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Digital Simulation-Based Learning for Reaction Engineering: Activity Design and Student Metacognition

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ABSTRACT

This study investigates the integration of digital simulation-based learning (DSBL) with Legitimation Code Theory (LCT) and problem-based learning (PBL) for a first-year undergraduate chemical engineering course on reaction engineering. The DSBL activity was designed to facilitate semantic shifts across the axes of semantic gravity and semantic density, enabling students to move between abstract concepts and simulation-based applications of varying complexity. Novel to this study is the coupling of DSBL with LCT to create a dynamic learning environment that promotes critical thinking and problem-solving skills. Student reflection, collected through a survey and processed through reflexive thematic analysis, reveals the positive impact of the DSBL activity on level of understanding, critical thinking, and student confidence in reaction engineering concepts. This triangulation of pedagogical learning theory, DSBL activity design, and student metacognition addresses an important implementation gap offering practical implications for engineering educators.

1 | Introduction

Digital simulation-based learning (DSBL) has emerged as a transformative approach in engineering education, leveraging the power of advanced computational tools to create immersive, interactive learning environments [1–4]. As the complexity of engineering problems continues to increase, traditional teaching methods often fall short in equipping students with the necessary skills since the gap between theory and practice is difficult to bridge [3–5]. DSBL addresses this challenge by providing a platform where students can engage with realistic scenarios and complex systems in a virtual environment, allowing them to apply theoretical knowledge to practical situations without the limitations of physical laboratories [6–8].

The pedagogical relevance of DSBL lies in its alignment with modern educational theories, particularly constructivism, which emphasises active learning, problem-solving, and the application of knowledge in real-world contexts [9]. By simulating professional engineering challenges, DSBL enables students to engage in self-directed learning, experiment and make mistakes, and learn from them in a risk-free environment, thus fostering deeper understanding and critical thinking skills [10–12]. Moreover, DSBL supports the development of procedural knowledge and competencies that are crucial in engineering practice, such as system analysis, decision-making, and collaborative teamwork [13–15].

A growing body of literature has explored the effectiveness of DSBL in enhancing student performance [16] and learning outcomes [17], where DSBL is particularly effective in helping students achieve the higher cognitive levels of 'analyse', 'evaluate' and 'create' as described in the Bloom's Taxonomy [18, 19]. Studies have demonstrated that students engaged in simulation-based learning exhibit improved problem-solving abilities, increased engagement, and greater retention of knowledge compared to those taught through traditional methods [20]. In a research study based on self-determination theory, Koh et al. found that students using simulation tools reported higher levels of satisfaction and motivation [21].

Similarly, the effectiveness of DSBL in improving conceptual understanding of complex engineering topics such as thermodynamics [22, 23] and fluid mechanics [24] have also been articulated. These findings are corroborated by meta-analyses that consistently show positive correlations between DSBL and student achievement across various engineering and non-engineering disciplines [7, 25, 26]. More recently, artificial intelligence (AI) has enabled improving the sophistication and capability of DSBL through AI-powered virtual agents and other pathways [27]. The shift from passive reception of information to active construction of knowledge is crucial in preparing students for the dynamic and complex challenges of the engineering profession. Particularly at introductory levels of engineering programmes, for example the first year of study of an undergraduate engineering programme, simulation-based learning design can have significant value [28].

Alongside the benefits of DSBL articulated above, the advantages of problem-based learning (PBL) has also been explored in the remit of engineering education [29–31]. Although PBL is well-established as a pedagogical approach, a recently published literature review highlights the "the lack of qualitative studies concerning students' articulation of their own competences" in the context of PBL environments [32]. Furthermore, an even more recent publication mentions "the lack of integration of DSBL with learning theories", such as PBL, in engineering education as a major implementation and research gap [33]. In an endeavour to address each of these limitations that have been surfaced in the literature cited above, this paper specifically targets two key research questions:

i. How can the design of a DSBL activity be informed by and integrated with a learning theory? (addressing gap identified in [33]).
ii. What are the student perceptions of the impact of the DSBL activity on their learning and understanding? (addressing gap identified in [32]).

The student metacognitive data from the latter question can be used to verify the degree to which learning gains articulated by students align with the instructor expectations during the design of the activity. Thereby, this piece of research addresses both the design of DSBL activities grounded in a pedagogical framework and assessment of the activity through student metacognition. Herein, the DSBL activity is designed for introductory content on reaction engineering, a core subject of training for chemical engineering students.

2 | Course Context and Methodology

The DSBL activity was designed for a module titled 'Introduction to Process Engineering' delivered to first-year undergraduate chemical engineering students. Approximately 6 weeks on the module (ca. 15 teaching hours) is dedicated to introducing concepts of reaction engineering addressing the following learning objectives (LOs):

- LO1: Apply concepts of chemical kinetics and stoichiometry to reaction engineering problems
- LO2: Apply material balances to ideal batch and continuous reactors to derive performance equations to determine reactor volume
- LO3: Operate a continuous stirred tank reactor (CSTR) under a chosen set of reaction conditions and critically analyse the resulting experimental data.

