JPPIPA 12(7) (2026)

Jurnal Penelitian Pendidikan IPA

http://jppipa.unram.ac.id/index.php/jppipa/index

Developing a Teaching Strategy for Mathematical Chemistry Using Maple-Assisted Experimental Data Modelling to Enhance Scientific Reasoning

Deklin Frantius[1*], Liliasari[1]

[1] Department of Natural Science Education, Faculty of Mathematics and Science Education, Universitas Pendidikan Indonesia, Bandung, Indonesia.

Received: May 02, 2026
Revised: June 30, 2026
Accepted: July 25, 2026
Published: July 31, 2026

Corresponding Author:
Deklin Frantius
deklinfrantius@upi.edu

DOI: 10.29303/jppipa.v12i7.15508

Abstract: This study developed a teaching strategy to strengthen scientific reasoning. The study proceeded through preliminary investigation, prototype design, iterative try-outs, and implementation. The preliminary study showed that differential and integral topics in classroom practice remained largely procedural and did not explicitly integrate modelling empirical data. In response, a strategy was designed to connect chemical phenomena, mathematical, and Maple-assisted. Participants were undergraduate students from two universities. Try-out I involved 17 Chemistry students and Try-out II involved 10 Chemistry Education students at university in Palangka Raya, Central Kalimantan, whereas the final implementation involved 30 undergraduate students at university in Bandung, West Java. Comprehension scores increased from 33.22 to 64.88 in Try-out I and from 33.82 to 70.59 in Try-out II. In the final implementation, mean scientific reasoning scores increased from 34.40 to 72.27 for the mathematical aspect and from 31.85 to 70.65 for the chemistry aspect. Gains in scientific reasoning were very strongly correlated with gains in differential–integral understanding ($r = 0.969$, $p < 0.001$). These findings indicate that the developed strategy supports scientific reasoning by linking chemical phenomena, mathematical modelling, and Maple. The strategy should be examined in larger samples and other chemistry topics.

Keywords: Maple; Mathematical Chemistry; Modelling; Teaching Strategy.

Introduction

Mathematical chemistry plays an essential role in undergraduate chemistry education because it provides the quantitative language needed to represent, analyse, and interpret chemical phenomena (Bain et al., 2019; Habiddin & Nagol, 2023; Merino et al., 2022). Differential and integral concepts are particularly important for describing rates of change, accumulation, kinetic processes, and other time-dependent chemical behaviours (Bain et al., 2018; Towns et al., 2025). Consequently, learning mathematical chemistry should extend beyond the manipulation of mathematical expressions. Students need to understand how equations represent chemical systems, how mathematical results relate to empirical evidence, and how those results can be interpreted within a scientifically meaningful context.

Mathematics may be easier to understand when instruction begins with mathematical modelling because students first engage with phenomena or data, identify patterns, determine relevant variables, and formulate the relationships they observe into mathematical representations (Alsina & Salgado, 2022; Hasibuan et al., 2024; Mukhlis et al., 2024; Paristiowati et al., 2022; Turner et al., 2022). Spanier (1980) conceptualized modelling as a process of translating real-world problems into mathematical forms, solving the resulting models, interpreting the results, and evaluating their consistency with the original phenomena. This view is reinforced by Frejd & Bergsten (2018), who identify description,

How to Cite:
Frantius, D., & Liliasari, L. (2026). Developing a Teaching Strategy for Mathematical Chemistry Using Maple-Assisted Experimental Data Modelling to Enhance Scientific Reasoning. *Jurnal Penelitian Pendidikan IPA*, *12*(7), 772–783. https://doi.org/10.29303/jppipa.v12i7.15508

understanding, abstraction, and negotiation as essential components of mathematical modelling. Accordingly, formulas are not introduced merely as finished symbols or procedures. They are constructed as formal expressions of patterns and relationships embedded in data. These enable students to understand the origins, functions, and meanings of the mathematical concepts involved (Alsina & Salgado, 2022; Evendi, 2022; Roslina et al., 2023; Turner et al., 2022).

Mathematical modelling also bridges reality and abstraction by requiring students to simplify situations, construct mathematical representations, and interpret the results within the original context (Cevikbas et al., 2022; Jablonski, 2023; Selvia et al., 2025). Therefore, beginning mathematics instruction with modelling can make mathematical concepts more meaningful and comprehensible while simultaneously fostering problem-solving, creativity, and the ability to use multiple mathematical representations in real-world situations (Lu & Kaiser, 2022; Mukhlis et al., 2024).

