

Need Analysis of Basic Chemistry Practicum Based on Computation

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Abstract: Computational chemistry is a branch of chemistry which is the theoretical translated into computer programs to calculate the properties of molecules and their changes. This study analyzes the need of computational-based chemistry practicum in the Basic Chemistry course at the Chemistry Education Study Program at Samudra University. This study was done by survey technique. Aspects analyzed in this study include: module analysis through a review of the Basic Chemistry practicum module used by the Chemistry Education study program, needs analysis through students' perceptions that has been carried out, and literatures analysis through computational studies for Basic Chemistry that have been developed. Basic Chemistry practicum implemented in Chemistry Education is a verification practicum (conventional), and it is necessary to implement a practicum that gives more freedom to students in exploring. Basic chemistry practicum in Chemistry Education is also not based on computational, so it is necessary to develop basic chemistry practicum activities that provide computational problem solving.

Keywords: Basic chemistry practicum; Chemistry computation; Molecules

Introduction

State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results. Basic Chemistry as a science course requires an emphasis on providing hands-on experience to develop students' competence in exploring nature and increasing knowledge (Fors, 2016; Bonney 2015). Giving immediate experience in the learning process can be done through practical implementation (Rakhman et al, 2020). Practicum is a student-centered learning, the teacher as a facilitator and not teaching immediately. Practicum is one of important activities in scientific process and scientific attitude (Subiantoro, 2010; Nasution, 2014; Sibuea, 2020). Anyhow, scientific process and scientific attitude is important factors in science investigation (Juhji, 2020). In addition, practicum can be used to train three skills, namely: (a) high cognitive skills include: deepening the theory that has been obtained for more understanding, and developing cognitive strategies; (b) affective skills

include: learning to plan activities independently, and learning to work together; (c) psychomotor skills include: learning to install the certain equipments so that it actually runs and learning to use its certain equipments (Utomo and Rijkes, 1991).

Implementation of the Basic Chemistry practicum can be hampered due to several factors: expensive cost to purchasing chemicals, limitation tools of chemical practicum, the dangers that may arise in chemistry practicum, no treatments of practical waste, and takes a long time to prepare practical. Along with science and technology advances, these problems can be solved by utilizing computational chemistry technology (Arifani et al, 2021; Hadisaputra et al, 2017; Jansen-van Vuuren, et al 2013).

Basically, Computational science is a field of science that has attention to the preparation of mathematical models and technical numerical solutions as well as the use of computers, to analyze and solve scientific problems. In practice, mathematical models and computer simulations as well as various forms of

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numerical computing not only used to solve scientific and technological problems, but also used to discover new principles of fundamental science (Ardisasmita, 2010). Computational science is concerned with the formulation of mathematical models and technical numerical solutions and the use of computers to analyze and solve scientific problems.

Computational chemistry is a branch of chemistry which is the theoretical translated into computer programs to calculate the properties of molecules and their changes. It is also simulated large systems (or many protein molecules of gases, liquids, solids, and liquid crystals) and apply the program to real chemical systems (Prianto, 2010; Cristopher 2004). This method is very flexible and almost all practical chemistry materials. Both simple and high levels of difficulty, it can be modeled using computational chemistry. There are various kinds of computational chemistry free software should be used as an alternative to chemistry practicum. These software are Hypercam, ChemLab, NwChem, Gaussian, ACD/ChemSketch dan lain- lain (Fortenberry et al, 2015). Another advantage of using computational chemistry as an alternative to chemistry practice is low fo cost, has a high level of accuracy, shortens practice time, is not dangerous, and of course can improve understanding of chemistry optimally (Ochterski, 2014; Sendlinger, 2010; Hadisaputra 2017).

Some uses of computational chemistry techniques for chemical modeling include: (1) designing initial process synthesis reaction desired, (2) studying and exploring possible reaction mechanisms from the designs that have been made, (3) performing reaction simulation in computer, (4) determine the properties of the reactant and product molecules (Prianto, 2008). Examples of molecular properties that can be calculated include structure (constituent atoms space), energy and energy difference, charge, dipole moment, reactivity, frequency of vibration and other spectroscopic quantities. Simulation of macromolecules (such as proteins and nucleic acids) and large systems include the study of molecular conformation and changes (eg protein denaturation), phase changes, and forecasting macroscopic properties (such as specific heat) based on behavior at the atomic and molecular level (Leach, 1996).