Table 1 presents a breakdown of the topics covered along with a mapping to the LOs identified above. The delivery style was through a combination of interactive lectures using integrated problem-solving i.e. new concepts were introduced and immediately followed up with application through numerical problem solving. This strong emphasis on problem solving was necessary to give students the best possible chance to meet the level of 'application' as stated in the first two LOs, making a PBL approach a natural fit for this course. Furthermore, the module also had a lab-component where students worked in groups to operate a bench-top CSTR under different conditions, and collected and analysed the resulting data (LO3). The proposed DSBL session was held after concluding teaching of the fifth chapter/topic listed in Table 1. The labs were completed in small student groups while the DSBL activity was the last session on reaction engineering. The content of this part of the module was assessed through a coursework based on the practical (LO3) and a closed-book examination (LO1 and LO2).

TABLE 1 | Content covered in the reaction engineering section of the course and mapping to learning objectives.

Chapter/topic	Sub-topics	LOs mapping
1. Introduction to reaction engineering	Definitions, types of chemical reactions, qualitative form of performance equation	Foundational knowledge for LO1, LO2
2. Chemical reaction kinetics	Rate of reaction, Stoichiometry, Reaction rate law, Arrhenius equation, Fractional conversion	Foundational knowledge for LO1, LO2
3. Ideal reactors	Qualitative introduction to batch reactor, continuous stirred tank reactor (CSTR) and plug flow reactor (PFR)	Foundational knowledge for LO2
4. Material balance on ideal reactors	Performance equations for batch reactor, CSTR and PFR, Levenspiel plots.	LO2, LO3
5. Experimental determination of rate law	Differential and integral methods of rate analysis for first and second order irreversible reactions	LO1

Although problem-solving requires application of foundational engineering knowledge, there could still be a barrier to deep understanding, if students merely distil a question to identify variables and data, and mathematically apply an equation to find the 'right' answer. Such an approach condenses an engineering problem into a mathematical problem, and in this translation, the rich engineering context of the problem is often lost, and students fail to appreciate how mathematics is a tool to model and describe complex engineering phenomena. This is even more of a possibility for first-year undergraduate students, who have very little understanding of the engineering discipline as a whole and could engage with mathematical equations and physicochemical phenomena as two different silos. In this context, digital simulations help preserve engineering complexity while marrying abstract theoretical concepts and mathematical equations to more concrete applications. The design of the DSBL activity and the underpinning theoretical construct used will be described in subsequent sections.

For a complete investigation of the DSBL intervention, the educator perspective of activity design is coupled with the student perspective of the effect of the DSBL activity on the learning experience. Immediately after the conclusion of the DSBL session, students were invited to complete an anonymous survey hosted on the JISC Online Surveys platform. Participation was voluntary and required approximately 5 min to complete. The survey questionnaire comprised Likert scale questions to gauge student satisfaction and the following open-ended free text question that asked students to reflect on how the DSBL activity had improved their understanding:

> *Describe briefly the impact this session has had on your learning. You can reflect on what you found useful and how it helped improve your understanding.*

The resulting qualitative data could then be used to evaluate the success of the DSBL activity in meeting the intended outcomes as envisioned by the instructor.

The qualitative data was analysed using the reflexive thematic analysis (RTA) approach [34–36]. Unlike other forms of thematic analysis, RTA does not use a codebook reliability approach, where structured codebooks are used to reach shared consensus among researchers. As opposed to attempting 'accurate' or 'reliable' coding, RTA is about "the researcher's reflective and thoughtful engagement with their data" [35, 37]. In the context of this study, RTA is an appropriate methodology as it allows to meaningfully evaluate the construct of the DSBL activity design in terms of its effect on student learning. Since RTA embraces subjectivity and reflexivity over correctness and reliability [36], student reflections can be analysed from the reflexive perspective of the author, which enables identifying links between student comments and the underlying pedagogical framework that the author used to design the DSBL activity. Following the six-phase analytical process [34], the author first familiarised themselves with the student responses collected in the survey and then began to generate initial codes. The coding approach followed was a combination of semantic coding (explicit meaning conveyed in the comments) and latent coding (identifies hidden meanings and ideas) [38]. The coding was done using the 'comments' feature in Microsoft Word. These codes were then organised to produce themes and sub-themes. The author also reflected on the connections between the various themes and sub-themes to develop a thematic map that informs the discussion of the results presented herein.

3 | Pedagogical Basis: Legitimation Code Theory (LCT)

LCT, an analytical framework developed by Karl Maton that extends and builds upon the ideas of Bourdieu and Bernstein [39], provides a way to understand knowledge practices, particularly how knowledge is constructed, communicated, and legitimated across different contexts [40, 41]. With its roots in social realism, LCT has been particularly influential in educational research as it offers a lens to analyse the underlying structures of knowledge that shape educational practices and student outcomes [41].