However, the integration of mathematics and chemistry presents persistent learning challenges. Chemistry students may be able to perform routine calculations but still experience difficulty applying mathematical concepts to chemical problems, interpreting graphs, coordinating multiple representations, and explaining the scientific meaning of mathematical results (Bain et al., 2019; Bunawan et al., 2023; Towns et al., 2025). Previous research conducted in a comparable instructional context also reported that students had difficulty understanding the relevance of differential and integral concepts to chemistry and using these concepts to interpret chemical phenomena (Frantius et al., 2025). Such difficulties are intensified when instruction relies heavily on symbolic and mathematical representations without adequately connecting them to macroscopic and submicroscopic phenomena. Students therefore require structured, representation-focused learning experiences that help them coordinate chemical and mathematical forms of representation (Becker et al., 2017; Cirkony et al., 2022; Murni et al., 2022).

These challenges are closely associated with scientific reasoning. Scientific reasoning involves identifying and controlling variables, examining quantitative relationships, interpreting correlations and probabilities, evaluating evidence, testing predictions, and drawing justified conclusions (Reith & Nehring, 2022; Syarqiy et al., 2023). Model-based learning is relevant to the development of these abilities because it engages students in constructing representations of phenomena, comparing models with empirical data, evaluating the adequacy of explanations, and revising models when necessary (Bolger et al., 2021; Shin et al., 2022). In mathematical chemistry, this process requires students to coordinate chemical knowledge with mathematical operations rather than treating the two domains separately. A mathematical equation should function not only as an operational device but also as a model through which students explain and predict chemical behaviour.

Computational software can support realtion between mathematics and real chemistry by reducing the burden of routine symbolic manipulation and enabling students to explore mathematical relationships through numerical, symbolic, and graphical representations. Maple, for example, can be used to visualize functions, solve differential equations, estimate parameters, and examine how changes in variables affect a mathematical model (Abramovich, 2023; Ionescu, 2021; Montgomery & Mazziotti, 2020; Olukemi Odumosu, 2018; Sallah, 2021). Nevertheless, the availability of computational software does not automatically promote scientific reasoning. Its pedagogical contribution depends on how it is integrated into activities that require students to connect phenomena, empirical evidence, mathematical representations, computational results, and scientific explanations. Without an explicit instructional structure, students may use software merely to obtain numerical answers without understanding the scientific meaning of the results.

Previous studies have separately examined students' mathematical reasoning in chemistry, model-based inquiry, representation-focused science instruction, and computational tools for scientific learning (Bain et al., 2019; Bolger et al., 2021; Cirkony et al., 2022; Montgomery & Mazziotti, 2020; Mustika et al., 2022; Sari et al., 2026). According to Spanier (1980), students should begin with an observable chemical phenomenon, formulate an initial mathematical equation, refine the equation into a form appropriate for analysis, use Maple to obtain a solution, and interpret the resulting model in relation to the empirical data. However, a teaching strategy that explicitly integrates observable chemical phenomena, differential–integral modelling, and Maple-assisted analysis within a coherent learning sequence remains limited. This study addresses that gap by introducing the PEE'SI (Phenomenon, Equation, Equation', Solution, Interpretation) strategy as a new instructional framework.

The novelty of this study, therefore, lies not merely in the use of Maple but in the systematic integration of chemical phenomena, mathematical modelling, computational analysis to support scientific reasoning. This integration is important because it positions scientific reasoning as an integral part of learning differential and integral concepts rather than as a separate, additional learning outcome. Accordingly, this study aimed to develop a Maple-assisted PEE'SI-based teaching strategy and to examine its potential to strengthen undergraduate students' scientific reasoning in mathematical chemistry.

Method

Research Procedure

This study employed an educational design research approach to develop teaching strategy for Mathematical Chemistry. The research consisted of four phases: preliminary investigation, prototype design, iterative try-outs, and final implementation as shown in Figure 1.

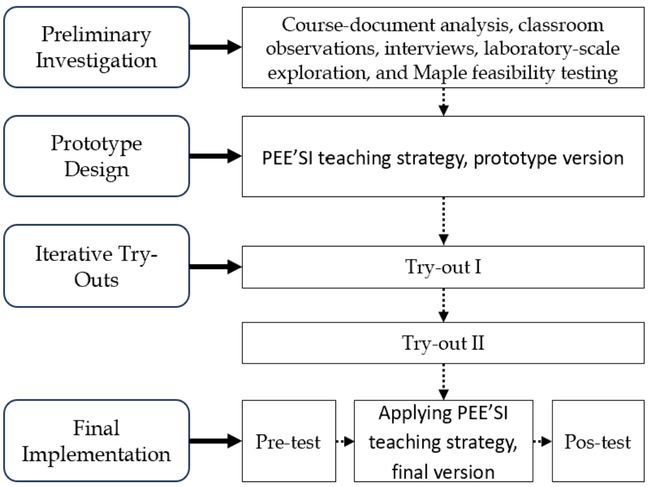

Figure 1. Research Procedure Flowchart

Preliminary Investigation

The preliminary investigation included course-document analysis, classroom observations, interviews, laboratory-scale exploration, and Maple feasibility testing. The findings from this phase were used to design the PEE'SI teaching strategy.

