



Enhancing Computational Thinking using Simulation Integrated Project-Based Learning (SIPrBL) in Chemical Reaction Engineering Course

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ABSTRACT (250 words)

BACKGROUND & CONTEXT

Students often struggle to grasp the fundamental concepts of reactor design through traditional lecture-based instruction alone, as the abstract nature of reaction mechanisms and system behaviour can be difficult to visualize. This paper presents a scholarly teaching practice that applied Simulation Integrated Project-Based Learning (SIPrBL) in the Chemical Reaction Engineering (CRE) course to foster computational thinking (CT).

PURPOSE OR GOAL

By integrating simulation into the PrBL, students are expected to visualize and predict reactor performance, enhancing conceptual understanding and enabling the development of CT through hands-on simulation experiences, inquiry-driven learning.

APPROACH OR METHODOLOGY

Constructive alignment (CA) model is adopted as the instructional design for SIPrBL project, where students were guided to conduct literature reviews, simulate reactor designs, and present their findings through ChemE Cube-UTM competition. The methodology involves both qualitative and quantitative data. Students' perception towards their ability on computational skill were obtained from after-project's feedback. The Focus Group Discussion (FGD) was conducted and analysed thematically to explore the CT skills experienced by the students using Weintrop's CT framework.

OUTCOMES

Students' perception shows 87% of students can effectively use computational tools for their project and 81% are highly confident in applying computational techniques in the project. The findings from FGD also proved that scaffolded SIPrBL enhances computational thinking such as data practice, modelling and simulation practice, computational problem solving and system thinking which aligns with key attributes for future engineers.

CONCLUSIONS

The intentionally designed scaffolding in SIPrBL fostered deeper understanding of reactor design concept with complex problem-solving and enhances students' ability in computational thinking through simulation practice.

KEYWORDS

Computational thinking; Chemical Reaction Engineering; Project-based learning.

Introduction

Computational thinking (CT) has become a fundamental competency for engineering graduates, enabling them to formulate, model, and solve complex problems systematically. Computational thinking, enabling graduates to approach problems systematically with logical methods. The Washington Accord indicated the ability to create, select, and apply appropriate techniques, resources, and modern engineering tools, including prediction and modelling as highly desirable skills in engineering curriculum output. Students form hypotheses, run experiments, analyse results, and refine models, mirroring scientific processes and fostering CT (Arjmandi et al., 2023). In chemical engineering programme, a strong foundation in CT prepares students for a fast-changing industry. The study showed students optimize reactor heat integration by balancing energy efficiency and throughput, then share findings for peer review (Lewin, 2003; Zapata and Agudelo, 2015). Computational tools enable dynamic visualization of chemical phenomena, helping students understand complex reactions that are often abstract or difficult to grasp using traditional methods. While these tools offer many advantages, promoting computational thinking in chemical reaction engineering course remain a challenge.

Chemical reaction engineering course has been a core part of chemical engineering education, requiring a solid understanding of kinetics, reactor design, and thermodynamics. Despite these advances in computational curriculum, chemical reaction engineering (CRE) remains one of the most conceptually challenging courses for undergraduates. Students often struggle with linking mathematical derivations, kinetic models, and reactor design principles to dynamic, real-world chemical processes. This difficulty limits their ability to apply knowledge flexibly and to develop higher-order problem-solving skills essential for engineering practice. The recent use of computational tools in this course helped students on the conceptual understanding was reported (Rodrigues et al., 2010; Moline et al., 2020). However, instructors incorporate these tools into lessons which these systems tend to be pre-made and are primarily used for application rather than for developing deeper computational skills on students.

Project-Based Learning (PrBL) has been shown to improve conceptual understanding, promote active engagement, and foster transferable skills such as teamwork, critical thinking as well as computational thinking (Saad and Zainuddin, 2022). Meanwhile, computational thinking must be coupled with disciplinary knowledge through the development of representational fluency by linking mathematical models with modelling and simulation practices, and the computational methods and techniques required to construct them (Magana and Silva, 2016). Thus, integrating simulation task could help student visualizing reaction dynamics and applying computational thinking to solve open-ended CRE problems. This creates a need for a more integrated pedagogical approach. This transformative educational approach adopted constructive alignment (CA) educational model to design scaffolded activities, formative assessments, and alignment with learning goals to foster computational thinking through the SIPrBL.