LCT is structured around several dimensions, but two key concepts that are often explored are semantic gravity (SG) and semantic density (SD). These concepts form the basis of what is known as the 'semantic plane', a conceptual space used to analyse and map shifts in meaning across educational discourse. While SG is a measure of the degree of abstraction i.e. 'the degree to which meaning relates to context', semantic density deals with the degree of complexity i.e. 'the degree to which meaning is condensed within symbols (terms, concepts, phrases, expressions, gestures, etc.)' [40]. Thereby, the SG axis runs from the abstract (SG−) to the concrete (SG+) while the SD axis runs from the simple (SD−) to the complex (SD+) (Figure 1). These semantic axes have been leveraged to particularly improve pedagogical practice in STEM education [42, 43], as students in these disciplines must frequently 'shift' or move across the different axes and quadrants in the semantic plane to develop solutions and problem solve. This process of moving back and forth across the semantic plane is crucial for developing what LCT describes as 'cumulative knowledge building' [44]. In engineering education, it ensures that

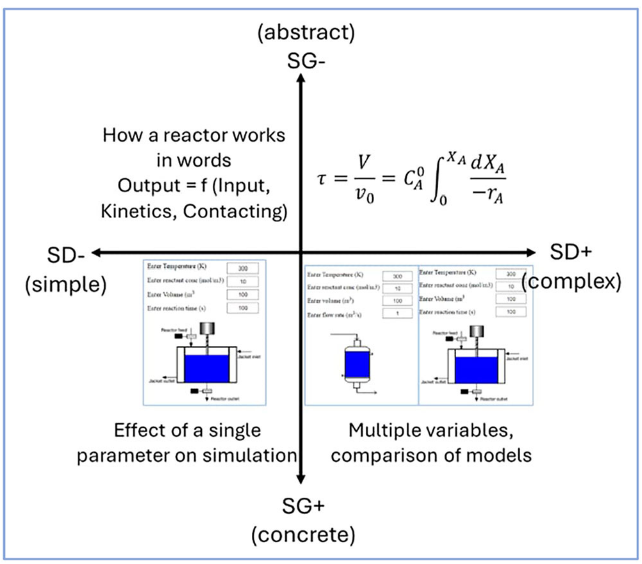

FIGURE 1 | Semantic plane for the reaction engineering content taught in the course.

students do not merely memorise isolated facts or procedures but understand the underlying principles that can be applied in novel contexts [24]. For example, understanding the concept of fluid dynamics in one scenario (airflow over a wing) allows students to apply similar principles in different scenarios (fluid flow in pipelines) [45]. Furthermore, the LCT does not merely advocate for anchoring abstract mathematical equations to practical engineering applications—that constitutes just a one-way movement along the SG axis; instead, LCT advocates for students to be able to engage in a two-way movement across both axes to develop holistic competence that is rooted in a deep understanding of underpinning concepts [24, 46]. Therefore, the LCT is a robust theoretical basis or framework that can inform the design and delivery of DSBL activities.

In the context of this course—reaction engineering content delivered to first-year undergraduate chemical engineering students—the semantic plane that the educator seeks to address is illustrated in Figure 1. The introduction of underpinning theoretical concepts can be done qualitatively (upper left quadrant, Figure 1) followed by the derivation of reactor performance equations (upper right quadrant, Figure 1). Although this translation scales the SD axis, the concepts are still abstract (SG−). The common approach to address this issue is the coupling to applications through numerical problem solving. However, as stated earlier, this is only a partial solution as students can end up treating an engineering problem as a purely mathematical equation to solve, in which case they would fail to appreciate the engineering context and nuances. In terms of the LCT, this would represent inadequate 'shifting' across the semantic plane, which has ramifications on students being able to meet the 'apply' cognitive level as stipulated in the module LOs.

Although lab practical sessions help enhance the movement towards SG+, as also addressed through the CSTR lab component in this course (LO3), such lab-based activities have several limitations. Firstly, lab sessions are usually a one-off opportunity in the course for students to engage with a 'concrete' application. They also tend to be rigid and highly prescriptive, for example, the reaction being investigated and reaction conditions are usually fixed by the instructor, especially for first-year undergraduate students. However, digital simulations do not suffer from any of these shortcomings. They can be student-led, run as many times as a student likes to, and allows varying variables and parameters that might not be possible in a physical lab environment. Simulation models can also inform design of questions that span the SD axis. Hence, a DSBL learning activity was designed to enable students to 'shift' across all quadrants of the semantic plane (Figure 1). Thereby, the DSBL approach was adopted not only for students to fully appreciate the context of reactor performance equations, but also to iterate between theory and equations to simulation results. The DSBL activity can also incrementally increase the level of difficulty, starting from investigating the effect of a single parameter or variable on reactor conversion (lower left quadrant, Figure 1), subsequently moving to studying effects of multiple variables and comparison of different reactors (lower right quadrant, Figure 1).

4 | DSBL Activity Design

In line with the teaching philosophy for the rest of the course, the DSBL activity was designed through a PBL approach. This was done to harness the advantages that PBL offers in a DSBL setting. The questions were designed with dual objectives of (i) providing appropriate scaffolding for the DSBL activity through PBL and (ii) enable students to iteratively traverse the SG and semantic density axes. The specific questions designed for each of the three ideal reactors and the rationale behind how these questions are formulated to facilitate shifting across the semantic plane are detailed below, starting with the batch reactor. The interactive simulations can be accessed from https://reactorlab.net/.

4.1 | Batch Reactor

Five questions were designed for the simulation based on the batch reactor (Figure 2):

Q1. What is the conversion of the reaction achieved in the batch reactor with the default parameter values as follows: Temperature = 300 K, reactant concentration = 10 mol/m^3, volume = 100 m^3, reaction time = 100 s, activation energy (Ea) = 60 kJ/mol, reaction order (n) = 1, rate constant (k) = 0.01?