Prototype Design

During the prototype design phase, the findings of the preliminary investigation were translated into a structured Maple-assisted PEE'SI teaching strategy. The prototype included learning objectives, instructional activities, student worksheets, Maple-assisted tasks, and scientific reasoning assessments organized through the Phenomenon, Equation, Equation', Solution, and Interpretation sequence. Each component was designed to connect observable chemical phenomena with mathematical representation.

Iterative Try-Outs

The prototype design was evaluated through two iterative try-outs. Try-out I examined time allocation, worksheet clarity, practical procedures, students' use of Maple, and the feasibility of the instructional sequence. The prototype was then revised based on observation notes, student worksheets, and interviews. Try-out II was conducted to evaluate the revised prototype before its final implementation.

Participants were recruited according to the purpose of each development stage. Try-out I involved 17 undergraduate Chemistry students and Try-out II involved 10 undergraduate Chemistry Education students at a university in Palangka Raya, Central Kalimantan. The try-out groups were used to identify implementation constraints and refine the instructional strategy rather than as comparison groups.

Final Implementation

In the final implementation phase, the revised teaching strategy was implemented with 30 undergraduate students enrolled in a Mathematical Chemistry course at a university in Bandung, West Java. The implementation focused on differential and integral concepts in chemical contexts and followed the PEE'SI sequence. Students completed the pre-test and the post-test. The tests were administered to examine changes in students' scientific reasoning.

Data Collection Techniques

Data were collected using observation sheets, questionnaires, interview guides, student worksheets, and scientific reasoning tests administered as pre-tests and post-tests. Scientific reasoning was assessed through five indicators: identification and control of variables, proportional reasoning, correlational reasoning, probabilistic reasoning, and hypothetico-deductive reasoning.

Data Analysis

Qualitative data were analysed descriptively to identify implementation constraints and guide prototype revision. Quantitative data were analysed using mean scores, raw gain, normalized gain, paired-sample *t*-test, and correlation analysis. Normalized gain was calculated using (see Eq. 1), proposed by Hake, (1998).

$$< g >= \frac{S_{\text{post}} - S_{\text{pre}}}{S_{\max} - S_{\text{pre}}} \quad (1)$$

where S_{post} is the post-test score, S_{pre} is the pre-test score, and $S_{\max}$ is the maximum possible score of 100. Normalized-gain values were categorized as low ($g < 0.30$), medium ($0.30 \leq g \leq 0.70$), and high ($g > 0.70$). Statistical significance was determined at $\alpha = 0.05$, with very small probability values reported as $p < 0.001$.

Result and Discussion

The findings of this study show that the development of a Maple-assisted PEE'SI-based instructional strategy grounded in a clear instructional need and resulted in a meaningful improvement in students' scientific reasoning (Table 1).

Table 1. Preliminary findings

Preliminary-study	Key findings	Design implications
Curriculum and classroom review	Differential–integral teaching remained procedural	The strategy should promote phenomenon-based learning.
Student learning evidence	Struggled to apply mathematical in chemical contexts.	Should strengthen scientific reasoning.
Laboratory-scale exploration	Glucose-solution heating exhibited nonlinear behaviour.	The phenomenon supported differential and integral.
Technology feasibility and synthesis	Maple supported multiple forms of mathematical exploration, but its classroom integration remained limited.	These findings supported developing the Maple-assisted PEE'SI strategy for reasoning-oriented learning.

The preliminary study indicated that differential and integral topics occupy a substantial portion of mathematical chemistry teaching, accounting for 38.20% of subtopics and 37.60% of instructional time, yet their treatment in classroom practice remained largely procedural. Course plans did not explicitly integrate empirical data, curve fitting, or symbolic computational tools such as Maple, and classroom activities dominated by symbolic derivation and routine exercises. Student responses further confirmed persistent difficulties in applying differential and integral concepts to chemistry, interpreting results, and understanding graphs. These findings revealed a mismatch between the curricular importance of differential and integral concepts and their predominantly procedural treatment, underscoring the need for instruction that explicitly connects mathematical representations with empirical phenomena and engages students in model-based scientific reasoning (Bain et al., 2019; Cirkony et al., 2022; Lazenby & Becker, 2019; Prain et al., 2023). This, in turn, justified the development of a more phenomenon-based and modelling-oriented strategy (Bolger et al., 2021; Kularajan & Czocher, 2025).

