22 (2), 2021, 315-323

Jurnal Pendidikan MIPA

e-ISSN: 2550-1313 | p-ISSN: 2087-9849

http://jurnal.fkip.unila.ac.id/index.php/jpmipa/

Molecular Simulation Assisted Discovery Learning to Improve Higher Order Thinking Skills in Chemical Equilibrium Concepts

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Abstract: The purpose of this study is to describe the effectiveness of discovery learning assisted by molecular simulation to improve higher order thinking skills in chemical equilibrium materials. The method used in this study was a quasi-experimental with the matching only pretest-postest control group design. The population were all students of XI MIA MAN 1 Bandar Lampung in the academic year 2019/2020. The sample was XI MIPA 5 as an experimental class and XI MIPA 6 as a control class obtained by purposive sampling technique. The data analysis technique used was the t test. The results showed the n-gain average of students' high-level thinking skills in the molecular simulation assisted learning class were 0.78 with high criteria, whereas in the control class was 0.58 with medium criteria. The t-test results showed students n-gain in the experiment class was significantly higher than control class. It can be concluded that the discovery learning model assisted by molecular simulations was effective in improving students' higher order thinking skills.

Keywords: chemical equilibrium, discovery learning models, higher order thinking skills, molecular simulation

Abstrak: *Penelitian ini bertujuan untuk mendeskripsikan efektivitas model pembelajaran discovery berbantuan simulasi molekul dalam meningkatkan keterampilan berpikir tingkat tinggi pada materi kesetimbangan kimia. Penelitian ini menggunakan metode kuasi eksperimen dengan desain penelitian the matching-only pretest-postest control group design Populasi dalam penelitian ini yaitu, seluruh siswa kelas XI MIA MAN 1 Bandar Lampung tahun ajaran 2019/2020. Sampel dalam penelitian yaitu kelas XI MIA 5 sebagai kelas eksperimen dan XI MIA 6 sebagai kelas kontrol yang dihasilkan dengan menggunakan teknik purposive sampling. Teknik analisis data yang digunakan adalah uji perbedaan dua rata-rata dengan uji t. Hasil penelitian menunjukan rata-rata nilai n-gain keterampilan berpikir tingkat tinggi siswa pada kelas pembelajaran discovery berbantuan simulasi molekul sebesar 0,78 berkriteria tinggi, sedangkan pada kelas pembelajaran menggunakan metode ceramah sebesar 0,58 berkriteria sedang. Hasil uji t menunjukkan n-gain pada eksperimen lebih tinggi secara signifikan daripada kelas kontrol. Berdasarkan hasil penelitian dapat disimpulkan bahwa model pembelajaran discovery berbantuan simulasi molekul efektif untuk meningkatkan keterampilan berpikir tingkat tinggi siswa.*

Kata kunci: *model pembelajaran discovery, kesetimbangan kimia, keterampilan berpikir tingkat tinggi, simulasi molekul.*

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DOI: http://dx.doi.org/10.23960/jpmipa/v22i2.pp315-323
Received: 08 October 2021
Accepted: 13 December 2021

▪ INTRODUCTION

Higher order thinking skills are students' thinking patterns by relying on the ability to analyze, evaluate and create all aspects and problems (Anderson & Krathwohl, 2001). Students with higher-order thinking skills must be able to really understand, apply what they already know and realize their ideas, so students must be trained to solve a problem Birgili, Seggie & Oğuz, 2021). One of the models that can improve students' higher order thinking skills is the discovery learning model.

The discovery learning model is rooted in constructivist understanding (constructivism). This constructivist theory states that students must find themselves and transform complex information, check new information, with old rules and revise them if the rules are no longer appropriate (Trianto, 2007). The stages in the discovery learning model are stimulation (providing stimulation), problem statements (problem identification), data collection (data collection), data processing (data processing), verification (proof), and generalization (drawing conclusions) (Syah, 2004). Chemistry learning with this model will produce students who are productive, creative, innovative and affective through strengthening integrated attitudes, skills and knowledge (Osman & Lay, 2020).