Design and Implementation

Chemical Reaction Engineering (CRE) Course

The CRE course is a core subject with 3 credits hour offered to third-year undergraduate students in the chemical engineering program. This course introduces students to the fundamental principles and design of chemical reactors, with a focus on both homogeneous and heterogeneous reaction systems. Key topics include reaction kinetics, reactor design equations, multiple reactions, and non-isothermal reactor operations, providing students with the theoretical foundation and practical skills to analyse and design chemical reaction systems. The course is delivered in parallel across four sections, each facilitated by one of four lecturers, ensuring consistent delivery of content and assessments.

SIPrBL Design using Constructive Alignment

SIPrBL was designed by adopting constructive alignment (CA) model to make sure the intended learning outcome (ILO) are achieved from the designed teaching and learning activities (TLAs) and assessments. The ILO which focuses on designing reactors under varying conditions using computer-aided tools. This reflects students' ability to apply modern computational tools and modelling techniques in problem-solving. This mapping ensures that the course not only strengthens technical competencies but also promotes responsible and sustainability-driven engineering practice.

Table 1 presents the CA for the ILO, the TLAs, and the assessment methods. This alignment ensures that students achieve the ILO through carefully scaffolded instructional strategies. Key topics include rate laws and mole balances, design equations and conversion, isothermal and non-isothermal reactor design, multiple reactions and selectivity were delivered during in-class lectures. Each topic is aligned with ILO such as the ability to derive reactor design equations, evaluate equilibrium conversion, or evaluate selectivity in complex systems. The teaching and learning activities combine lectures with project-based learning, where students conduct literature reviews, design reactor systems using AutoCAD, run simulations, and prepare video presentations. Assessment is conducted through project deliverables, including a final presentation and a video report, ensuring students demonstrate applied understanding of both theory and practice.

Project Overview

The CRE course incorporates this SIPrBL model through a cornerstone project titled ChemE Cube-UTM 2024 competition. This initiative engages the students to work collaboratively in groups for solving real-world chemical engineering problems. Students are tasked with designing a miniature chemical plant (1×1×1-foot cube) that transforms greenhouse gas (GHG) emissions into useful products (Figure 1). A complete synthesis reaction route should be selected for a chemical product using the specified reactant such as carbon dioxide, methane, nitrous oxide, ozone, sulfur hexafluoride, chlorofluorocarbons, hydrofluorocarbons, and perfluorocarbons. Students should analyze the chemical process system by applying theoretical knowledge and practical skills from various chemical engineering disciplines such as chemical reaction engineering, thermodynamics, separation, computer programming, numerical method and optimization which they are required: (1) To model and simulate the process using appropriate software tools (e.g., MATLAB, Polymath, AutoCAD); (2) To apply numerical methods and optimization techniques to improve system performance; (3) To analyse reactor design and performance based on chemical kinetics and reaction engineering principles.

Project Design and Implementation

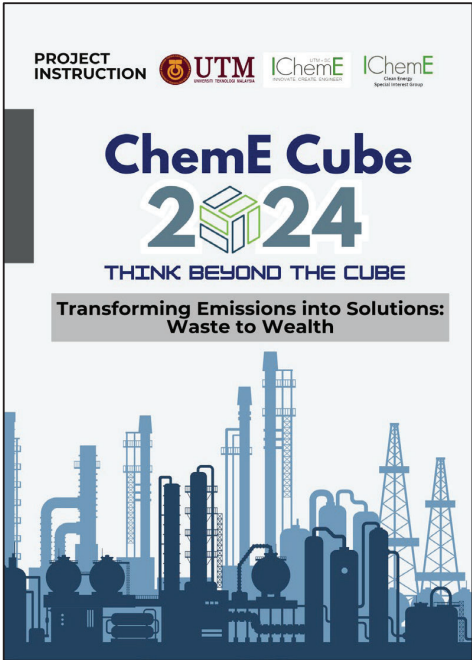
The design of project was structured using a flowchart of integrated activities (Figure 2), organized across three interdependent lanes: (1) Lecturer Activities, (2) Scaffolding Mechanisms, and (3) Student Activities. These activities are carefully aligned with ILO and pedagogical goals to promote progressive and supported learning.