An important result of the preliminary phase was the identification of glucose-solution heating as a suitable phenomenon for model-based instruction. The laboratory-scale study produced consistent nonlinear temperature–time curves characterized by an initial acceleration phase, an inflection region, and a final asymptotic toward maximum temperature (Figure 2).

In this study, laboratory-scale trials on glucose-solution heating produced nonlinear temperature–time data with acceleration, inflection, and asymptotic behavior, making the phenomenon suitable for differential interpretation and Maple-assisted modelling. Students' responses further indicated that Maple helped them visualize concepts, construct models from data, and reflect on model adequacy.

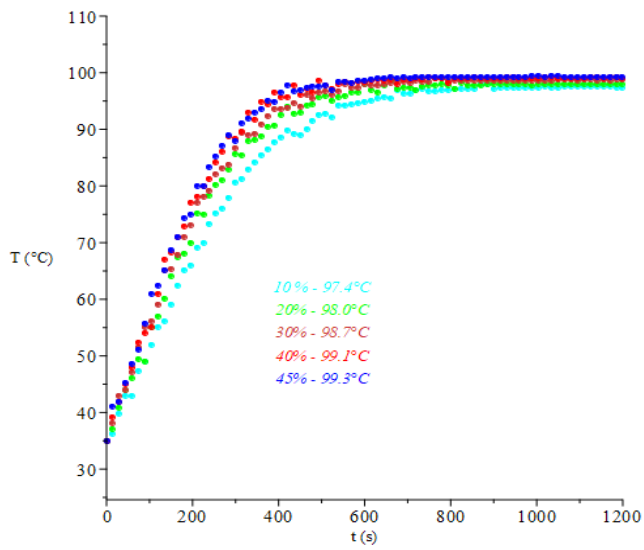

Figure 2. Empirical Glucose-Heating Curves

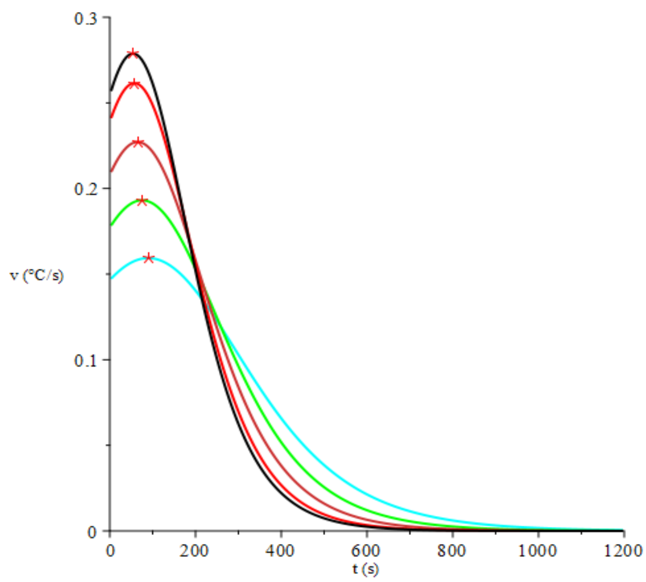

Figure 3. Maple Visualization Across Concentrations

These features made the phenomenon highly relevant for connecting empirical observation, differential interpretation, nonlinear modelling, and parameter-based reasoning. Figure 3 shows the display of Maple visualization of inflection behaviour (marked with *) and asymptotic tendency. In pedagogical terms, this choice was important because it enabled students to engage with mathematical ideas as tools for explaining real chemical behaviour rather than as isolated symbolic procedures (Bain et al., 2019; Bolger et al., 2021).

On the basis of these findings, the study produced a PEE'SI sequence consisting of Phenomenon, Equation, Equation', Solution, and Interpretation. This structure functioned not merely as a lesson sequence, but as a reasoning scaffold (Table 2). Figure 4 shows the PEE'SI strategy flowchart designed in this research.

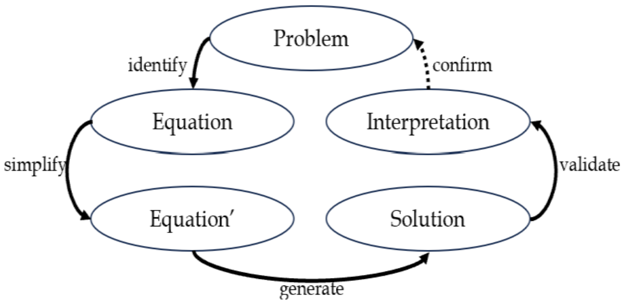

Figure 4. PEE'SI strategy flowchart

Table 2. Pedagogical roles of each PEE'SI phase

PEE'SI phase	Pedagogical role	Expected student engagement
Phenomenon	Introduces an observable chemical situation as the basis.	Students identify and relate the phenomenon to prior knowledge.
Equation	Translates the phenomenon into an initial mathematical.	Students formulate and propose a model.
Equation'	Refines the initial equation into a form suitable for deeper analysis.	Students reinterpret the model to chemical context.
Solution	Uses Maple to analyse and interpret the model.	Students generate graphs, solve expressions, fitting, and evaluate model.
Interpretation	Returns the mathematical results to the original phenomenon.	Students interpret parameters, and evaluate the adequacy and limitations.

