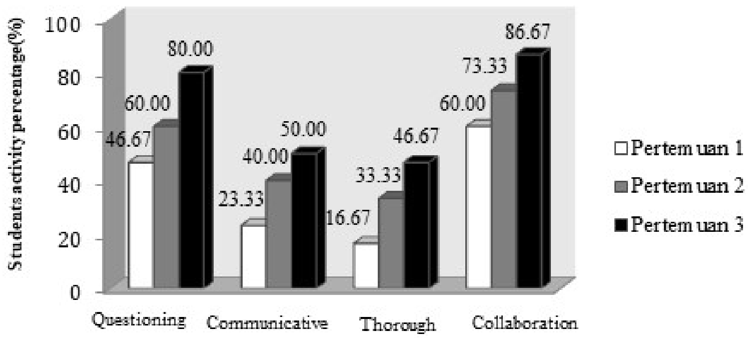

Figure 3. Percentage of students activity in MSADL class

In Figure 3, it can be seen that the average percentage of student activity in the class using discovery learning assisted by molecular simulations from the first meeting to the third meeting has increased.

Stage 1. Stimulation (providing stimulation)

At this stage the teacher raises the phenomenon of factors that affect chemical equilibrium. This is done to raise problems and grow students' curiosity, so that students are interested in being involved in solving these problems. In students' worksheet 1 in stimulation activities, the teacher shows the phenomenon of the concentration factor to a shift in the direction of equilibrium in the form of a discourse on the equilibrium of iron (III) thiocyanate solution and pictures of the first iron (III) thiocyanate solution, and after the addition of $FeCl_3$, KSCN, and NaOH solutions. The teacher provides the opportunity for students to identify problems based on the discourse given, then students are asked to ask questions about what students have observed and identified.

In students' worksheet 2 in stimulation activities, students are asked to observe the phenomenon of the temperature factor towards the shift in the direction of equilibrium in the form of the discourse of NO_2 gas initially, after being cooled or heated. The teacher then asks students to ask questions about what the students have observed and identified. In students' worksheet 2 students can ask questions correctly without being directed by the teacher.

It can be seen the difference between students' worksheet 1 and 2. In students' worksheet 1 student observation skills are still not visible, this is indicated by students still confused about what questions they want to ask because students are not used to observing phenomena. As time goes by, students begin to get used to and be trained so that it is clear that the student's development is quite good in students' worksheet 2, Students have curiosity about the material to be studied according to the stimulation given. This can also be seen in the percentage of student activity at the first meeting, student questioning activities were still lacking, only around 46.67%, while at the next meeting students were more active, reaching 80.00% in expressing questions.

This stimulation stage is included in the observation skill which is shown by students observing carefully the phenomenon of factors that affect the shift in the direction of equilibrium. At this stage, students use their sensory tools to observe the phenomena provided by the teacher so that their observation skills have been trained at the stimulation stage.

Stage 2. Problem statement (problem identification)

At this stage students are trained to formulate hypotheses (temporary answers) based on the problems they ask at the stimulation stage. The formulation of hypotheses is carried out in groups based on the results of discussions with each group, then students write them down in the students' worksheet.

In students' worksheet 1, before students formulate hypotheses, students are asked to identify changes that occur in the first iron (iii) thiosinate solution and after the addition of concentrated FeCl3 solution, concentrated KSCN and concentrated NaOH. This activity leads students to think analytically. In students' worksheet 2, students identify the changes that occur in NO2 gas after heating and cooling, then students can write their hypotheses according to the questions in the stimulation section posed by students.

It can be seen the difference between students' worksheet 1 and 2. In students' worksheet 1 student observation skills are still not visible, this is indicated by the answers of students who are still not right in proposing hypotheses because students are not used to it. As time goes by, students begin to get used to and be trained so that it is clear that the student's development is quite good in students' worksheet 2, students are able to put forward the correct hypothesis based on the results of observations.

At this stage, the student's observation skills have been trained by the teacher. Students identify discourses, figures, and tables related to factors that influence the shift in the direction of equilibrium. The activities carried out at this stage are in accordance with the indicators of observation ability, namely identifying the characteristics of the object in terms of shape, color and size.