Q2. Next, you perform the same reaction under the same conditions but in a bigger batch reactor of volume 200 m^3. What is the conversion of the reaction achieved after 100 s in this bigger reactor? How does it compare to the conversion you got in the previous question? Can you reason your findings?

Q3. Let us go back to using a batch reactor of volume 100 m^3. We are now interested in determining the evolution of the reaction over time. What is the conversion of the reaction in this batch reactor after 100, 200, and 300 s? What is the trend you observe of conversion versus time? Can you reason why this trend is observed?

Q4. We are currently working with a first order reaction. Hence, what will the units of rate constant 'k' be? What is the conversion of the reaction when $k = 0.02$ and $k = 0.03$? How does this compare to the case of $k = 0.01$? How do these three conversion values compare to the values you got in Q3 earlier? Can you explain the similarities in values?

Q5. The next task is to compare the conversion achieved in the batch reactor for a first-order reaction with that of a second-order reaction. For the same reactor volume and the other conditions remaining unchanged, what is the conversion for a 2nd order reaction? Is it lower or higher than what was achieved for a 1st order reaction? Can you explain why?

As formulated, Q1 starts in the bottom left quadrant of the semantic plane (Node A: SD−, SG+), asking students to merely input parameter values and check the reported conversion value (Figure 2). It is a simple task (SD−) performed on a virtual reactor without reference to abstract reaction engineering concepts (SG+). For Q2, students would need to re-run the simulation for a bigger batch reactor and subsequently engage

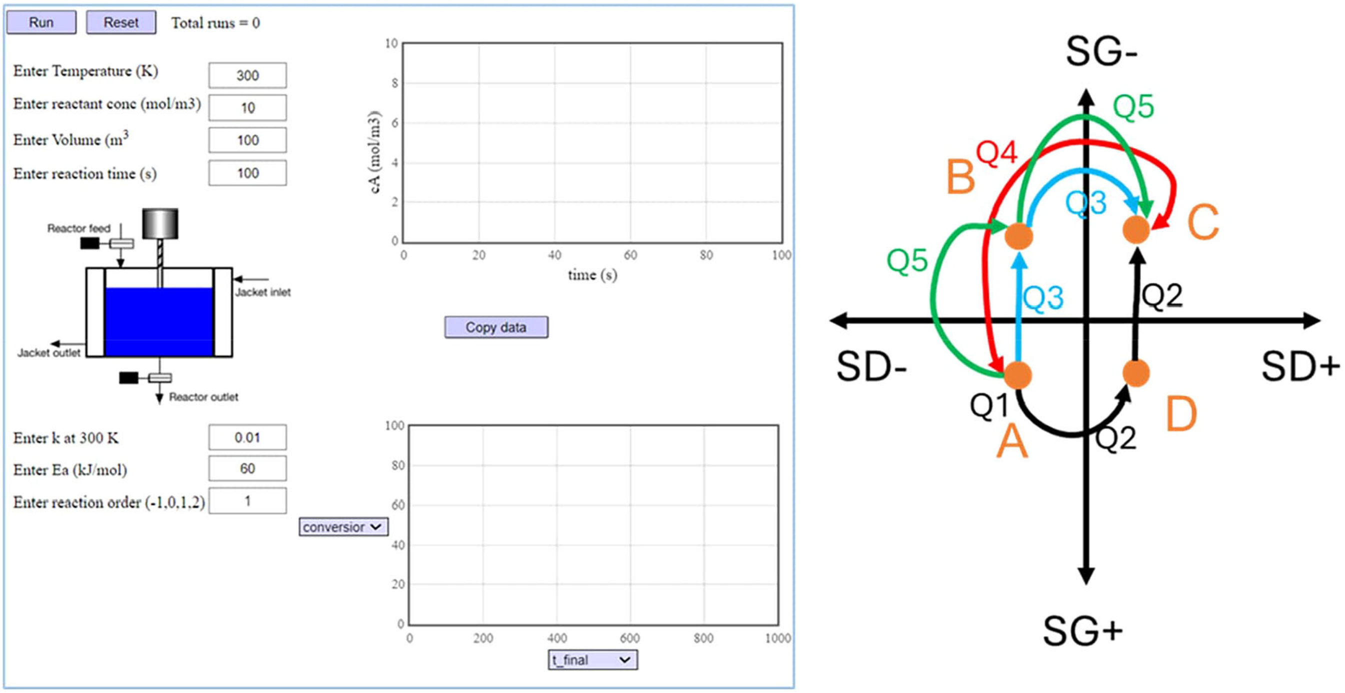

FIGURE 2 | Left: The user interface for batch reactor simulator (https://reactorlab.net/web_labs/web_lab_13/index.html). Right: Mapping of question prompts designed for the DSBL learning activity on the semantic plane (SD v/s SG) for the batch reactor simulation.