The phenomenon stage directed students to observe, identify variables, and recognize patterns (Mesci et al., 2020; Mustika et al., 2022; Vasconcelos & Kim, 2022). Students did experiments first to collect real data (Figure 5).

Figure 5. Phenomenon Stage in Experiment

The equation and equation' stage guided them from empirical data toward formal mathematical structure and then toward chemically meaningful representation (Bielik et al., 2018; Kohen & Nitzan-Tamar, 2022; Sanjari & Manouchehri, 2024; Schuchardt & Schunn, 2016). Using Maple, students formulated mathematical modelling based on collected empirical data (Figure 6).

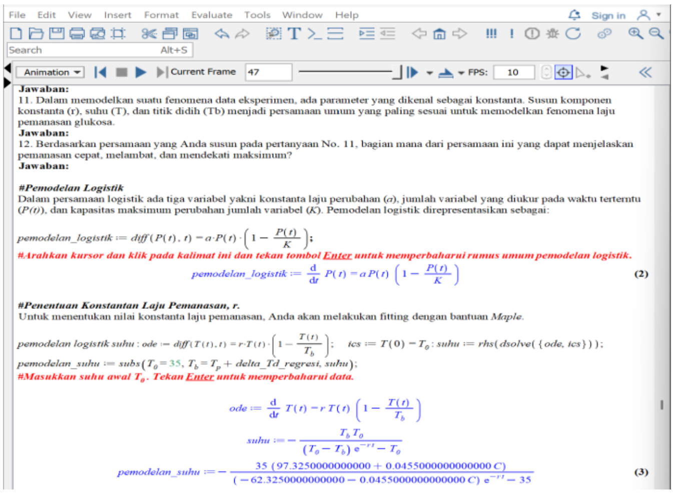

Figure 6. Equation and Equation' Stage in Maple

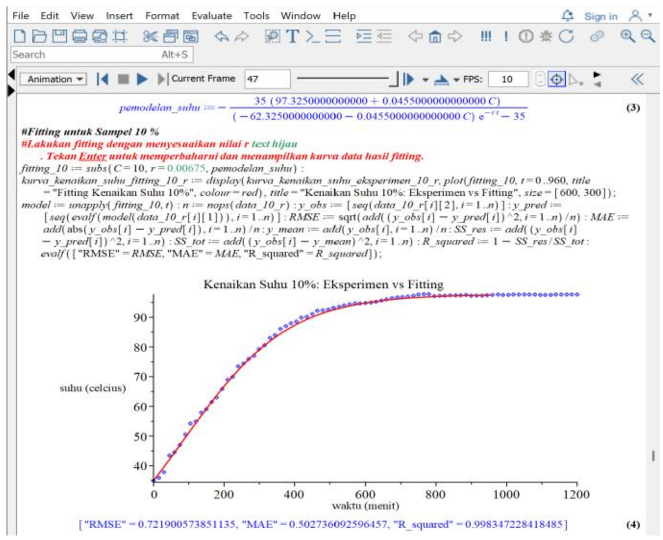

Figure 7. Solution Stage in Maple

Next, the solution stage used Maple to support plotting, symbolic or numerical processing, parameter estimation, and quantitative evaluation through indicators such as R^2, RMSE, and MAE (Kwadzo et al., 2021; Shekaari et al., 2019; Shin et al., 2022). These activities were done to generate final model (Figure 7).

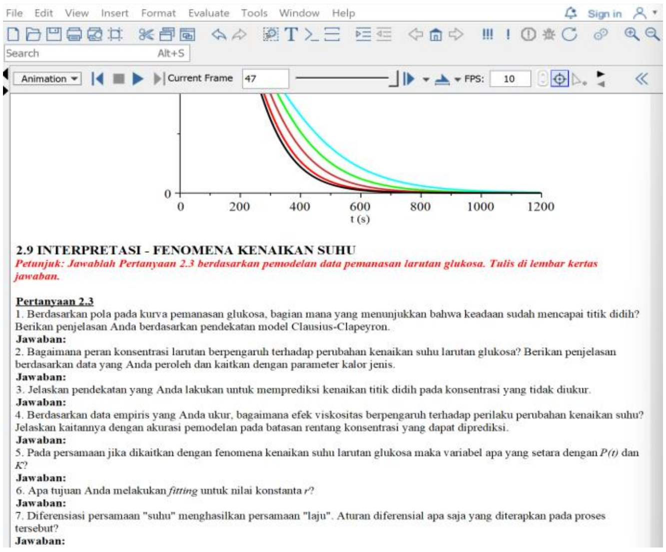

Figure 8. Interpretation stage in Maple

Finally, the interpretation stage required students to relate the mathematical results back to the chemical phenomenon by explaining parameter meanings, interpreting model behavior, and evaluating the model's assumptions and limitations (Khan, 2007; Lazenby & Becker, 2019; Markauskaite et al., 2020). Students were given some questions to confirm their understanding. The give questions guided them to deeper comprehension (Figure 8).