Stage 3. Data collection (data collection)

At this stage, students find out the truth of the hypothesis they wrote down through experiments and seek information through their chemistry books. In students' worksheet 1 students conducted experiments on the effect of concentration on shifting the direction of equilibrium using a solution of iron (III) thiocyanate, $FeCl_3$, KSCN, and NaOH. The experiments conducted by these students provided the opportunity for students to use their five senses to the maximum extent possible in observing the color change of iron (III) thiocyanate solution before and after adding concentrated $FeCl_3$, concentrated KSCN, and concentrated NaOH solutions.

In students worksheet 2, students also conducted experiments on the effect of temperature on the shift in the direction of equilibrium using copper and concentrated HNO_3 solution. This activity also trains students' observation skills shown by the students observing the color of the gas produced from the reaction between copper and concentrated HNO3 solution. Students also observe the color changes that occur in the gas produced at both cold and hot temperatures.

At the first meeting, when conducting the first experiment, namely the effect of concentration on the shift in the direction of the chemical equilibrium in students' worksheet 1, students were still not careful in measuring solutions, observing changes in color, and using laboratory tools, this was because students were not used to practicing, but in experiments Next, in the next meeting the students were good enough in using the tools, observing changes in gas color and measuring the volume of the solution.

This is also supported by the percentage of student activity, namely student thoroughness activities, at the first meeting the students were still not thorough, as indicated by the low score of student activity, namely 16.67% and increased at the next meeting reaching 46.67%. Based on the explanation above, it is clear that at this stage students' observation skills have been trained in accordance with the indicators of student observation skills, namely using one or more sensory devices to collect information about objects or events.

Stage 4. Data processing (data processing)

This stage is a continuation of the data collection stage. The data that has been collected in the data collection section is then processed by students with guidance and direction from the teacher. Students process experimental data by making observations tables, analyzing them, and discussing with their group friends in answering the questions available in the data processing section of the students' worksheet.

In students' worksheet 1, students were asked to observe the equilibrium reaction of iron (iii) thiocyanate. Students also observe available discourses relating to the equilibrium that occurs in iron (iii) thiocyanate solutions. The activities carried out by the students then answered several questions that were available on data processing so that some processed data were obtained. At this stage, students are still led to analyze the table of observations they have obtained until they find the answer to the effect of concentration on the shift in the direction of equilibrium according to students.

In students' worksheet 2, students are guided by the teacher in writing down the reaction equations that occur based on the experiments that have been carried out. Students are able to answer several questions from the teacher, one of which is whether the copper reaction and the HNO3 solution produce gas or not. The student answers "yes, the gas is brown ma'am." The student is then asked by the teacher to write down the equation for the reaction. At this stage, students are asked to answer several questions based on the results they get from the experiment by observing the table of observation results such as the color of the gas produced when the temperature is raised and lowered. Students also answered correctly according to the observations they had obtained. The teacher then guides, guides, and directs students in processing data by answering the available questions.

It can be seen the difference between students' worksheet 1 and 2. In students' worksheet 1 students are still confused about communicating with the group, so the teacher guides students to analyze the table of observation results, this is because students are still not used to discussing in groups, but at the next meeting students can discuss with good with the group without the need to be directed by the teacher in answering the questions in the students' worksheet. This is also supported by the percentage value of students' communication activities, at the first meeting the percentage of students' communication was still quite small, namely 23.33%, at the next meeting the percentage of students' communication activities increased to 50.00%.

The activities carried out at students' worksheet 1 and 2 show that at this stage students 'communication skills have been trained, which is shown by processing data in the form of tables of observation results then discussing it with the group to answer questions, this is in accordance with the indicators of students' communication skills namely Providing / describing empirical data from experiments or observations with tables, and discussing the results of activities of a problem or an event.

Stage 5. Verification

At this stage, students have found the answer to the problem, then students carry out careful examinations to prove whether or not the hypothesis is determined and then linked with the results obtained in data processing. In students' worksheet 1, students are asked to discuss with their groups to prove whether the hypothesis is true or not by connecting the observations obtained from the experiment and from the results of molecular simulation animation data processing. An animated display of the concentration factor towards the shifting direction of chemical equilibrium can be seen in Figure 5.

