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The Effectiveness of Computer Program-Aided Assignments to Solve Differential Equations in Chemical Engineering Course

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ABSTRACT
Chemical Engineering is a field of applied science that aims to develop technology that can be implemented in the chemical industry. Several courses in this field use a mathematical approach to determine the condition of a process requiring high accuracy. Mathematical modeling for solving problems in the field of chemical engineering is generally in the form of differential equations that can be solved analytically or numerically. Analytical methods are usually used for problems with limited and simple models, while numerical methods are more suitable for complex problems in the chemical process. Numerical method solutions are easier to obtain with the help of computer programs, including Solver in Excel, Polymath, or Matlab. The use of the computer program provides a relatively fast solution with high accuracy. This study was conducted to evaluate the use of computer programs by students in Chemical Reaction Engineering (CRE) courses. The assessment was carried out based on the exam results. The considered parameters include the duration of the exam, accuracy of answers, as well as understanding of concepts or algorithms of problem-solving.

Keywords: *Chemical Engineering, Differential Equation, Solver, Polymath*

1. INTRODUCTION

The curriculum designed by the Chemical Engineering study program is intended to educate students with chemical engineering expertise. This is in accordance with the requirements specified by ABET accreditation [1], i.e. engineering graduates can work in multi-disciplinary teams and apply mathematics and science for solving engineering problems [2]. One of the skills needed by chemical engineering graduates is the ability to analyze, process, evaluate, and solve problems related to chemical processes. The chemical process can operate by controlling several variables expressed in complex process conditions. A mathematical model approach is needed to describe the relationship between these complex variables. Teaching mathematical modeling requires practice to solve problems based on real case studies [3], [4]. To achieve an understanding of complex modeling, appropriate teaching methods are needed that can align the perspectives of teachers and students, then direct them according to the right solution to the problems being studied [5], [6].

Mathematical modeling has been introduced to several courses taught to the Chemical Engineering Study Program undergraduate students, including the Chemical Reaction Engineering (CRE) course. This course implements the use of mathematical models to solve various problems in the field of chemical engineering. To find out the relationship between several variables related to chemical processes, a mathematical model approach is required which is generally in the form of a dynamic model. The mathematical model is in the form of a differential equation that can be solved by analytical or numerical methods. Solving numerical differential equations tends to be preferred because it can be implemented in relatively more complex mathematical models. These numerical methods can be solved more easily and quickly using computer programs, such as Solver in Excel, Polymath, or Matlab with high accuracy.

The ability to use computer programs to solve differential equations from a mathematical model of chemical processes is an important skill for graduates of chemical engineering. Therefore, efforts are needed to increase student proficiency in using various computer programs in the learning process. Applying the use of computer programs to solve mathematic problems in the learning process can increase student understanding and identify gaps in understanding of the concepts being taught [7]. Furthermore, it can show the student's perspectives in solving problems and encourage the development of traditional teaching methods towards computer program-based teaching for solving differential equations. This becomes the basis for further development so as to encourage the effectiveness of learning. Previous studies, including those reported by Kwon et. al. [8], Tabach et. al. [9], and Rasmussen et. al. [10], [11], were built based on the linearity of inquiry that seek to link the learning outcomes with the instructional paradigm in differential equations and to identify and overcome student difficulties in learning subjects.

In this study, an assessment was made of the use of computer programs in conducting the exams for Chemical Engineering Study Program students. The aim of the study is to determine the effectiveness of learning, i.e., the student's understanding of the concept of solving differential equations using a conventional analytic technique approach compared to numerical solutions assisted by computer programs. The research was conducted based on class observations and student learning outcomes.

2. METHODS

The research aimed to observe the differences in learning instructions conventionally and with the help of computer programs applied to learning processes. The research was conducted following a quantitative design, i.e., a prospective, causal-comparative, quasi-experimental study with the class as the independent variable [7]. The performance of the two groups of students was measured based on the results of the exams. The creation and scoring of questions are described in detail below. Data were generated through the observation of 16 sessions in each classroom and the detailed examination of students' written responses to the final exam tasks.