These sequences are significant because they shifted instruction from procedural manipulation toward the epistemic practices of scientific reasoning. Students were trained to connect evidence, model, and explanation (Bielik et al., 2018; Malone & Schuchardt, 2023; Shin et al., 2022; Vaesen & Houkes, 2021).

The iterative try-out process further clarified how the strategy worked in practice (Table 3). Try-out I showed that students were generally able to generate empirical curves, regression equations, and model-fit statistics but several implementation constraints emerged. Especially in time allocation, worksheet clarity, and the technical demands of entering symbolic expressions into Maple. These issues were pedagogically important because they showed that the success of technology-supported modelling depends not only on the availability of software, but also on the clarity of scaffolding and the manageability of learning tasks (Chiu & Lin, 2019; Kaldaras & Wieman, 2023; Siller et al., 2023; Tay & Toh, 2023). After revision, including simplification of procedures, clearer worksheet prompts, and additional time for discussing differential interpretation, Try-out II became more systematic and manageable. This improvement suggests that the effectiveness of the strategy strengthened through iterative refinement, which is consistent with the logic of design research (McKenney & Reeves, 2021).

Table 3. Main revisions across the two try-out cycles

Issue identified in try-out I	Revision introduced	Outcome in try-out II
Insufficient time for modelling	An additional session allocated, and some topics redistributed across meetings.	Implementation became more systematic and manageable within the available time.
Practical procedures were inefficient	Technical procedures simplified to improve model efficiency.	Practical activities completed more efficiently.
Worksheet prompts were not sufficiently explicit	Questions revised with clearer wording and explicit references.	Students were better able to follow tasks and interpret the intended context.
Students had difficulty entering symbolic into Maple	Analytical responses first written on paper before entered directly into Maple.	Technical obstacles reduced, allowing students to focus more on modelling and interpretation.

The feasibility of the assessment instrument also supported the study. Expert validation of the integrated test yielded an overall mean score of 3.30 (good), with an average item relevance score of 3.50, indicating that the instrument was appropriate for assessing differential–integral understanding, scientific reasoning, and related higher-order thinking. Empirical testing with 32 students allowed the revision of weak items based on difficulty and discrimination indices. This process was essential because the quality of the conclusions about students' reasoning depends on the appropriateness of the instrument used to measure it. All 32 students had completed the Mathematical Chemistry course and had studied differential and integral concepts comparable to those assessed in the research instrument.

Analysis of the post-test scores from try-out I, try-out II, and the final implementation showed that instrument test demonstrated acceptable to good internal consistency, with Cronbach's alpha coefficients ranging from 0.710 to 0.858. The coefficient increased from 0.849 in try-out I to 0.858 in try-out II, indicating improved internal consistency following the instrument revision. During the final implementation, the coefficient decreased to 0.710 but remained within the acceptable reliability threshold (Taber, 2018). This decrease does not necessarily indicate a decline in instrument quality, as Cronbach's alpha may be affected by differences in participant characteristics or ability homogeneity. Therefore, the instrument was considered reliable, although its level of internal consistency varied according to the participant group and measurement conditions.

Table 4. Cronbach's alpha coefficients for evaluation test

Phase	Cronbach's alpha coefficients	Category
Try-out I	0.849	Good
Try-out II	0.858	Good
Implementation	0.710	Good

Across the developmental stages, the mean comprehension scores increased from 33.22 to 64.88 in Try-out I and from 33.82 to 70.59 in Try-out II, indicating that the revised prototype functioned more effectively than the initial version. In the final implementation, further gains of scientific reasoning observed in both the mathematical aspect and chemistry aspect of scientific reasoning.