Higher order thinking skills such as the ability to analyze and evaluate can be improved at several stages in molecular simulation-assisted discovery learning, namely at the data collection stage (data collection), data processing (data processing), and verification (proof). At the data collection stage (data collection). Most of the material in chemistry lessons has abstract characteristics (Treagust, 2003). One of the Basic Competencies (KD) in chemistry class XI SMA which contains abstract material, namely KD 3.9 Analyzing the factors that affect the shift in the direction of equilibrium and its application in industry and KD 4.9 Designing, conducting, and concluding and presenting experimental results factors that affect the shift in the direction of the equilibrium. Chemical equilibrium is a chemical material in which it describes reversible and irreversible reactions and the factors that affect equilibrium. Changes that occur in the equilibrium state in a reaction are at the submicroscopic (molecular) level so that it is difficult to observe with the naked eye (macroscopic level). One of the learning media that can explain the concept of chemical equilibrium submicroscopically is molecular simulation.

Molecular simulation is a simplification model to imitate and model the behavior of molecules so that it can be used to study the molecular system of a particular molecule that reflects the actual situation or situation (Imaniastuti, 2011). Molecular simulation is recommended because the effect of changes in concentration, temperature, volume and pressure on a shift in chemical equilibrium will be difficult to understand if it is explained only through experimental observation or expressed symbolically by using a reaction equation. By molecular simulation, it easy to show the dynamics that actually occur at the submicroscopic level (Allen, 2007; Stull, Gainer & Hegarty, 2018; Bennie et.al., 2019; Edwards et.al., 2019; O'Connor, 2019)

Molecular Workbench is one of the molecular simulations that can explain the concept of chemical equilibrium such as the temperature factor to the shift in the direction of chemical equilibrium. Molecular Workbench was created by Nation Science Foundation grants which was later developed by Charles Xie (Xie & Tinker, 2006). Molecular Workbench can assist teachers in visualizing how the effect of temperature on the shift in the direction of the chemical equilibrium when the system temperature is raised and lowered.

Research with molecular simulation-assisted learning using Molecular Workbench has been applied to many topics in chemistry (Al-Moameri, Jaf & Suppes, 2018; Kurniawan et.al., 2019; Sharma & Asirwatham, 2019; Al Mamun, Lawrie & Wright, 2020; Zohar & Levy, 2021). In the learning process students can easily start, stop, and check the simulation frame-by-frame and can change the initial conditions and parameters. Interactive simulation and visualization of chemistry at the atomic scale can help students understand the relationship between chemical equations and atomic interactions. Learning chemical reactions and atomic interactions that have been carried out with the help of molecular simulations using Molecular Workbench has very good results on student activity (Xie & Tinker, 2006).

This study aimed to determine the effectiveness of discovery learning assisted by molecular simulation using molecular workbench in improving higher order thinking skills in chemical equilibrium materials. The following are the research questions that the study seeks to answer:

1. Is the discovery learning assisted by molecular simulation effective in improving students higher order thinking skills in chemical equilibrium materials?
2. Why does discovery learning assisted by molecular simulation effective in in improving students higher order thinking skills in chemical equilibrium materials?

▪ METHOD

The method used in this study is a quasi-experimental method with a research design of The Matching-Only Pretest-Postest Control Group Design (Fraenkel, Wallen, & Hyun, 2012). The population in this study was all students of class XI MIA MAN 1 Bandar Lampung for the academic year 2019/2020 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 with the sample selection technique used, namely the purposive sampling technique. The instruments used in this study included discovery learning model worksheets with the help of molecular simulations, pretest and posttest lattices, pretest and posttest rubrics, and pretest and posttest questions in the form of description questions to measure higher order thinking skills.

The data analysis carried out in this experiment is on quantitative data, including the calculation of student scores and the calculation of n-gain. Hypothesis testing in this study used a difference test of two averages. The normality test and a homogeneity test were carried out first before difference test of two averages. The normality test and the homogeneity test used SPSS version 23.0. The two-mean difference test was used to determine how effective the treatment is on the sample by looking at the n-gain value of higher order thinking skills. The test criteria used are accept H0 if the value of sig (2-tailed) > 0.05 and accept H1 if the value of sig (2-tailed) < 0.05.

▪ RESULT AND DISCUSSION

Based on the results of the pretest and posttest scores of students' higher order thinking skills in the molecular simulation-assisted discovery learning class and the lecture-based learning class (conventional learning), which is presented in Figure 1.