2.1. Participants and Classroom Observations

Participants were 100 undergraduate students enrolled in the Chemical Reaction Engineering courses in the even semester 2021/2022 and 20 students in the even semester 2022/2023 from the Chemical Engineering Study Program at Semarang State University. Each class meets 18 times during one semester, with a time of 3 x 50 minutes for each session.

2.2. Assessment of student learning outcomes

Four problems were created and embedded in the final exam, representing applied, procedural, and conceptual components of ordinary differential content. All the problems were designed to target the connections between a differential equation and its solution. Students were permitted graphing calculators and computers.

An example of the topics taught in Chemical Reaction Engineering courses is the mathematical model approach used to solve problems in chemical reactors. The physicochemical processes that occur can be presented as ordinary differential equations (1). Two examples of problems applying differential equations that can be solved by numerical methods are as follows:

First question

A chemical reaction is described by schematic as follow:

$$A \overset{k_1}{\to} B \overset{k_2}{\to} C \qquad (1)$$

The reactions take place consecutively in a 500-dm^3 batch reactor. It is assumed that the reaction takes place in the liquid phase with negligible volume changes. The combination of mass balance and rate law for each component can be written as follow:

$$\frac{dC_A}{dt} = -k_1 C_A \qquad (2)$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad (3)$$

$$\frac{dC_C}{dt} = k_2 C_B \qquad (4)$$

Where C_A, C_B, dan C_C are the concentrations of the three chemical components of the reaction. These equations are a set of linear first-order ordinary differential equations, which describe the dynamic behavior of a chemical reaction. The initial concentration of A is 1.6 mol/dm^3. Plot and analyze the concentration of A, B, and C as a function of time. Assume that each reaction is irreversible with $k_1 = 0.4h^{-1}$ and $k_2 = 0.1h^{-1}$.

Second question

The reaction of $A \to B + C$ was carried out in a constant-volume batch reactor where the following concentration measurements were recorded as a function of time.

t (min)	0	5	10	15	20	25	30	35
C_A (mol/dm^3)	2	1.6	1.35	1.1	0.87	0.70	0.53	0.35

Use nonlinear least squares (i.e., regression) and numerical differentiation formula to determine the reaction order (α) and the specific reaction rate constant (k). Compare the result!

Solution of the questions above can be solved numerically both by hand and using computer programs, such as Polymath, Matlab, or Solver in Excel. The assessment of student performance was conducted using qualitative and quantitative methods.

3. DISCUSSIONS

3.1. Calculation using Numerical Methods

First question

The first problem can be solved numerically using the Euler method [12] to determine the concentration variation of A (C_A) over time (t) in the reactor, by selecting the time step $h = 0.5$. In this problem, the independent variable is time (t) and the dependent variable is the concentration of component i (C_i), with i is A, B, and C. Thus, with $t \equiv x$ and $C_i = y$ the equation can be written as follows:

$$\frac{dC_i}{dt} = f(t, C_i) = r_j \qquad (5)$$

Where r_j is the reaction rate for each reaction in equations 2-4. With initial conditions $C_A(0) = 1.6\ mol/dm^3$, the detailed solutions from the first and second steps were done manually by hand and then continued using Excel until step $t = 50$.