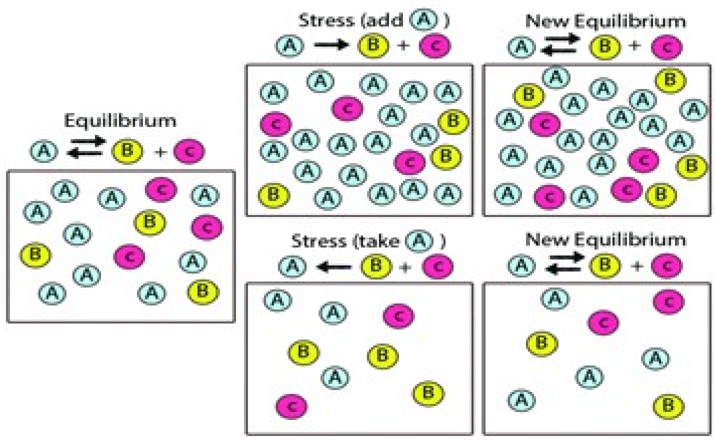

Figure 5. The screenshots of animation used in MSADL class

Based on Figure 5 it can be seen that there are atoms A, B and C, where A is the reagent, B and C are the product with the initial equilibrium position, the new equilibrium after the addition of the reagent A, and the new equilibrium after the reduction of the reagent A. During the learning process, students together the group was led to observe the animation presented so that it was able to identify and calculate the ratio of product and reactant concentrations at initial equilibrium (Kc) and when equilibrium was disturbed (Qc). Students are then also able to compare the Kc and Qc values obtained from the calculations so that in the end the students get answers about whether the hypothesis is true or not. In the learning process students are good enough in working together with their groups to discuss molecular animation and answer questions in students' worksheet 1, this is supported by the percentage of student cooperation activities that are quite good, reaching 60.00% and getting better at the next meeting until they reach 86.67%

In students' worksheet 2, just like students' worksheet 1, students are asked to discuss with their groups to prove whether the hypothesis is true or not by connecting the observations obtained from the temperature effect experiment with the results using molecular simulations. Before students use molecular simulations, students have been given the guidelines contained in their respective student worksheets, when opening the Molecular Workbench application students will see the initial view of the temperature factor molecular simulation towards the direction of the shift in chemical equilibrium as shown in Figure 6.

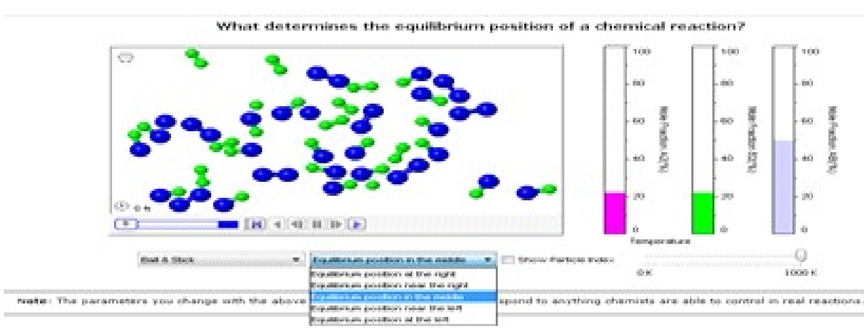

Figure 6. Initial display of the molecular simulation

Based on Figure 6, it can be seen that there are molecules consisting of AB molecules, A_2 molecules, and B_2 molecules. There are several tools that users can adjust, including molecular shape, equilibrium position, and temperature (K), because students will see the temperature factor towards the shifting direction of chemical equilibrium, the tools that are changed are the temperature tools located at the far right, while for the shape of the molecule and the position of the equilibrium are made the same, after adjusting it according to the needs of the students, students can see what changes occur in these molecules. The temperatures used for this molecular simulation are temperatures of 250 K, 300 K, and 350 K. The display images of molecular simulations at temperatures of 250 K, 300 K, and 350 K can be seen in Figures 7, 8 and 9.