Seeing the importance role of computational chemistry, it is necessary to analyze the need of computational-based chemistry practicum in the Basic Chemistry course at the Chemistry Education Study Program at Samudra University.

Method

This study is part of research and development (R&D) of basic chemistry practicum based on computation. It is followed research flow on Figure 1.

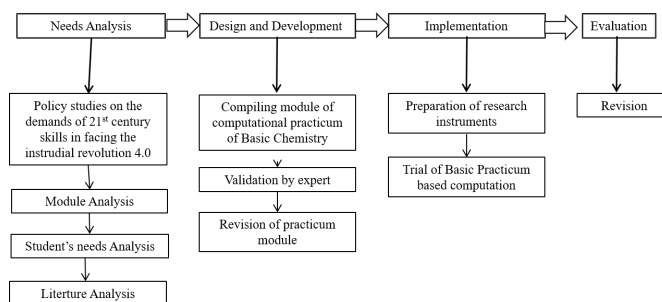


Figure 1. Research Flow

This analysis research was done by survey technique. Survey is a data collection technique by asking questions about opinions, characteristics and behaviors that have been/are happening (Groves et al., 2010). Aspects analyzed in this study include: module analysis through a review of the Basic Chemistry practicum module used by the Chemistry Education study program, needs analysis through students' perceptions that has been carried out, and literatures analysis through computational studies for Basic Chemistry that have been developed.

The module analysis is carried out using a review sheet which is grouped into 3 aspects, including: the component aspects of the practicum worksheets, the aspects of computational elements, and aspects of skills that are trained in the implementation of the practicum. The review sheet is filled out by a Basic Chemistry 1 course lecturer.

Needs analysis is done by using a closed questionnaire with a rating scale. Closed questionnaire is a type of questionnaire in which the answer has been provided, the respondent can choose one of the available answers by marking (Suharsimi, 2006). The respondents in this analysis are active students of the Chemistry Education who have taken Basic Chemistry class. There are 54 students from 87 active students who have taken Basic Chemistry class. Data analysis was carried out descriptively, namely by describing the collected data as it is (Sugiyono, 2013). The data description provides in simple form percentage using interpretation criteria: no one, for 0%; few, for 0%-25%; almost half, for 25-50%; half, for 50%; most of, for 50-75%; almost everyone, for 75-100%; and the whole, for 100%. (Lestari and Yodhanegara, 2017). The instrument sheet used to analyze these two aspects has been validated by experts and has been tested to be valid and reliable.

Literature analysis meant for finding relevant literature by reading articles. Here, it done by describing previous research to map and assess the research are. Analysis conducting used the systematic literature review method for identifying and critically appraising relevant research. (Snyder, 2019). Literature analysis was carried out descriptively qualitatively through three activity lines: data reduction, data presentation, and conclusion drawing (Miles and Huberman, 1984).

Result and Discussion

Practicum Module Analysis

Generally, the module is one of teaching materials packaged in a complete and systematic way, which contains a set of planned learning experiences to help students master specific learning goals (Daryanto, 2013). So, practicum module as a guideline for practicum must also meet the criteria as a learning module. Practicum is one of learning methods which is accordance to constructivism learning theory that emphasizes the activities of students to gain their own knowledge (Suparlan, 2019). Thus, a good practicum module must be able to train students' process skills.

Computation as a mainstay in solving chemistry experiment problems (Arifani et al, 2021; Hadisaputra et al, 2017; Jansen-van Vuuren, et al 2013), so practicum module must consist of computational elements. These

elements can include: low cost for require tools and materials, directed experimental method (not repeated), combines technical and mathematical, computational problem solving easily, provides simulation modeling and visual representation of abstract concepts (Ardisasmita, 2010).

This research has reviewed the Basic Chemistry module used by the Chemistry Education Study Program UNSAM. The module review is carried out in three aspects of the review, that is: (1) Components of the Practicum Worksheet to see the completeness of the elements as a practicum module in general (conventional), (2) Computing elements to see the use of computational science as a solution to problems in Basic Chemistry practicum, and (3) Skills that are trained to see the function of the module in developing student process skills. Table 1, Table 2 and Table 3 are the review results of Basic Chemistry practicum module in these three aspects.