Table 1: Constructive alignment of Chemical Reaction Engineering (CRE) course

Intended Learning Outcome	Stage	Teaching and Learning Activity	Assessment
To design a reactor for a range of conditions using computer aided tools	Project instruction and briefing	Lecture on topic, Introduction and briefing to ChemE Cube project, Problem analysis, worked examples	Submission of project topic
	Stage 1: Literature review	Lecture on topic, Team formation, Literature search (chemical reaction equation)	Facilitation and feedback in problem analysis,

		submission of literature review
Stage 2: Computational analysis	Lecture on topic, Peer teaching (industrial reactor case study), worked examples, guided discussion, open forum (e-Learning), team interim milestone discussion, industrial seminar	Progress check, submission of simulation draft, presentation (Instructor and peer feedback)
Stage 3: Reactor selection	Lecture on topic, worked examples, guided discussion, open forum (e-Learning), team interim milestone discussion, video and hands-on tutorial on simulation	Progress check, submission of preliminary design
Stage 4: Video Presentation	Lecture on topic, worked examples, guided discussion, open forum (e-Learning), team interim milestone discussion	Draft presentation review, ChemE Cube presentation, competition, self-reflection

Project planning and briefing initiates the scaffolding process. A detailed project briefing is conducted to explicitly communicate expectations, outcomes, and deliverables, providing cognitive scaffolding to help students structure their project planning. Content delivery and early engagement involves delivering core CRE concepts such as reaction kinetics, reactor design, and sustainability scaffolded by class activities to build conceptual understanding and introduce the context in which simulation and analysis tools will later be applied. To reinforce skill acquisition, worked examples and guided discussions are provided. Lecturers demonstrate how to use computational tools to simulate reactor performance, offering models that students can adapt in their own work. Open discussion platforms, such as e-learning forums, allow for clarification and peer-to-peer engagement, further supporting learners as they develop computational confidence.



PROJECT INSTRUCTION UTM IChemE IChemE

ChemE Cube 2024

THINK BEYOND THE CUBE

**Transforming Emissions into Solutions:
Waste to Wealth**

ChemE Cube 2024 OBJECTIVES

The ChemE Cube 2024 competition aims to provide third-year students in chemical reaction engineering (CRE) course and related disciplines with an opportunity to engage in an innovative, team-oriented, presenting design project centered around the manufacture of a mini chemical plant within a 1x1x1-foot cube. Participants will be expected to:

- Solve Industrial Problems:**
Design a process that addresses current challenges in the chemical engineering industry, utilizing creative and practical solutions.
- Propose a Safe Operational Design:**
Include justification on the design and operational safety of a complete chemical process (including both reaction and/or separation) within scale, employing advanced manufacturing techniques and intensified processing technology.
- Perform Scalability through Calculation and Pitching:**
Perform calculations to determine how the designed process can be scaled up to meet product demand. Participants will pitch their product's business case to a panel of industry judges, effectively communicating the process's viability and market potential.
- Utilize Computational Tools:**
Employ computational tools such as AutoCAD, MATLAB etc for system design and simulation, reinforcing the integration of modern technology in chemical engineering practices.
- Promote Sustainability:**
Incorporate principles of sustainability into the design, ensuring that the chemical process aligns with environmental goals and promotes responsible consumption and production.
- Instill Core Values:**
Encourages team working, creativity and innovation, sustainable development, and diversity and inclusion.

Figure 1: Project Instruction of ChemE Cube-UTM 2024 Competition

Interim milestones and formative feedback are strategically embedded to break down complex tasks into manageable stages. Students are required to submit components such as literature reviews, draft simulations, and preliminary designs. Lecturers provide formative feedback at each checkpoint, guiding improvements and encouraging iteration. To connect theory with practice, an industrial seminar is conducted featuring an invited speaker from chemical engineering industry, who shares insights into real-world chemical process engineering. This session includes interactive elements such as open question and answer, promoting two-way engagement.