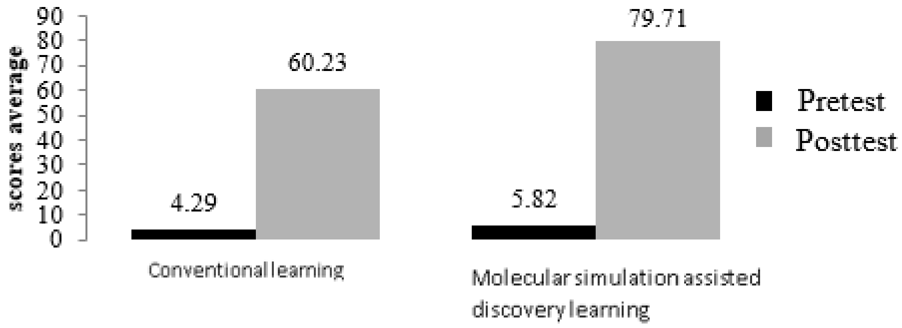

Figure 1. The average of the pretest and posttest

Figure 1 shows that both classes have the different average of pretest and postest scores. The average pretest and posttest scores in the molecular simulation-assisted discovery learning class was higher than the conventional learning. The similarity test of pretest scores was conducted to check the initial students higher order thinking skills. Before conducting the similarity test of the two averages, a prerequisite test was carried out, namely the normality test and the homogeneity test using SPSS version 23.0. The homogeneity test is a prerequisite test that aims to determine whether the variance between the data groups being tested is uniform or not based on the sample data obtained (Arikunto, 2006). The results of the normality tests are presented in Table 3.

Tabel 3. The result of normality test of pretest scores

Class	Normality test		Conclusion
	sig	Test criteria	
Molecular simulation asissted-discovery learning	0.000	*Sig*> 0,05	Not normally distributed
Conventional learning	0.000		

Then the homogeneity test was carried out using SPSS version 23.0 with the acceptance test criteria H_0 if the value of sig. from Levene Statistics > 0.05, in other cases reject H_0. Based on the results of the homogeneity test on the pretest score, the sig value was obtained. From Levene Statistics 0.59. These results indicate that the value of sig. From Levene Statistics it is greater than 0.05, so the decision of the test is to accept H_0, which is significantly the two research classes have homogeneous variance. Because the pretest data obtained were not normally distributed and homogeneous, then a similarity test of the two averages was carried out using the Mann-Whitney U test (U test).

The similarity test of these two averages was used to find out that the students' initial higher order thinking skills in the discovery learning class assisted by molecular simulation and the class using the lecture method were significantly the same. Based on the test results using SPSS 23.0 obtained the value of sig. (2-tailed) obtained from the U test of 0.605. Because the value of sig. (2-tailed) obtained > 0.05 then accept H0 where the hypothesis criteria are, the average value of the pretest of students' higher order thinking skills in the discovery learning class assisted by molecular simulation is the same as the average value of the pretest of students' higher order thinking skills in the learning class using the lecture method on chemical equilibrium material. It can be concluded that both classes have the same initial higher order thinking skills. The average n-gain of students' higher order thinking skills obtained is presented in Figure 2.

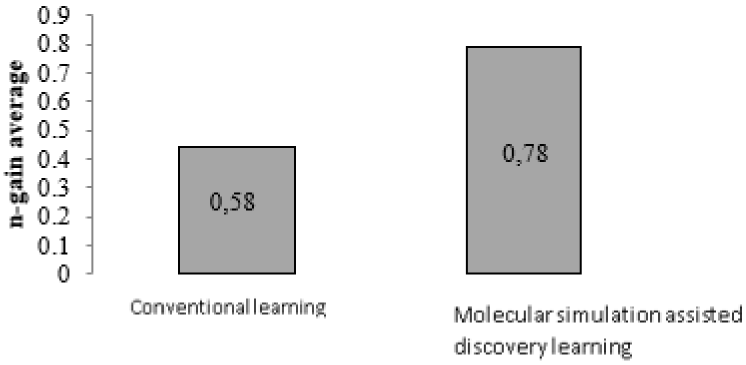

Figure 2. Average n-gain of students higher order thinking skills

Based on Figure 2, it can be seen that the average value of n-gain in the discovery learning class assisted by molecular simulation is higher than the average value of the n-gain class using the lecture method. To find out whether the mean n-gain of the two samples is significantly different, then a difference test of the two means is carried out. Before testing the difference between the two averages, a prerequisite test was carried out, namely the normality test and the homogeneity test. The results of normality tests are presented in Table 4.