Table 1. Worksheet Aspect

Review Aspect	Review Target	Yes	No	%
Worksheet Practicum Components	Title	√		76.9%
	Aims of practicum	√		
	Basic Theory	√		
	Practicum Tools and Materials	√		
	Problem Formulation		√	
	Hypotheses		√	
	Practicum Procedures	√		
	Observation Data Table	√		
	Data Analysis	√		
	Preliminary assignments	√		
	Practicum final assignments		√	
	Practice questions	√		
	Reference lists	√		

Based on Table 1, the completeness of the component aspects in practicum worksheets reached 69.2% of all review targets, which included: title, aims of practicum, basic theory, practicum tools and materials, problem formulation, hypotheses, practicum procedures, observation data tables, data analysis, preliminary assignments, practicum final assignments, practice questions and reference lists. This percentage

refers to "good". So, as a conventional module, the Basic Chemistry module has a good completeness of worksheet. Uncomplete items only for problem formulation, hypotheses, and final assignment. This incompleteness because the module was used for verified experiment, where the students were guided to do the whole experiment in detail.

Table 2. Computation Elements Aspect

Review Aspect	Review Target	Yes	No	%
Computation Elements	Low cost for require tools and materials		√	16.7%
	Directed experimental method (not repeated),		√	
	Combines technical and mathematical	√		
	Computational problem solving easily		√	
	Provides simulation modeling		√	
	Visual representation of abstract concepts		√	

The computational elements contained in the Basic Chemistry practicum module are only 16.7% of the overall targets reviewed, including: low cost for require tools and materials, directed experimental method (not repeated), combines technical and mathematical,

computational problem solving easily, provides simulation modeling and visual representation of abstract concepts. This percentage refers to "low". It is only agreed for combines technical and mathematical,

but the mathematic that used in that practicum module is simple mathematic.

Table 3. Trained Skill Aspect

Review Aspect	Review Target	Yes	No	%
Skills that are trained	Lead instructions in understand the basic theory ability of practical implementation	√		44%
	Lead instructions in practical planning skills		√	
	Lead instructions in assembling practical equipment skill	√		
	Lead instructions in direct the skills to operate practical equipment	√		
	Lead instructions in do practicum skills	√		
	Lead instructions in formulating skills practical steps		√	
	Lead instructions in data processing and analysis skills		√	
	Lead instructions in applying software in data solving and analysis skill		√	
	Lead instructions in applying technology to represent data from practicum results skill		√	

The skills trained in the use of Basic Chemistry practicum module reached 44.4% of the overall target of the process skills review that should have been. These skills are: lead instructions in understanding the basic theory ability of practical implementation, instructions in assembling practical equipment skill, and lead instructions in direct the skills to operate practical equipment. However, the basic theory in the Basic Chemistry practicum module has been presented, students are only directed to read the theory presented and are not directed to find their own theoretical concepts. Likewise, with assembling and operating practicum equipment, the Basic Chemistry practicum module provides a schematic for assembling and operating practicum tools. In this case, students are not directed to think the right equipment for doing practicum. As for the skills aspect of doing practicum, the module presents practical steps in detail so that students can easily have the ability in doing practicum. However, this instruction does not provide an opportunity for students to develop their own way in practical activities.

Based on the review results of the Basic Chemistry module into the three component aspects, the practicum worksheet, computation elements, and skill that are trained, it can be seen that the Basic Chemistry practicum in the Chemistry Education Study Program of UNSAM still uses conventional modules. Here, the students only work according to activity orders, both planning practicum, assembling and operating

equipment, and doing practicum. The module is not enough to provide opportunities for students to develop good process skills. In other hand, a good practicum module is expected to improve students' science process skills well. Science process skills (SPS) can be categorized into basic PPPs which include observing, classifying, measuring, calculating, using space and time relationships, predicting, inferring, and communicating; and integrated PPP which includes defining and controlling variables, formulating and testing hypotheses, operational definitions, designing experiments and interpreting data (Curriculum Development Centre, 1993; Turiman et al, 2012; Hikmah et al, 2018). Likewise, the computational elements contained in Basic Chemistry practicum are still very low. So, it is necessary to add computational elements in the implementation of the practicum so that the Basic Chemistry practicum advantages of applying computational science itself.