In the final preparation and evaluation phase, lecturers review draft presentations and provide detailed and constructive feedback. Students synthesize their findings into a comprehensive technical presentation supported by simulation results, AutoCAD schematics, and reactor analysis. Students present their ChemE Cube project in the form of pitching session to a panel of judges from industry professionals and academic lecturers, simulating an industrial pitching environment. Table 2 outlines the project assessment rubric, which evaluates students' performance across criteria assessing ILO, promoting clear expectations and transparency in evaluating both technical competencies and transferable skills.

Finally, students presented their project output in IChemE Cube-UTM competition. Judges provide immediate feedback on technical feasibility, innovation, and presentation clarity, which helps students reflect and refine their understanding of their designs. The competition mimics real-world expectations of technical communication, professionalism, and client-centred problem solving. Following the live competition, each team is required to submit a video report, which involves recording a comprehensive presentation of their ChemE Cube project. This ensures that every team's work is captured in a consistent and structured format for further assessment. Finally, in the reflection and completion phase, students submit self-reflections to consolidate their learning experiences, documenting both technical insights and personal growth.

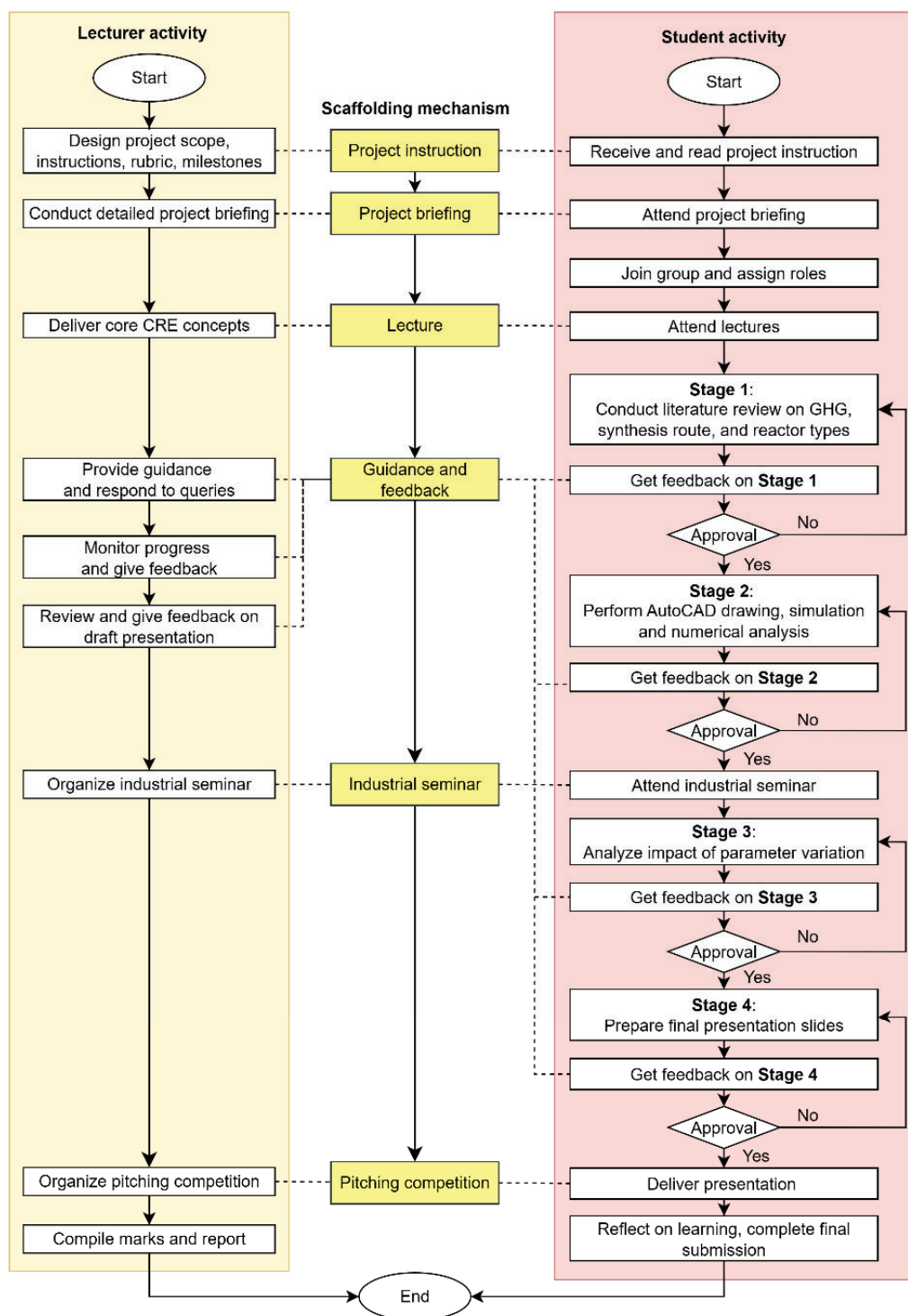


Figure 2: Integrated activities of lecturers and students in the ChemE Cube project, explicitly highlighting the scaffolding structure

Table 2: Project assessment rubrics

Criteria	1	3	5
Mini Plant Design	- Reactors and operating units are poorly designed without labels. - Unclear or incomplete AutoCAD drawing of the process flow diagram. - Drawing does not meet specifications. - No evidence of innovation.	- Reactors and operating units are well designed with incomplete labels. - Inaccurately AutoCAD drawing of process flow diagram lacks detail. - Drawing meets some specifications. - Minimal innovation.	- Reactors and operating units are perfectly designed with complete labels. - Detailed and accurate AutoCAD drawing of the process flow diagram. - Drawing meets the required specification. - Unique and impactful innovations.