The first problem can be solved using the Euler method according to the following equation:

$$y_{i+1} = y_i + hf(x_i, y_i) \qquad (6)$$

The initial values are $i = 0, t_0 = 0, C_{A,0} = 1.6$

For the next step time ($i = 1, t_1 = t_0 + h = 0.5$), concentration is calculated as follows:

$$C_{A,1} = C_{A,0} + h(-k_1 C_{A,0})$$

$$= 1.6 + 0.5(-0.4 \times 1.6) = 1.280$$

For the 2nd time step ($i = 2, t_2 = t_1 + h = 1$), so that:

$$C_{A,2} = C_{A,1} + h(-k_1 C_{A,1})$$

$$= 1.280 + 0.5(-0.4 \times 1.280) = 1.024$$

The calculation for the concentration of component B (C_B) follows the steps:

The initial values are $i = 0, t_0 = 0, C_{A,0} = 1.6, and\ C_{B,0} = 0$

For the next step time ($i = 1, t_1 = t_0 + h = 0.5$), concentration is calculated as follows:

$$C_{B,1} = C_{B,0} + h(k_1 C_{A,0} - k_2 C_{B,0})$$

$$= 0 + 0.5(0.4 \times 1.6 - 0.1 \times 0) = 0.320$$

For the 2nd time step ($i = 2, t_2 = t_1 + h = 1$), so that:

$$C_{B,2} = C_{B,1} + h(k_1 C_{A,1} - k_2 C_{B,1})$$

$$= 0.320 + 0.5(0.4 \times 1.280 - 0.1 \times 0.320) = 0.560$$

The calculation for the concentration of component C (C_C) follows the steps:

The initial values are $i = 0, t_0 = 0, C_{A,0} = 1.6, C_{B,0} = 0, and\ C_{C,0} = 0$

For the next step time ($i = 1, t_1 = t_0 + h = 0.5$) concentration is calculated as follows:

$$C_{C,1} = C_{C,0} + h(k_2 C_{B,1})$$

$$= 0 + 0.5(0.1 \times 0.320) = 0.016$$

For the 2nd time step ($i = 2, t_2 = t_1 + h = 1$), so that:

$$C_{C,2} = C_{C,1} + h(k_2 C_{B,2}) = +0.5(0.1 \times 0.560) = 0.044$$

Calculations for the next steps can be done in the same manner using Excel as presented in Table 1.

Table 1 Calculation of concentration profile using Euler method

Euler Method				
i	t	C_A	C_B	C_C
0	0	1.60	0.00	0.00
1	0.5	1.28	0.32	0.02
2	1	1.02	0.56	0.04
3	1.5	0.82	0.74	0.08
4	2	0.66	0.86	0.12
5	2.5	0.52	0.95	0.17
6	3	0.42	1.01	0.22
7	3.5	0.34	1.04	0.27
8	4	0.27	1.06	0.33
9	4.5	0.21	1.06	0.38
10	5	0.17	1.05	0.43
11	5.5	0.14	1.03	0.48
12	6	0.11	1.01	0.53
13	6.5	0.09	0.98	0.58
14	7	0.07	0.95	0.63
15	7.5	0.06	0.91	0.68
16	8	0.05	0.88	0.72
17	8.5	0.04	0.84	0.76
18	9	0.03	0.81	0.80
19	9.5	0.02	0.77	0.84
20	10	0.02	0.74	0.88
21	10.5	0.01	0.71	0.91
22	11	0.01	0.67	0.95
23	11.5	0.01	0.64	0.98
24	12	0.01	0.61	1.01
25	12.5	0.01	0.58	1.04
26	13	0.00	0.56	1.07
27	13.5	0.00	0.53	1.09
28	14	0.00	0.50	1.12
29	14.5	0.00	0.48	1.14
30	15	0.00	0.46	1.17
31	15.5	0.00	0.43	1.19
32	16	0.00	0.41	1.21
33	16.5	0.00	0.39	1.23
34	17	0.00	0.37	1.25
35	17.5	0.00	0.35	1.26
36	18	0.00	0.34	1.28
37	18.5	0.00	0.32	1.30
38	19	0.00	0.30	1.31
39	19.5	0.00	0.29	1.33

This problem can also be solved numerically by using the ODE Solver in Polymath following the equations:

Polymath Equation
k2=0.1
k1=0.4
Cc(0)=0
Cb(0)=0
Ca(0)=1,6
*d(Cc)/d(t) = k2*Cb*
*d(Cb)/d(t) = k1*Ca-k2*Cb*
*d(Ca)/d(t) = -k1*Ca*
t(0)=0 ; t(f)=50

The calculation results with the ODE Solver are shown in Table 2 and the resulting graph is presented in Figure 1. The results obtained using both methods are relatively the same.