Tabel 4. The result of normality test of n-gain scores

Class	Normality test		Conclusion
	sig	Test criteria	
Molecular simulation asissted-discovery learning	0.181	*Sig* > 0.05	Normally distributed
Conventional learning	0.200		

The homogeneity test was carried out using the Levene statistical test, with the assumption that it was homogeneous if the sig. value> 0.05. Obtained a sig value of 0.133. Based on the test criteria, it means that you accept H0 which means that both samples have homo-gene variance. After the normality test and homogeneity test were carried out on the n-gain, then the hypothesis was tested using the independent samples t-test, using SPSS version 23.0. Obtained the value of sig. (2-tailed) < 0.05 is 0.00. It means that reject H_0 and accept H_1, with the hypothesis criteria being that the average value of the n-gain value of students' higher order thinking skills in the discovery learning class assisted by molecular simulation is higher than the n-gain average value of students' higher order thinking skills in the learning class using the lecture method (conventional learning).

Based on the result, there was significant difference in the n-gain average value of students' higher-order thinking scores between classes that use discovery learning models assisted by molecular simulations and classes whose learning uses the lecture method, so it can be concluded that the simulation-assisted discovery learning model molecules on the material factors that affect the shift in the direction of chemical equilibrium was effective for improving students' higher order thinking.

Discovery learning cosisted of six stages, namely stimulation (providing stimulation), problem statements (problem identification), data collection (data collection), data processing (data processing), verification (proof), and generalization (drawing conclusions) . The first stage is stimulation, at this stage students are given the phenomenon of chemical equilibrium in everyday life, this aimed to raise problems and encourage students' curiosity so that students are interested in being involved in problem solving. Students are given discourses and pictures of a solution of iron (III) thiocyanate in its initial state, given the addition of $FeCl_3$, KSCN, and NaOH to observe, recognize, and identify the color changes that occur.

Then students were asked to formulate problems based on the discourse that has been read. After that the teacher guides students in the second stage of the discovery learning model, namely the problem statement (problem identification). At this stage, students observed and identified the problems contained in the stimulation stage and then made the hypothesis. The hypotheses made will be used to guide the data collection process. In data collection, students were asked to find out the truth of the hypotheses they have made. In students worksheet, students were given a discourse about experiments related to the effect of concentration on the shift in the direction of chemical equilibrium. Students were asked to determine the independent variables, dependent and control variables, experimental tools and materials based on the discourse. Then they arranged an experimental procedure. Because this activity requires students to analyze variables, tools and materials to make an appropriate experimental procedure, so this activity can train students' analytical skills. They compared the procedure with the procedure made by the teacher. This activity can train students' ability to evaluate. At this stage, students also conduct experiments. After conducting the experiment, students were asked to fill in the table of observations where they had to analyze the color change in the equilibrium system when it was given treatment, determined which direction the chemical equilibrium shifted after being treated based on the color changes that occurred. This activity can train students' ability to analyze. Student activities at the data collection stage train students' abilities in analyzing and evaluating so that they can improve students' higher-order thinking skills (Saputri, 2019)

The second meeting was started by the fourth stage of discovery learning model, namely data processing. At this stage the teacher guides students in processing the data collected. Students discussed in groups to answer questions. In the fifth stage, namely verification, students observed the animations regarding the effect of concentration on the shift in the direction of chemical equilibrium. The animation of the concentration factor towards the direction of the chemical equilibrium shift can be seen in Figure 3.

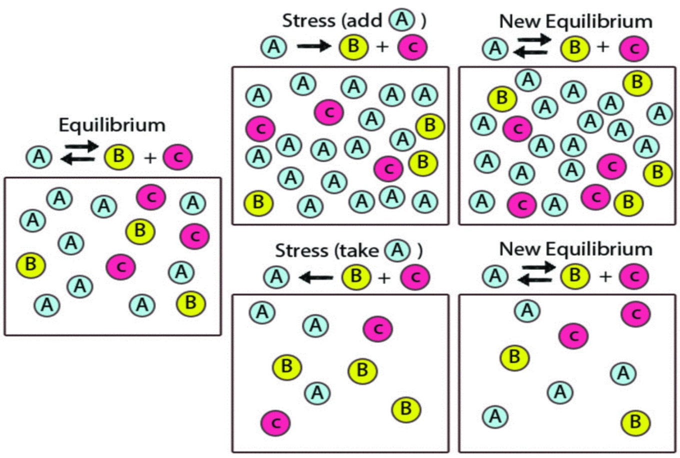

Figure 3. Animation of the concentration factor in the direction of the shift in chemical equilibrium