Synthesis Route Analysis	- Present only 1 synthesis route for the reaction. - Unclear explanation or scientifically inaccurate understanding with no justification of the chosen route. - Inappropriate reactor type with no justification.	- Explored only 2 possible synthesis routes for the reaction. - Brief explanation with moderate scientific understanding and justification of the chosen route. - Appropriate reactor type with reasonable justification.	- Explored several possible synthesis routes for the reaction. - Detailed explanation with clear scientific understanding and justification of the chosen route. - Reactor type is well-justified with strong technical reasoning.
Simulation and Numerical Analysis	- Assumptions are not stated. - Conversion and yield calculations are incomplete or inaccurate. - Use only 1 computational tool for analysis. - No parameter is manipulated.	- Assumptions are stated. - Conversion and yield calculations are less accurate and incomplete. - Use 2 computational tools for analysis. - Only one parameter is manipulated.	- Assumptions are clearly stated. - Accurate and detailed calculations of conversion and yield. - Use more than 2 computational tools for analysis. - Various parameters are manipulated.

Lecturers evaluate the project and provide final marks and qualitative feedback, reinforcing learning outcomes and identifying areas for future development. This structured, scaffolded approach ensures that students are supported at every stage of the learning journey, with progressively reduced guidance to encourage independence. The integration of simulations, industrial relevance, and authentic assessments makes this SIPrBL model highly effective in developing computational thinking, sustainable design skills, and professional competencies in undergraduate chemical engineering students.

Data Collection and Analysis

Students' responses from after-project survey related to the ILO was collected to determine students' perceptions in SIPrBL through computational tool usage. The questions in the survey were: (1) How effectively did the project help you develop skills in using computational tools for modelling and prediction? (2) How confident are you in your ability to use modern computational techniques after completing the project?

Focus group discussion (FGD) was conducted for 10 volunteered students undergo the course. The FGD transcription was thematically analysed guided by Braun and Clarke's thematic analysis. The thematic analysis used deductive approach to search the evidence that support four interrelated themes based on the Weintrop et al.'s (2016) CT framework that illustrate how CT was embedded in students' project work as summarized in Table 3.