Table 2 Calculation of concentration profile using ODE Solver in Polymath

Polymath			
t	C_A	C_B	C_C
0	1.60	0.00	0.00
1.4	0.91	0.64	0.05
1.8	0.78	0.74	0.08
2.2	0.66	0.83	0.11
2.6	0.57	0.89	0.14
3.4	0.41	0.97	0.22
3.8	0.35	0.99	0.26
4.2	0.30	1.00	0.30
4.6	0.25	1.01	0.34
5.4	0.18	1.00	0.42
5.8	0.16	0.98	0.46
6.2	0.13	0.97	0.50
6.6	0.11	0.95	0.54
7	0.10	0.93	0.57
7.8	0.07	0.88	0.65
8.2	0.06	0.86	0.68
8.6	0.05	0.83	0.71
9	0.04	0.81	0.75
9.8	0.03	0.76	0.81
10.2	0.03	0.73	0.84
10.6	0.02	0.71	0.87
11	0.02	0.68	0.90
11.8	0.01	0.64	0.95
12.2	0.01	0.61	0.97
12.6	0.01	0.59	1.00
13	0.01	0.57	1.02
13.8	0.01	0.53	1.07
14.2	0.01	0.51	1.09
14.6	0.00	0.49	1.11
15	0.00	0.47	1.13
15.8	0.00	0.44	1.16
16.2	0.00	0.42	1.18
16.6	0.00	0.40	1.20
17	0.00	0.39	1.21
17.8	0.00	0.36	1.24
18.2	0.00	0.34	1.25
18.6	0.00	0.33	1.27
19.4	0.00	0.31	1.29
19.8	0.00	0.29	1.31
20.2	0.00	0.28	1.32
20.6	0.00	0.27	1.33

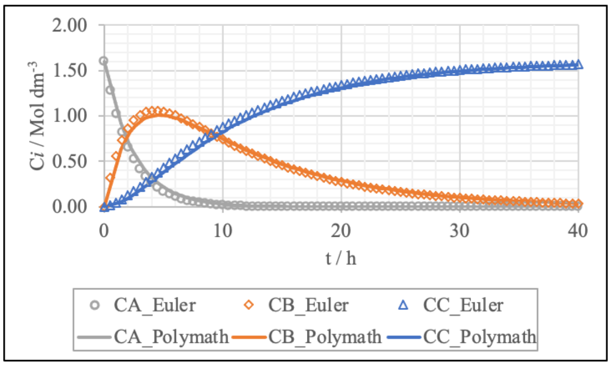

Figure 1 Concentration profile of components A, B, and C calculated using the Euler method and ODE solver Polymath

Second question

The second question can be solved using numerical differentiation formulas or using nonlinear regression [13]. The non-linear regression method is done by minimizing the sum squares of the differences between the measured values and the calculated values for all the data points. The steps for solving the 2nd problem are explained.

It is assumed that the reaction takes place in a constant volume batch reactor so that the combined rate law and mole balance can be written as follows:

$$\frac{dC_A}{dt} = -kC_A^{\alpha} \qquad (7)$$

Integration of Eq. 7 for $\alpha \neq 1$ results

$$C_{A0}^{1-\alpha} - C_A^{1-\alpha} = (1-\alpha)kt \qquad (8)$$

Rearrange Eq. 8 to obtain the concentration as a function of time.

$$C_A = [C_{A0}^{1-\alpha} - (1-\alpha)kt]^{1/(1-\alpha)} \qquad (9)$$

Then, calculations are performed using Solver to determine α and k which will minimize s^2 from the following equation:

$$s^2 = \sum_{i=1}^{N} (C_{Aim} - C_{Aic})^2$$

$$= \sum_{i=1}^{N} \left[C_{Aim} - [C_{A0}^{1-\alpha} - (1-\alpha)kt_i]^{1/1-\alpha}\right]^2 \quad (10)$$

Iterative calculation using Solver in Excel obtained α dan k values of 0.7 and 4.57 x 10^{-2}, respectively, with a sum of squared error of 5.07 x 10^{-3}.