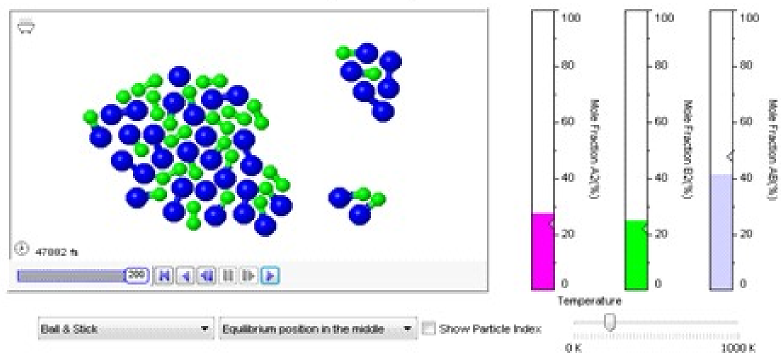

Figure 7. Molecular simulation of reaction in 250 K

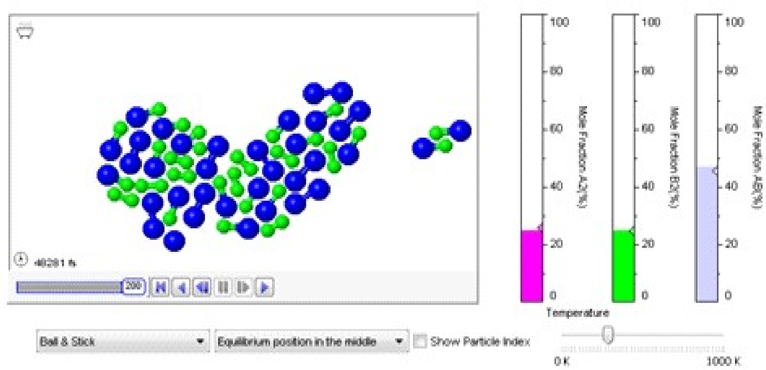

Figure 8. Molecular simulation of reaction in 300 K

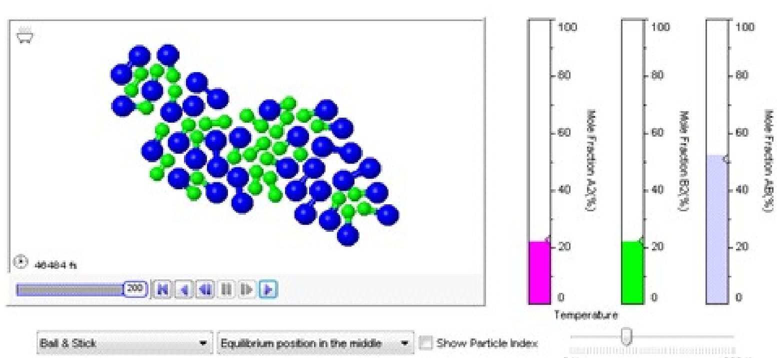

Figure 9. Molecular simulation of reaction in 350 K

Based on Figures 7, 8, and 9 it can be seen that there are molecules consisting of AB molecules, A_2 molecules, and B_2 molecules, where the equilibrium position is used, namely the equilibrium position in the middle, the ball and molecular shape. stick and the temperatures used were 250 K, 300 K, and 350 K after adjusting as needed, students were led to compare the number of molecules present in the reactants and products at room temperature (300 K), when the temperature was increased (350 K), and when the temperature is lowered (250 K), so that students can explain the relationship between the experimental data and the molecular simulation results. In the end, students get answers about whether the hypothesis is true or not.

Activities carried out in students' worksheet 1 and 2 indicate that students' inference skills have been trained at this stage, according to the indicators of student inference skills, namely proposing explanations for symptoms based on observations.

Stage 6. Generalization

Generalization is the final stage of the discovery learning model. At this stage students are asked to draw conclusions from the knowledge that has been obtained during the learning process based on the results of group discussions. The teacher then asks students to present the results to another group. Students' answers vary, but the teacher guides students to get relevant answers so that students are able to draw conclusions appropriately. At first the students were still confused in making conclusions, the conclusions made were not based on the problems given, but gradually the students were able to make conclusions on teacher guidance.

This activity also shows that at this stage students 'inference skills have been trained in accordance with the indicators of students' inference skills, namely being able to make a conclusion about an object or phenomenon after collecting, interpreting data, and information. The above stages clearly provide good achievement in the experimental class because they can train students 'SPS (observation, communication, and inference) at all stages of discovery learning, so that students' SPS can improve. This is also supported by research by Sukawati (2016), which states that the discovery learning model is effective in improving grouping and communicating skills on buffer solution material.

CONCLUSIONS

Based on the results of data analysis, the average n-gain value of students SPS who applied the discovery learning model assisted by molecular simulation was higher than the average n-gain value of students' SPS who applied conventional learning models on the factors that affect the shift in the direction of chemical equilibrium, It can be concluded that the discovery learning model assisted by molecular simulation is effective in improving science process skills on the factors that affect the shift in the direction of chemical equilibrium.

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