Needs Analysis

Table 4 is the result of students' responses to the Basic Chemistry practicum activities in the Chemistry Education. Respondents are 54 students of 87 active students who passed Basic Chemistry course. The assessment statement was developed from several aspects which include the benefits of practicum activities, practicum equipment, computing utilization, and practicum activities.

Table 4. Students' Response for Benefits of Practicum Activities

Statements	Approval Rate				
	SS	S	KS	TS	STS
1 Practical activities can improve my understanding and mastery of Basic Chemistry concepts	81.48 %	18.52%	0%	0%	0%
2 Laboratory activities can practice skills in applying the scientific method	74.7%	25.93%	0%	0%	0%
3 Practical activities help me to understand concepts at the microscopic level	55%	40.7%	3.7%	0%	0%

Based on Table 4, it can be seen that in terms of the benefits of practicum activities : almost everyone

strongly agrees (81.48%) and a few agree (18.52%), that the implementation of Basic Chemistry practicum can

improve understanding and mastery of Basic Chemistry concepts ; most strongly agree (74.7%) and almost half agree (25.93%), that laboratory activities can practice skills in applying the scientific method ; most of students strongly agree (55%), almost half agree (40.7%), and a

few undecided (3.7%), that practicum activities can help in understanding concepts at the microscopic level. That is, in term of practical activities benefit, the Basic Chemistry practicum has provided good benefits based on the three statements above.

Table 5. Students' response for Practical Equipments

Statements	Approval Rate				
	SS	S	KS	TS	STS
4 Equipments in Basic Chemistry practicum available in the laboratory and function properly	20.4%	57.41%	16.67%	0%	1.85%
5 Available practicum tools can be used to explore abstract concepts	27%	53%	18.52%	0%	0%

For practicum equipment (Table 5): a few strongly agree (20.4%), most students agree (57.41%), a few undecided (16.67%), a few strongly disagree (1.85%), that the Basic Chemistry practicum equipment available in the laboratory and can be functioned properly; a few strongly agree (27%), most agree (53%), a few undecided (18.52%), and no one disagree, that available practicum tools can be used to explore abstract concepts. This means that the availability of Basic Chemistry practicum equipment is quite good based on these two statements.

disagree (1.85%), that practical activities in the laboratory are carried out virtually using software for abstract and microscopic concepts ; almost half students strongly agree (35%), most of students agree (55.56%) and a few students undecided (7.41%), no one disagree, and a few strongly disagree (1.85%), that carried out practicum activities require me to use computational calculations to organize data and analyze data. In these two aspects, no one strongly agree for the two statements. This means that the students have not felt the use of computing in Basic Chemistry practicum activities sufficiently.

For computing utilization aspect (Table 6): almost half of students strongly agree (31.48%) most of students agree (57.41%), a few undecided 9,26%, and a few

Table 6. Students' Response for Computing Utilizing

Statements	Approval Rate				
	SS	S	KS	TS	STS
6 Practical activities in the laboratory are carried out virtually using software for abstract and microscopic concepts	31.48%	57.41%	9.26%	1.85%	0%
7 Carried out practicum activities require me to use computational calculations to organize data, and analyze data	35%	55.56%	7.41%	0%	1.85%

For computing utilization aspect: almost half of students strongly agree (31.48%) most of students agree (57.41%), a few undecided 9,26%, and a few disagree (1.85%), that practical activities in the laboratory are carried out virtually using software for abstract and microscopic concepts ; almost half students strongly agree (35%), most of students agree (55.56%) and a few

students undecided (7.41%), no one disagree, and a few strongly disagree (1.85%), that carried out practicum activities require me to use computational calculations to organize data and analyze data. In these two aspects, no one strongly agree for the two statements. This means that the students have not felt the use of computing in Basic Chemistry practicum activities sufficiently.