3.2. Quantitative Analysis of Student Performance

Student performance is measured quantitatively according to the values obtained from participatory activity scores, project results scores, assignment scores, quiz scores, midterm exams, and final semester exams. The weight of scores applied to each criterion are 25%, 25%, 10%, 10%, 15%, and 15%. In this study, the assessment evaluation was carried out based on the midterm exams of CRE course in the even semester 2022/2023. The assessment of learning outcomes is in accordance with the guidelines in Table 3.

Table 3 Guidelines for assessing student learning outcomes of the UNNES Chemical Engineering study program

Score	Letter	Weight	Predicate
86-100	A	4	Very well
81-85	AB	3.5	More than good
71-80	B	3	Good
66-70	BC	2.5	More than enough
61-65	C	2	Enough
56-60	CD	1.5	Less than enough
51-55	D	1	Not enough
≤ 50	E	0	Failed (did not pass)

As a benchmark, the assessment is based on student scores for the CRE course in the even semester 2021/2022. The learning process and the exams were conducted conventionally using manual calculation without using a computer program. The results of the midterm exams of the CRE course are shown in Figure 2.

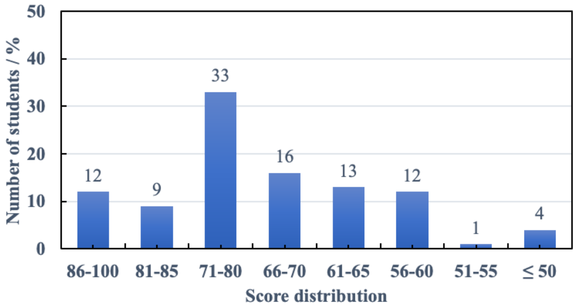

Figure 2 Midterm exam scores of CRE course in the even semester 2021/2022

Out of a total of 100 students (in 3 groups of classes) who took CRE course, 54% of students scored more than 71 with A, AB, and B predicates. This shows that more than 50% of students taking CRE courses were able to understand the material taught and can solve the questions given.

In order to evaluate the effectiveness of using computer programs to solve questions in the CRE course, observations were made on students participating in the course which was held in the even semester of 2022/2023. Evaluation of the implementation of lectures in the CRE course is based on the midterm exam results. The results of student scores are presented in following Figure 3.

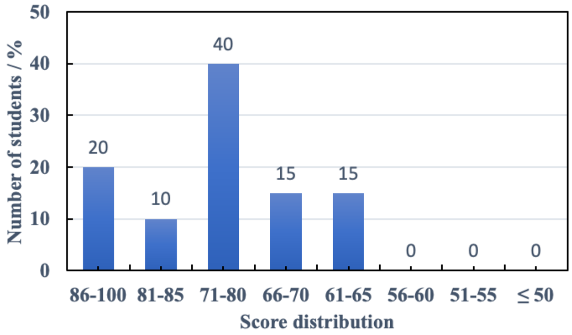

Figure 3 Midterm exam scores of CRE course in the even semester 2022/2023

Based on the results of the exams conducted, 100% of students used computer programs to complete calculations of the questions given. Compared to the previous trend in the 2021/2023 even semester, there was an increase in student scores in the 2022/2023 even semester of the CRE course. As many as 70% of students who took the CRE exam scored more than 71. This shows that the method applied is effective in supporting the learning process, especially for the CRE course where there are many problems that must be solved numerically with the help of computer programs.