in a comparative analysis with Q1, inducing a degree of complexity (Node D: SD+ , SG+), that requires coupling the simulation results to the underpinning mathematical performance equation of the batch reactor (Node C: SD+ , SG−). Likewise for Q3, students again go from a well-defined simulation input (Node A: SD−, SG+) to interpreting the simulation output qualitatively (Node B: SD−, SG−), then to reasoning the trend through the performance equation (Node C: SD+, SG−) (Figure 2). Unlike the earlier questions, Q4 asks students to start from the abstract (SG−)—units of rate constant need to be derived from the general rate law expression—then move towards examining the effect of increasing the value of the rate constant on conversion (Node A: SD−, SG+), followed by a comparative analysis that requires reasoning through the performance equation (Node C: SD+, SG−). Lastly, Q5 examines the effect of reaction order on conversion, which after the simulation is run (Node A: SD−, SG+), allows students to interpret the findings qualitatively (Node B: SD−, SG−) and quantitatively (Node C: SD+, SG−). Hence, the coupling of PBL and DSBL should enable multiple rounds of shifting across the semantic plane (Figure 2).

4.2 | Continuous Stirred Tank Reactor

Three questions were designed for the simulation based on the CSTR (Figure 3):

Q6. Input the following default parameter values for the CSTR simulation (temperature = 300 K, reactant concentration = 10 mol/m^3, volume = 100 m^3, flow rate = 100 m^3/s, Ea = 60 kJ/mol, $n = 1$, $k = 0.01$). Based on the given data, what is the value of space time τ in seconds? What is the conversion achieved in the CSTR under these conditions?

Q7. You perform the same reaction but in a smaller CSTR of volume 50 m^3. What is the conversion achieved now? How does it compare to the conversion you got in Q6? Can you reason your findings? Also, how are the findings different to Q2, where you investigated the effect of batch reactor volume on conversion?

Q8. Go back to using the CSTR of volume 100 m^3. How does the CSTR conversion change when volumetric flow rate is changed from 1 to 2 m^3/s? How does this conversion compare to Q7? Can you reason the similarity in conversion values?

As was the case with the simulation on the batch reactor, the activity on the CSTR begins with a standard question (Q6) on computing conversion based on a set of reaction parameters (Node E: SD−, SG+). In addition, the simulator also returns the value of the space time, which the students can easily calculate as the ratio of the reactor volume to the volumetric flow rate (Node F: SD−, SG−) (Figure 3). Q7 is formulated to address two aspects: the effect of CSTR volume on conversion is firstly interpreted through the corresponding performance equation and then the comparison to changing reactor volume in the case of the batch reactor. The former elicits interpretation of results through the underpinning mathematical equation (SG+ to SG−) while the latter increases complexity in terms of having to contrast space time with batch time (SD− to SD+). As a whole, Q7 should facilitate multiple code shifts starting from the simple concrete through to the complex concrete (Figure 3). Q8 again addresses the effect of space time on conversion but through changing volumetric flow rate (Nodes F to G). This is further intended to help students understand the physical manifestations of space time, which can otherwise be conceived as an abstract concept (Figure 3).

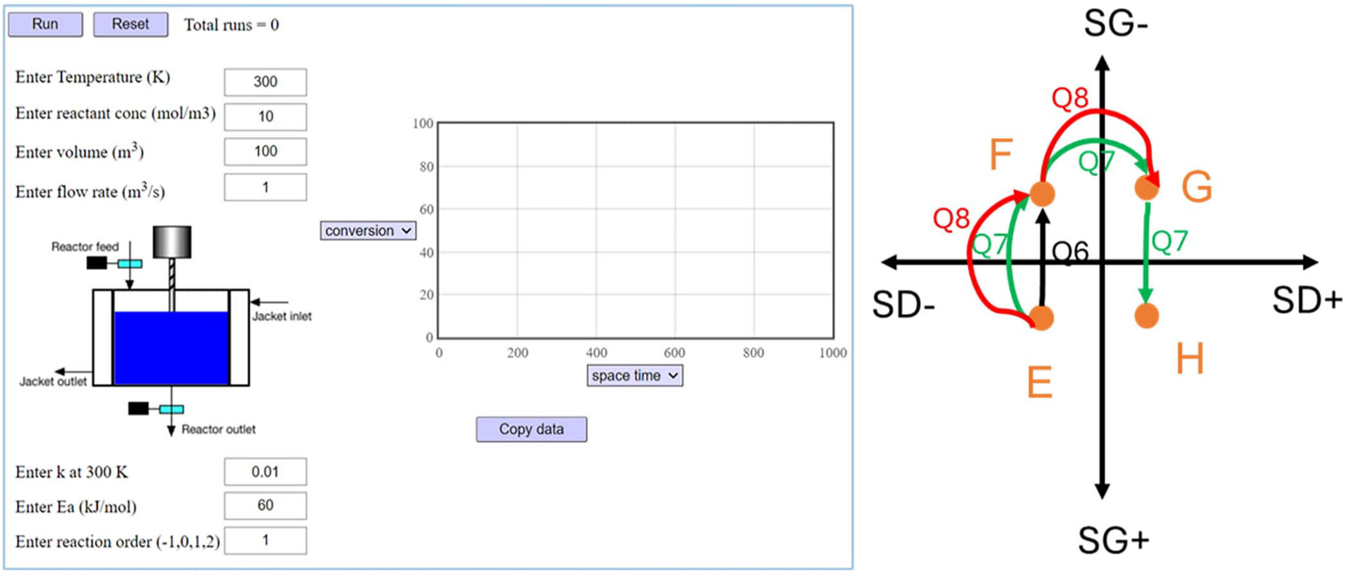

FIGURE 3 | Left: The user interface for CSTR simulator (https://reactorlab.net/web_labs/web_lab_14/index.html). Right: Mapping of question prompts designed for the DSBL learning activity on the semantic plane (SD v/s SG) for the CSTR simulation.