Findings and Discussion

Students' Perception in ChemE Cube Competition

Students' perception on two criteria which are: (1) the effectiveness of using computational tools for modelling and prediction (2) the confidence in using modern computational techniques were obtained from after-project survey. Figure 3 shows 87% of students can effectively use computational tools for their project and 81% are highly confident in applying computational techniques in the project. The course was designed using CA principles, with a focus on enhancing structured scaffolding activities throughout the SIPrBL approach. This design introduced intentional support mechanisms such as staged deliverables, formative feedback loops, progress monitoring, and an industrial style pitching competition. These activities were carefully sequenced to guide students through the logical structuring of problems, simulation of chemical reactions using computational tools, and iterative design improvements based on analytical interpretation. The impact of these scaffolding enhancements is evident to enhance students' confidence in applying computational thinking and tools in learning. This improvement is directly reflected in the attainment of ability to apply modern computational tools, confirming that structured scaffolding effectively supported the development of technical competencies and computational reasoning. In overall, students were able to construct AutoCAD designs of mini plant systems (Figure 4), perform accurate conversion and yield calculations, and demonstrate a strong understanding of synthesis routes using appropriate reactor types. Moreover, students showed increasing competence in manipulating process parameters (e.g., concentration, flow rate) using multiple computational tools, such as MATLAB, Polymath, Python, and Excel.

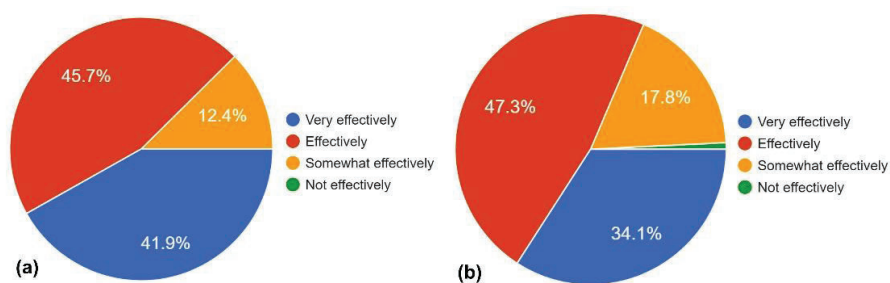


Figure 3: Student perceptions on computational tools experience for academic session 2024/2025-1: (a) Effectiveness of computational tools for modelling and prediction, (b) Confidence in ability to use computational techniques

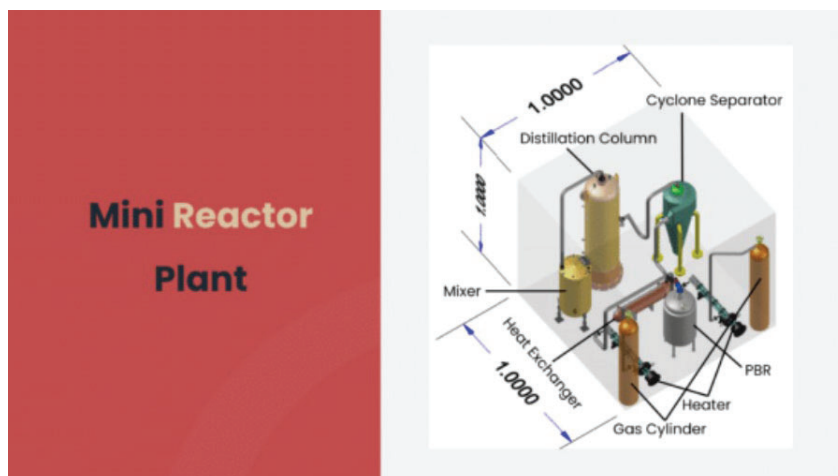


Figure 4: Chemical mini plant within a 1x1x1-foot cube presented by one of the teams

Computational Thinking Skills

Focus group discussion (FGD) was conducted for 10 volunteered students undergo the course. The FGD transcription was thematically analysed guided by Braun and Clarke's thematic analysis. Findings revealed four interrelated themes based on the Weintrop et al.'s (2016) CT framework that illustrate how CT was embedded in students' project work as summarized in Table 3. The CT framework developed by Weintrop et al. (2016) categorizes CT into four interrelated dimensions as presented in Table 3.