3.3. Qualitative Analysis of Student Performance

Qualitative assessment is carried out based on the results of student answers. The following is an example of student answer sheets for solving the questions given. Midterm exam question sheets (Figure 4) and the results (Figures 5 and 6) are presented as examples.

From the student answer sheet (Figures 5 and 6), it can be seen the level of understanding based on the score obtained for each question. The order of questions number 1-4 has a level of difficulty from low to high. The average student scores for each question number (from 1-4) are 21.25, 22, 20.8, and 13.5.

Midterm Exam
Chemical Reaction Engineering
28^{th} of March 2023
Time: 13.00-15.30 (Western Indonesian Time)

1. **Topic: Rate Law (score: 25)**
Write the rate law for the following reactions assuming each reaction follows an elementary rate law. Give the unit of k_A for each,
    a) $C_2H_6 \rightarrow C_2H_4 + H_2$
    b) $(CH_3CO)_2O + H_2O \leftrightarrow 2CH_3COOH$

2. **Topic: Activation Energy (score: 25)**
The initial reaction rate for the elementary reaction
$$2A + B \rightarrow 4C$$
Was measured as a function of temperature when the concentration of A was 2 M and that of B was 1.5 M.

$-r_A(mol/dm^3 \cdot s)$	0.002	0.046	0.72	8.33
$T(K)$	300	320	340	360

    a) What is the activation energy?
    b) What is the frequency factor?
    c) What is the rate constant as a function of temperature using the following equation and $T_0 = 27°C$ as the base case?
$$k(T) = k(T_0)exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

3. **Topic: Analysis of rate data (score: 25)**
The reaction
$$A \rightarrow B + C$$
was carried out in a constant-volume batch reactor where the following concentration measurements were recorded as a function of time.

t (min)	0	5	9	15	22	30	40	60
C_A (mol/dm^3)	2	1.6	1.35	1.1	0.87	0.70	0.53	0.35

Use nonlinear least squares (i.e., regression) and one other method to determine the reaction order α and the specific reaction rate constant, k

4. **Topic: Reaction in series (score: 25)**
The elementary liquid-phase series reaction
$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$$
is carried out in a 500-dm^3 batch reactor. The initial concentration of A is 1.6 mol/dm^3. The desired product is B, and separation of the undesired product C is very difficult and costly. Because the reaction is carried out at a relatively high temperature, the reaction is easily quenched.
    a) Plot and analyze the concentrations of A, B, and C as a function of time. Assume that each reaction is irreversible, with $k_1 = 0.4h^{-1}$ and $k_2 = 0.01h^{-1}$
    b) Plot and analyze the concentration of A, B, and C as a function of time when the first reaction is reversible, with $k_{-1} = 0.3h^{-1}$