Table 8. Students' for Practical Activities

Statements	Approval Rate				
	SS	S	KS	TS	STS
8 Practical activities are carried out to verify the truth of concepts/theories previously presented in class	68%	31.48%	0%	0%	0%
9 Carried out Basic Chemistry Practicum trains real problem-solving strategies in everyday life	64.81%	33.33%	1.85%	0%	0%
10 Practical activities begin with providing contextual problems related to daily life and solutions are investigated through practical activities	55.56%	42.59%	1.85%	0%	0%
11 Practicum activities begin by formulating hypotheses, then testing them using their own practicum procedures prepared by students	51.8%	33.33%	9.26%	3.70%	1.85%
12 Practical activities use the steps that have been determined in detail in the practical guide book	64.81%	35.19%	0%	0%	0%
13 Practical activities take a long time	29.63%	50%	18.52%	0%	1.85%

For practical activities aspect : most of students strongly agree (68.00%), almost half agree (31.48%), and no one give response do not agree, that practical activities are carried out to verify the truth of concepts/theories previously presented in class ; most of students strongly agree (64.81%), almost half agree (33.33%), a few disagree (1.85%), and no one who disagree, that carried out Basic Chemistry Practicum trains real problem solving strategies in everyday life ; most of students strongly agree (55.56%), almost half agree (42.59%), a few undecided (1.85%), and no one who disagree, that practical activities begin with providing contextual problems related to daily life and solutions are investigated through practical activities ; most of students strongly agree (51.8%), almost half agree (33.33%), a few undecided (9.26%), a few disagree (3.70%), and a few strongly disagree (1.85%), that practicum activities begin by formulating hypotheses, then testing them using their own practicum procedures prepared by students ; most of students strongly agree (64.81%), almost half agree (35.19%), and no one who disagree, that practical activities use the steps that have been determined in detail in the practical guide book ; almost half students (29.63%), half (50.00%), a few undecided (18.52%), no one disagree, and a few strongly disagree (1.85%). This result confirms the previous analysis of module, where the students are nor free to use their own practicum procedures and only work according to the instructions in the practicum guide/module. Beside that the practicum that used to do take a long time.

Literature Analysis

This part, discuss how far implementation of computing had been used in practicum or Chemistry learning. Computational chemistry has advantages in visualizing quantum mechanical scales or describing the shape of molecules, and can create animations of particle motion based on their vibrational motion and visualize molecular shapes in three-dimensional structures (Hasibuan et al., 2020).

Siregar and Harahap (2020) have conducted research on the development of an E-Module based on project-based learning integrated hypercam computing media in molecular form. The result shows that computing media integrated modules can improve learning outcomes. Hasibuan et al (2020) also found that there were differences in learning outcomes between computational method-based learning using NWChem software and using ChemsSketch software. NWChem software is a computational chemistry software that can be used to calculate molecular quantities and the periodic system using quantum mechanical functions or wave density. In addition, NWChem can also be used to predict the structure, reactivity and reaction mechanisms and can determine your transition state, the

activation energy of organic reactions (Valiev et al, 2010; Hasibuan et al., 2020). While ChemsSketch is used to draw the shape of the molecular structure of hydrocarbons, and chemical bonds in 2D and 3D, and can visualize the movement of atoms in the molecule (Marpaung et al., 2020). Another popular software that can be used for Chemistry computation are Gamess-US, Gaussian, Molcas, Molpro, MPQC, Open Mopac, Orca dan QChem, Hyperchem, Chemlab, WebMo. Software-software tersebut ada yang berbasis web dan ada yang tidak (Allouche, 2010; Hadisaputra et al, 2017). Thus, computing media can also improve creative thinking skills (Hulyadi & Khotimah, 2016), increase motivation in doing chemistry practicum (Hadisaputra et al, 2017), and improve spatial ability and predict stability of organic molecules (Setyarini, 2017).

Purwiandono (2017) in his research found that the use of computational based visualization methods in the Physical Chemistry practicum provides a positive value in the Physical Chemistry learning process. However, there are problems related to the ability of students to input data into computing software, so the software cannot display the evaluation model such as in practicum for viscosity and activation energy and kinetic of phenolphthalein solubility in alkaline solution. To apply the computing capabilities, it is necessary to pay attention in general problems faced by students in computing. Anggraini et al (2019) explained that the problem was caused by a lack of ability to decipher complex problems into simple ones, analyze the general differences and similarities of a problem so that students were unable to generalize problem solving patterns.

Conclusion

Basic Chemistry practicum implemented in Chemistry Education is a verification practicum (conventional), and it is necessary to implement a practicum that gives more freedom to students in exploring. Basic chemistry practicum in Chemistry Education is also not based on computational, so it is necessary to develop basic chemistry practicum activities that provide computational problem solving

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