Modelling and simulation practices involve constructing, refining, and using computational models to represent real-world systems. From the FGD data, students reported that simulation task helped them move from theoretical confusion to practical clarity. Before engaging with the simulation, many expressed difficulties in relating chemical kinetics and reactor design equations to overall plant performance. By simulating reactor behaviour under varying parameters, students gained insight into how their choices affected conversion, selectivity, and yield. This simulation practice functioned as a cognitive scaffold for reaction system understanding and served as a design validation mechanism (Yan et al., 2025). Students used it to test assumptions, evaluate reactor configurations and optimize operational conditions. The output graphs and numerical results helped them confirm whether their numerical analysis was functionally sound before proceeding to reactor design.

Data practices refer to how learners engage with data through activities such as collecting, organizing, interpreting, and using data to support claims or inform design decisions. In engineering contexts, this often involves sourcing data from literature, validating parameters, and visualizing outputs (Peters-Burton *et al.*, 2022). In this SIPrBL, students primarily sourced simulation inputs from scientific literature. They validated those inputs by checking whether simulation outputs aligned with expected output such as reaction behaviour trend, reactor design simulation and optimized reaction parameters. These actions highlight a type of data practices such as collecting, selecting, validating, and interpreting data within constraints. This dimension of computational skill is much related to the problem abstraction of CT foundation by managing data efficiently, filtering the necessary data from the literatures.

Table 3: Computational Thinking Skills Emerged from Focus Group Discussion

CT Categories	Emerging Themes	Supporting Quotes
Modelling and Simulation Practices	Simulation as a learning scaffold	"After doing the simulation... the picture got clearer... before that, we were kind of lost."
	Optimization of reaction parameters	"We simulated different temperatures... what is the conversion when the temperature is 0, 1..."
	Tool integration	"All the AutoCAD and MATLAB arrangements are interconnected..."
Data Practices	Literature-Informed data practice	"We need to take the reactor volume, gas constant, exponential factor... from research papers."
	Data Validation	"We code using data obtained... then we check whether our computation is valid or not through the profile"
Computational Problem Solving	Use of Iterative Debugging	"If you are talking about only by calculations with hands, I think it is a lot of work to do."
Systems Thinking	Understanding Interconnected Processes	"Changing the feed affected everything else... we need to consider scrubbers, spargers..."
	SDG-Linked Systems Design	"We realized this project is highly related to SDG goals... how it helps environmentally."

Another key computational thinking dimension by Weintrop is computational problem-solving practices. Students' experience iterative debugging, particularly in the way they refined simulation outputs through repeated parameter adjustments and validation against expected trends. While the simulation tasks were structured around chemical reaction modelling, students did not execute these in a single, linear step which they used various simulation approaches, data, algorithms and outputs. Instead, their approach was depending on the programming objectives. Simulations were also used iteratively to improve design logic, where student use AutoCAD to visualize 3D engineering drawing of the reactor design.

System thinking practices encourage learners to understand the structure and behavior of interconnected components within a system, considering system' factors. Students reflected on how components interact in a chemical plant by analysing the system parameter through simulated output. Students also linked their decisions to broader environmental concerns, guided by the SDGs. For example, the use of wet scrubbers to reduce ozone emissions, or converting methane to syngas for cleaner energy, reflects deliberate systems thinking embedded in CT.

While the project required students to engage in simulation-based problem solving, the FGD data also revealed a limitation in their application of system thinking practice. However, in this context, students often approached the problem in segregated task assignments, where each student focused on a specific aspect in relative isolation. Some students admitted they were not fully involved in or aware of the simulation process or the design rationale applied by other team members. The result was a compartmentalized workflow that risked turning the project into a collection of parallel efforts rather than a coordinated, integrative problem-solving experience. Such separation may hinder the development of computational thinking, as students are not consistently challenged to navigate the interdependencies of CT dimensions. Future implementation of this learning experience could benefit from more intentional scaffolding of collaborative problem decomposition.

Conclusion

The overall assessment of learning outcome attainment, particularly on simulation-based reactor design shows that SIPrBL approach provides an effective and supportive environment for students to acquire both technical expertise and transferable skills. By incorporating structured scaffolding mechanisms in SIPrBL project through CA based design including staged project milestones, formative feedback loops, computational tool guidance, and an industrial-style pitching session, the course effectively supported students in developing computational thinking skills, system-level reasoning, and technical competency in reactor design. Future enhancements will focus on strengthening support for sustainability literacy and collaborative system thinking practice.

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