Figure 4 Exam question sheet

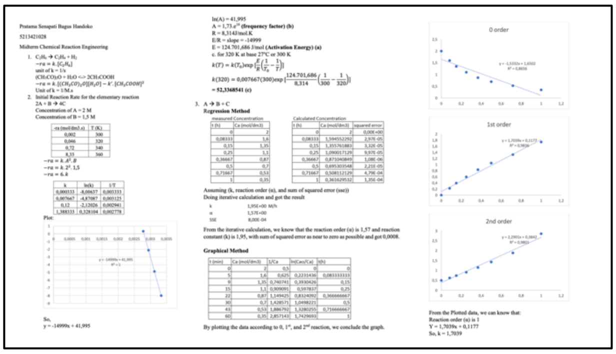

Figure 5 Answer sheet of student 1 for the solution of questions number 1-3

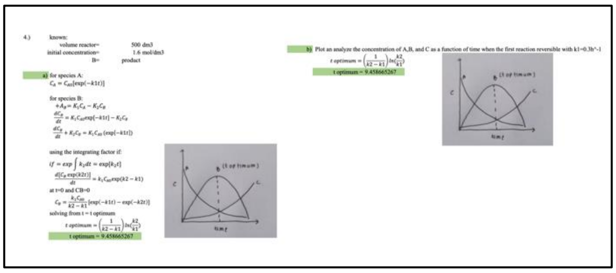

Figure 6 Answer sheet of student 2 for the solution to question number 4

Problem number 2 can be done using the linear regression method and question number 3 can be done using non-linear regression with Solver in Excel. More than 90% of students cannot solve question number 4 correctly, because the level of difficulty is high. From the answer sheet, it can be seen that students are trying to solve question number 4 with the analytic method using integrating factors. These problems can be solved more easily and quickly numerically with the ODE solver on Polymath. However, none of the students used the ODE solver in Polymath to solve problem number 4.

From the results of the evaluation carried out, it can be seen that the level of student ability in using computer programs is quite good, although it is limited to using Solver in Excel. Students also quite understand the flow chart or problem-solving algorithm given. In addition, students are also able to complete the exam within 150 minutes. This shows that the use of the computer is effective in assisting with calculations of the questions given.

These results are consistent with the explanation presented by Litzinger et. al. [6] which describes several examples of practical instructions that can create effective learning experiences, which are classified based on the abilities achieved which include affective, meta-cognitive, and cognitive abilities. Based on the affective aspect, instructional practices that can be carried out include varied learning that can increase the interest of students who have different abilities and goals. Based on the metacognitive aspect, instructional practice is carried out by providing constructive feedback so students can understand what they know and can do it well. From the cognitive aspect, instructional practice is carried out by paying attention to students' initial knowledge by selecting learning assignments according to the level of difficulty, supporting appropriate content through the design and assignments that require interaction between students, and using assessments that can be used to determine students' thinking processes so that the level of understanding can be assessed. Based on these aspects, giving the assignment and exam with the assistance of a computer program is a part of the learning method that can increase student creativity and increase their interest in understanding the problems given. In addition, the assignments given also provide opportunities for students to interact and have discussions for solving the problems. This is an appropriate instructional practice to support metacognitive aspects. Meanwhile, the assessments carried out were also prepared based on assessments with different levels of difficulty, so that they could be used to determine students' thinking processes and levels of understanding.

The learning process applied was problem-based learning, where students learn to solve a problem related to mathematical modeling in chemical reaction processes [14]. Practice questions that are given regularly can improve students' abilities in analyzing, managing time, and increase students' understanding of more diverse problems. This can also be seen from the qualitative analysis of the exam results, where students who are more active in doing problem excercises regularly find it easier to understand step-by-step solving problems and are able to manage the duration of time to answer the questions more efficiently. The assessment results obtained in this study are in accordance with those stated by Mousoulides et. al. [15] that the student's abilities in modeling increase through a series of problem-solving activities, as well as several influential factors such as student grades, experience with modeling activities, and modeling abilities that influence their modeling process. The availability of tools that can be used effectively for modeling activities is also influential in developing students' abilities to understand modeling concepts and solve problems related to these modeling activities.

4. CONCLUSIONS

This study aims to determine the effectiveness of the exam assisted by a computer program. The results of quantitative assessments show that 70% of students score more than 71, which indicates a fairly good level of understanding of the questions. This percentage has increased compared to the evaluation results based on midterm exam scores in the previous semester, which shows the effectiveness of the learning being carried out. In addition, from observations based on student answer sheets in working on midterm exam questions, it can be seen qualitatively that students were able to work on questions number 1-3 with a moderate level of difficulty, but experienced difficulty when solving question number 4 with a high level of difficulty. From the results of observations, it is also known that the level of ability of students is quite good in using computer programs, although it is still limited to using solvers in Excel. From the student exam answers it shows that there is still limited understanding in solving ODE numerically. In addition, it can be seen that the level of student's ability to use computer programs other than Solver in Excel, such as Polymath is still low. The results of this study also show that a series of exercise activities that are given routinely based on problem-based learning can increase students' understanding of modeling concepts and improve students' ability to manage problem-solving given more efficiently.

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