4.3 | Plug Flow Reactor (PFR)

Three questions were designed for the simulation based on the PFR (Figure 4):

Q9. When using the same default reaction conditions as we used for the CSTR (see Q6), what final conversion is achieved for the same reaction in a PFR? Is the conversion higher or lower than that obtained in a CSTR? Why is it so? Can you explain this through a graphical representation of the performance equation of a CSTR and PFR?

Q10. For the same reaction, compute the size of the PFR (or reactor volume) needed to get the same conversion as you got with the 100 m^3 CSTR in Q6.

Q11. Evaluate the impact of initial reactant concentration on the final conversion achieved in a PFR for a 1st order and 2nd order reaction. First, consider the case of a 1st order reaction. How does the final conversion change when initial concentration is halved from 10 to 5 mol/m^3? Next, repeat the same thing for a 2nd order reaction: how does the final conversion change when initial concentration is halved from 10 to 5 mol/m^3? How are the findings different from what you observed in the case of 1st order reaction?

Q9 asks students to compute conversion in a PFR for the identical reaction conditions as used for the CSTR in Q6. This allows for comparison of reactor performance in terms of the performance equation and the classical Levenspiel plot (SG−, Figure 4). Q10 helps demonstrate the smaller PFR volume required to achieve the same conversion as that of the CSTR for a positive order reaction. For this question, calculating the PFR volume via the simulation interface requires a trial-and-error methodology (Nodes I to L). Finally, Q11 builds in a layer of complexity to the PFR simulation by investigating the combined effects of initial reactant concentration and reaction order (Figure 4). Interpretation of the results requires students to diligently apply the performance equation in each case to realise that fractional conversion is independent of initial concentration only for a first-order reaction but not for a second-order reaction (Nodes I to K).

The mapping of the questions to the LCT semantic plane (Figure 5) ensures coverage across all quadrants and illustrates the shifts that students should ideally undertake when engaging in the DSBL activity. However, Figure 5 is only the ideal blueprint of semantic plane movement as envisioned by the instructor. We proceed to investigate how students perceive engagement on the activity and its impact on their learning.

5 | Student Reflections

Student feedback on the DSBL activity is very positive (Table 2). Even without adopting any gamification strategies, 75% of the survey respondents state the activity to have been enjoyable. The activity received even more positive feedback for its impact on enhancing understanding of reaction engineering concepts. An overwhelming 97% of the students either 'agreed' or 'strongly agreed' to the activity improving their understanding of ideal reactors and that the activity helped reinforce the reaction engineering knowledge they had acquired thus far (Table 2). The strong student opinion in favour of the DSBL session 'reinforcing' knowledge is the first indicator of students having successfully moved around the semantic plane bringing together theory and application. Likewise, coupling PBL to DSBL was successful in engaging students in critical thinking—with 97% of the students again being in agreement to the equivalent statement (Table 2). The DSBL activity also had a positive impact on student self-efficacy with 91% of the students reporting feeling more confident in their understanding of reaction engineering fundamentals after the session. There was also a broader appeal among students of wanting to have more such sessions in their programme of study (Table 2).