Table 5. Gain scores in mathematical aspect

Students	Pretest	Postest	Gain	N-gain	Category
S1	22.00	68.00	46.00	0.59	Medium
S2	48.00	76.00	28.00	0.54	Medium
S3	50.00	88.00	38.00	0.76	High
S4	24.00	68.00	44.00	0.58	Medium
S5	38.00	80.00	42.00	0.68	Medium
S6	22.00	84.00	62.00	0.79	High
S7	40.00	66.00	26.00	0.43	Medium
S8	38.00	80.00	42.00	0.68	Medium
S9	40.00	72.00	32.00	0.53	Medium
S10	18.00	74.00	56.00	0.68	Medium
S11	24.00	80.00	56.00	0.74	High
S12	24.00	74.00	50.00	0.66	Medium
S13	36.00	70.00	34.00	0.53	Medium
S14	22.00	84.00	62.00	0.79	High
S15	36.00	76.00	40.00	0.63	Medium
S16	24.00	76.00	52.00	0.68	Medium
S17	36.00	70.00	34.00	0.53	Medium
S18	38.00	74.00	36.00	0.58	Medium
S19	24.00	68.00	44.00	0.58	Medium
S20	38.00	66.00	28.00	0.45	Medium
S21	60.00	90.00	30.00	0.75	High
S22	28.00	64.00	36.00	0.50	Medium
S23	38.00	68.00	30.00	0.48	Medium
S24	46.00	74.00	28.00	0.52	Medium
S25	46.00	70.00	24.00	0.44	Medium
S26	26.00	52.00	26.00	0.35	Medium
S27	42.00	74.00	32.00	0.55	Medium
S28	38.00	56.00	18.00	0.29	Low
S29	40.00	66.00	26.00	0.43	Medium
S30	26.00	60.00	34.00	0.46	Medium
Average	34.40	72.27	37.87		

On the mathematical aspect (Table 5), the mean score rose from 34.40 in the pre-test to 72.27 in the post-test. The average of gain score is 37,87 with most students reaching the medium gain category and several reaching the high gain category. Indicator-level analysis showed improvement across all observed components, with particularly strong gains in identification and control of variables, hypothetico-deductive reasoning, and probabilistic reasoning.

On the chemistry aspect (Table 6), the same general trend appeared. The mean score rose from 31.85 to 70.65 and the average of gain score is 38.81, with especially notable increases in hypothetico-deductive, correlational, and probabilistic reasoning. These results suggest that scientific reasoning strengthened when students were required to move repeatedly between phenomenon, model, computation, and interpretation (Kularajan & Czocher, 2025; Prain et al., 2023; Reith & Nehring, 2022).

Table 6. Gain scores in chemistry aspect

Students	Pretest	Postest	Gain	N-gain	Category
S1	38.39	67.86	29.46	0.48	Medium
S2	43.75	75.00	31.25	0.56	Medium
S3	45.54	85.71	40.18	0.74	High
S4	33.04	78.57	45.54	0.68	Medium
S5	26.79	82.14	55.36	0.76	High
S6	34.82	86.61	51.79	0.79	High
S7	31.25	62.50	31.25	0.45	Medium
S8	16.96	66.96	50.00	0.60	Medium
S9	27.68	75.89	48.21	0.67	Medium
S10	25.00	80.36	55.36	0.74	High
S11	36.61	77.68	41.07	0.65	Medium
S12	26.79	72.32	45.54	0.62	Medium
S13	25.89	67.86	41.96	0.57	Medium
S14	25.89	71.43	45.54	0.61	Medium
S15	34.82	70.54	35.71	0.55	Medium
S16	25.89	65.18	39.29	0.53	Medium
S17	22.32	62.50	40.18	0.52	Medium
S18	17.86	69.64	51.79	0.63	Medium
S19	25.00	67.86	42.86	0.57	Medium
S20	48.21	78.57	30.36	0.59	Medium
S21	44.64	82.14	37.50	0.68	Medium
S22	36.61	72.32	35.71	0.56	Medium
S23	35.71	61.61	25.89	0.40	Medium
S24	36.61	62.50	25.89	0.41	Medium
S25	31.25	64.29	33.04	0.48	Medium
S26	33.93	50.89	16.96	0.26	Low
S27	35.71	75.89	40.18	0.63	Medium
S28	41.07	57.14	16.07	0.27	Low
S29	19.64	58.93	39.29	0.49	Medium
S30	27.68	68.75	41.07	0.57	Medium
Average	31.85	70.65	38.81		

The difference between pre-test and post-test scores in the final implementation was also examined statistically to determine whether the observed gain represented a meaningful improvement. The normality of the gain scores was examined using the Shapiro–Wilk test (Table 7). The gain scores were normally distributed for both the mathematical aspect ($p = 0.124$) and the chemistry aspect ($p = 0.464$).

Table 7. Normality of the gain scores

Aspects	Statistic	df	Sig.
Mathematical	0.945	30	0.124
Chemistry	0.967	30	0.464

Therefore, paired-sample *t*-tests were conducted (Table 8). The results showed that post-test scores were significantly higher than pre-test scores for the mathematical aspect, with a mean difference of 37.87 ($p = 0.001$) and for the chemistry aspect, with a mean difference of 38.81 ($p = 0.001$). These results provide inferential support for the descriptive improvements and indicate that students' scientific reasoning increased significantly following the implementation of the Maple-assisted PEE'SI strategy.