Atom A acts as reactant while B and C act as products. After observing the animation, students were asked to identify what happens in the animation by answering the questions in worksheet 1. Students calculated the ratio of the concentrations of products and reactants in an equilibrium system initial (Kc) and when the equilibrium system is disturbed (Qc) then compared the value of Qc with Kc. The sixth stage is generalization (drawing conclusions). Students are asked to conclude the effect of concentration on the shift in the direction of the equilibrium based on the value of Qc with Kc. The next material is the temperature factor for the shift in the direction of chemical equilibrium. In this material, students were trained their order thinking skill by an application named Molecular Workbench. At the stimulation stage, students were asked to observe the discourse along with pictures of NO_2 gas at first, after being heated and cooled. At the problem statement stage (problem identification) students were asked to identify changes that occur in NO_2 gas after being heated and cooled, then students wrote their hypotheses based on questions in the stimulation section. The hypotheses made will be used to guide the data collection process.

In the third stage, namely data collection, students were asked to design experiments on the effect of temperature on the shift in the direction of chemical equilibrium in groups. Students determined the independent variables, dependent and control variables, experimental tools and materials based on the discourse then arrange experimental procedures. This activity can train students' analytical skills. After that they compared the procedure they have made with the procedure made by the teacher. This activity can train students' ability to evaluate. Students observed the color of the concentrated HNO_3 + Cu mixture at first, when the temperature was lowered (cooled), and when the temperature was raised (heated). Data processing stage asked students to write down the equation for the reaction that occurs between Cu and concentrated HNO3 solution and analyze the changes that occur based on experimental data on the effect of temperature on the shift in the direction of chemical equilibrium. This activity train students' ability to analyze chemical process so they can train students' higher order thinking skills. The verification stage asked students to observe reactions experimental results of the effect of temperature on the shift in the direction of chemical equilibrium and analyze the changes that occur in the reaction by relating the entalphy of the reaction. Students observed a molecular simulation Workbench to determine the effect of temperature on the submicroscopic shift in chemical equilibrium from the equilibrium reaction equation as shown in Figure 4.

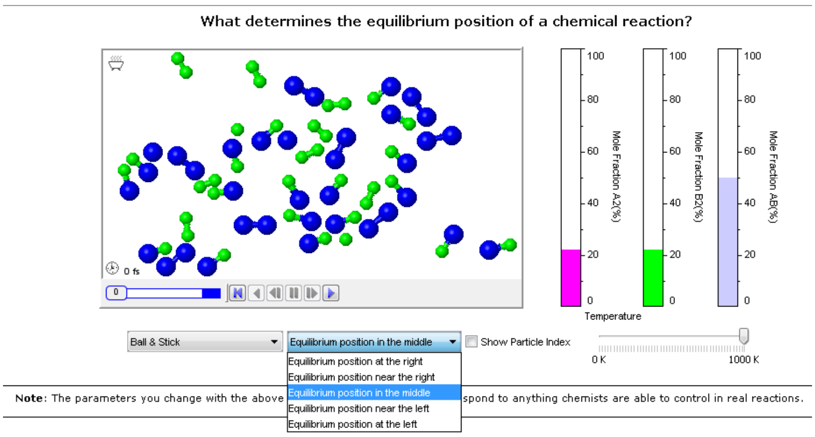

Figure 4. Initial view of molecular workbench molecular simulation of temperature factor on the direction of shift in chemical equilibrium

$$A_2 + B_2 \rightleftharpoons 2AB \qquad \Delta H = +X\ kJ$$

After observing the molecular simulation, students analyzed the number of product and reactant molecules based on the molecular workbench simulation then compare the entalphy at the various temperatures of 250K, 300K and 350K. These activity train students' higher-order thinking skills. In the generalization stage (drawing conclusions) students concluded the effect of temperature on the shift in the direction of chemical equilibrium based on experiments and molecular simulations.

▪ CONCLUSION

Based on the results of the research and discussion, it was concluded that the discovery learning model assisted by molecular simulation was effective in improving students' higher-order thinking skills on the material on the factors that influence the shift in the direction of chemical equilibrium. The discovery learning model assisted by molecular simulation can train students ability in analyzing, evaluating and drawing conclusion.

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