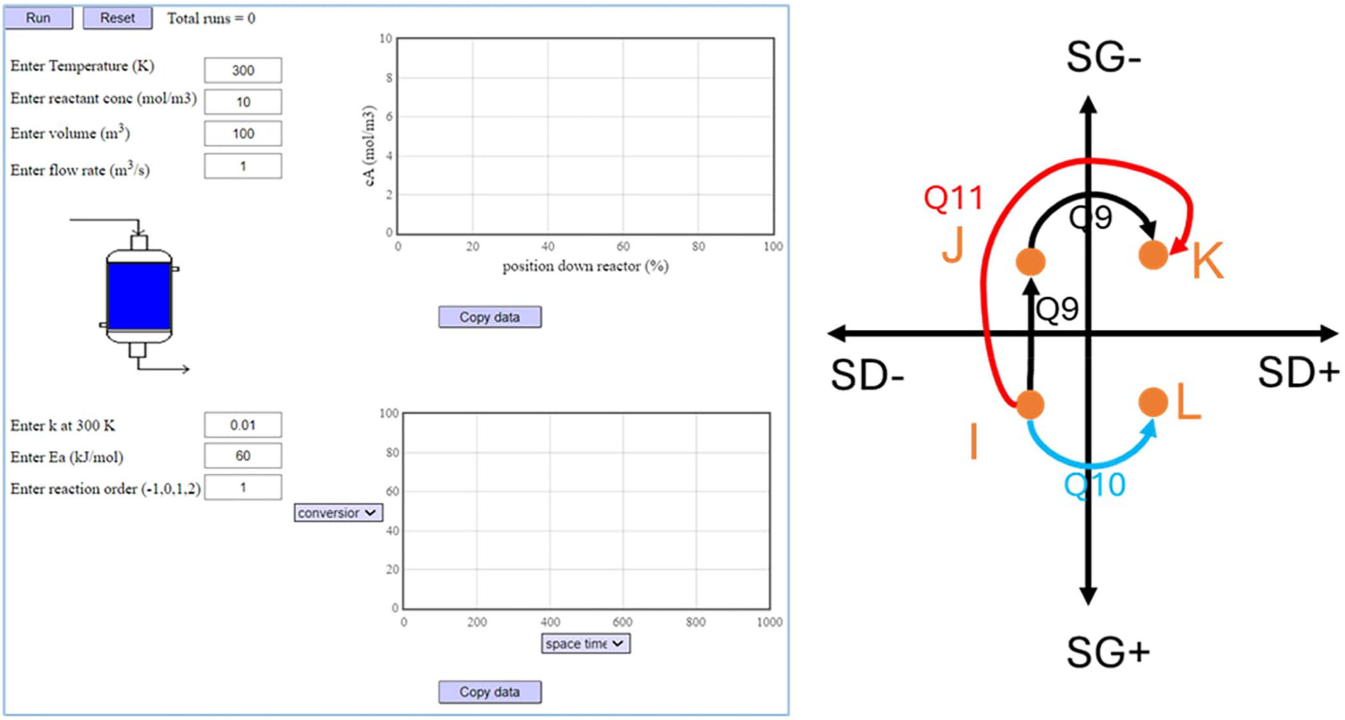

FIGURE 4 | Left: The user interface for PFR simulator (https://reactorlab.net/web_labs/web_lab_15/index.html). Right: Mapping of question prompts designed for the DSBL learning activity on the semantic plane (SD v/s SG) for the PFR simulation.

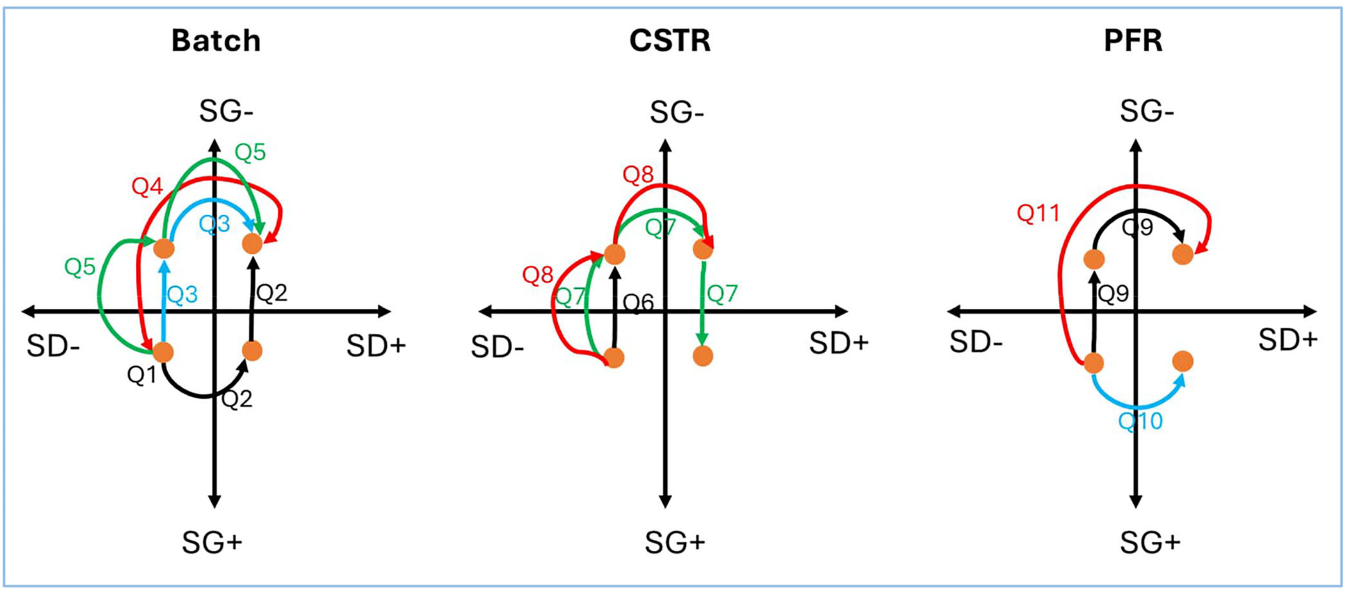

FIGURE 5 | Mapping of question prompts designed for the DSBL learning activity on the semantic plane (SD v/s SG). Q1 to Q5 are on the batch reactor, Q6 to Q8 on the CSTR, and Q9 to Q11 on the PFR.

Although the Likert scale questions are a good instrument to gauge the overall success of the DSBL approach on student learning, it only provides a high-level perspective that is insufficient to investigate the exact ways in which the activity enhanced student understanding. Hence, students were asked to articulate the impact of the DSBL session on their learning by reflecting on how the activity was useful to them, which fosters reflective thinking and metacognition. RTA of the qualitative data was undertaken by the author to develop a thematic map of student reflections (Figure 6). The coding of student comments resulted in two key themes: (i) the activity enabled a deeper understanding of reaction engineering and (ii) the learner-led nature of the activity triggered a greater sense of student ownership that enhanced learning (Table 3 and rectangles in Figure 6).