Table 8. The paired-sample *t*-tests

Aspects	Mean	df	Sig.
Mathematical	37.87	29	0.001
Chemistry	38.81	29	0.001

These findings also clarify the role of Maple. The results do not indicate that software alone improved students' reasoning; rather, Maple became effective because it embedded in a structured modelling sequence. Its main contribution was to reduce routine algebraic burden and make mathematical relationships more visible, allowing students to focus more on interpretation, comparison of models, and evaluation of evidence (Bolger et al., 2021; Montgomery & Mazziotti, 2020). In this study, Maple was not the starting point of instruction, but a tool used within the solution and interpretation stages to support deeper engagement with the model. This explains why the gains in scientific reasoning were strongest in indicators that required students to reason about variables, relationships, and evidence rather than merely calculate (Bain et al., 2019; Reith & Nehring, 2022).

Another important result is the very strong positive correlation between gain in differential–integral mastery and gain in scientific reasoning (r = 0.969, p = 0.001, N = 30). This finding indicates that the development of scientific reasoning did not occur separately from disciplinary learning, but together with students' increasing ability to interpret, model, and explain differential–integral ideas in mathematical chemistry. In other words, scientific reasoning in this context appears embedded in conceptual understanding rather than added on top of it. This strengthens the argument that mathematical chemistry instruction should not separate content mastery from reasoning development (Bain et al., 2019; Bolger et al., 2021).

Overall, the results and their interpretation suggest that the Maple-assisted PEE'SI strategy provided a coherent pedagogical framework for moving students beyond the procedural treatment of differential and integral concepts toward more interpretive and evidence-based reasoning. Its contribution did not derive from the introduction of technology alone. Maple was embedded within a structured modelling cycle that connected chemical phenomena, mathematical representations, computational exploration, and scientific interpretation. This design is consistent with evidence that students' mathematical reasoning in chemistry is strengthened when they engage meaningfully with models rather than relying on algorithmic procedures. Digital tools are also most effective when integrated into guided instructional sequences (Bolger et al., 2021; Lazenby & Becker, 2019; Palacios et al., 2024).

From a pedagogical perspective, these findings suggest that mathematical chemistry instruction may benefit from a shift from procedural teaching toward epistemic learning, in which students are positioned as active knowledge constructors who develop, test, and interpret models of chemical phenomena (Berland et al., 2016; Bolger et al., 2021; Schukajlow et al., 2023). However, the findings should be interpreted cautiously because of the relatively small implementation group and the need for adequate scaffolding and student preparation when computational tools are introduced (Chiu & Lin, 2019; Orosz et al., 2023; Tay & Toh, 2023). Nevertheless, the results provide preliminary evidence that a phenomenon-based, Maple-assisted modelling strategy may support scientific reasoning in mathematical chemistry (Kwadzo et al., 2021; Malone & Schuchardt, 2023; Morris, 2025; Widiastuti & Kariadinata, 2021).

Conclusion

This study developed a Maple-assisted PEE'SI teaching strategy that integrates chemical phenomena, mathematical representation, and computational analysis in Mathematical Chemistry course. In the final implementation, students' scientific reasoning scores increased significantly in both the mathematical and chemistry aspects, with mean gains of 37.87 and 38.81 points, respectively ($p < 0.001$). Gains in scientific reasoning were also very strongly correlated with gains in differential–integral understanding ($r = 0.969; p < 0.001$). It indicates that reasoning development was closely associated with students' increasing ability to model and interpret chemical phenomena.

These findings suggest that the Maple-assisted PEE'SI strategy has potential to support scientific reasoning and conceptual understanding in Mathematical Chemistry. However, the findings should be interpreted cautiously because the final implementation involved only 30 students, was conducted in a limited institutional context, and covered a relatively short teaching period. Further studies should examine the strategy with larger and more diverse samples, longer implementation periods, comparison groups, and direct measures of instructional practicality and implementation fidelity.

Acknowledgments
The authors would like to thank all those people and institutions that helped us in this research. We extend our thanks to the Indonesian Education Scholarship, the Centre for Higher Education Funding and Assessment, and the Indonesian Endowment Fund for Education for supporting this research.

Author Contributions
Conceptualization, D.F. and L.; formal analysis, D.F.; investigation, D.F.; methodology, D.F. and L.; supervision, L.; writing-original draft preparation, D.F.; writing–review and editing, L. All authors have contributed to the completion of this manuscript. They have read and agreed to the published version of the manuscript.

Funding
This research received no external funding.

Conflicts of Interest
The authors declare that there are no conflicts of interest.

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