These two themes were drawn from several sub-themes (ovals in Figure 6) identified in the student comments; starting with the theme of the 'learner-led' approach, students opined that learner independency, interactivity and the participatory nature

TABLE 2 | Student responses to Likert-scale survey questions ($n = 32$).

Statement	Strongly agree (%)	Agree (%)	Neutral (%)	Disagree + strongly disagree (%)
How much fun was the activity?	44	31	25	0
This session has improved my understanding of ideal reactors	56	41	3	0
This session helped in reinforcing the reaction engineering knowledge that I have acquired so far	53	44	3	0
The questions we worked through helped in critical analysis of simulation results	63	34	3	0
I am more confident of my reaction engineering fundamentals after this session	47	44	9	0
I would like to have more such sessions in the programme	53	38	6	3

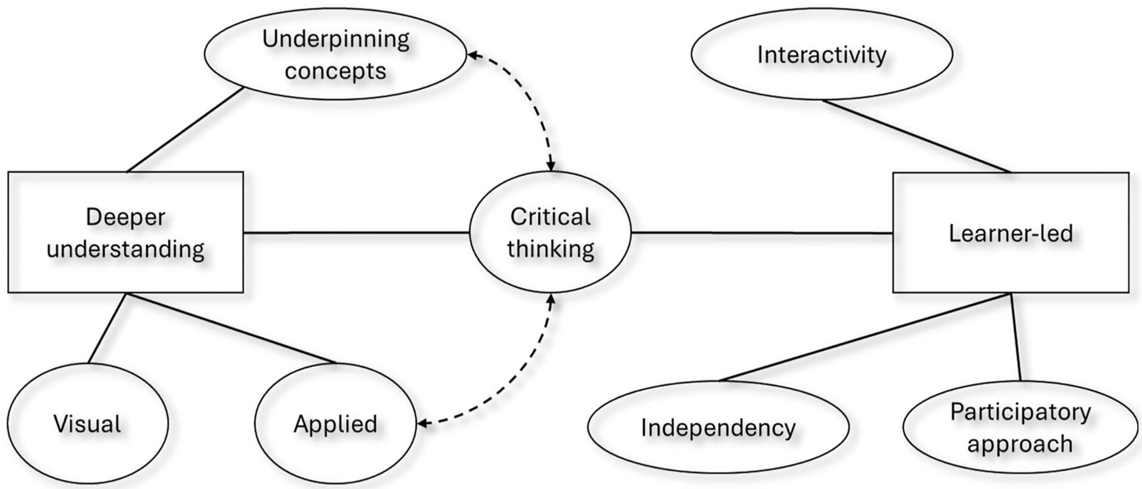

FIGURE 6 | Thematic map of student reflections. Main themes are shown as rectangles and sub-themes as ovals. Relationships between themes and sub-themes are shown with a solid line. The dotted line highlights the transition in the semantic plane mediated through critical thinking.

of the exercise was particularly useful (see Table 3 for exemplar student quotes).

These findings are consistent with the wider pedagogical literature on how students are more likely to engage in active learning if the learning activity is designed to be interactive and participatory [47, 48]. Furthermore, structuring the DSBL activity with a series of prompts/questions (PBL) forces students to engage in critical thinking associated with problem solving. This is vital for students to evaluate the results output by the simulation software and not merely take them at face value.

> *way of asking questions made me think critically and understand every reason behind every number*

> *People came up with their ideas and various ideas made the lecture active.*

Hence, the intertwining of an interactive, participatory approach with critical analysis of simulation results helps address the dual objectives of student engagement and student attainment. This is further strengthened by the connections between critical thinking and the other sub-themes that constitute the 'Deeper understanding' theme. Several student respondents suggested that the 'visual explanation' offered through the DSBL activity helped them 'understand the concept even further'. Importantly, the multiple student comments referring to the 'visual' mode of learning with respect to their metacognition should not be perceived as conflicting the large body of work that has debunked the idea of 'learning styles' [49, 50]. As mentioned in the activity design, the purpose of the activity was not to cater to different 'learning styles' but to use DSBL as a tool to empower students to move across the semantic plane. Thereby, the DSBL activity facilitates a more holistic learning experience for students, particularly helping them make the transition from abstract mathematical reactor performance equations (SG−) to visual reactor effects (SG+) (Table 3).

Further evidence of students having traversed the SG axis during the DSBL activity is surfaced through the two sub-themes: 'underpinning concepts' and 'applied'. The two-way reversible connection between these two sub-themes is facilitated through 'critical thinking' (Figure 6). The 'underpinning concepts' here primarily refer to the reactor performance equations, which can come across as very 'abstract' (SG−) when first introduced to students and the simulation environment presents in a more

TABLE 3 | Summary of themes and sub-themes identified in reflexive thematic analysis with exemplar quotes.

Theme	Sub-theme	Exemplar quote
Learner-led approach	Independency	*“Helpful to be involved and do it ourselves sometimes”*
	Interactivity	*“Interactive work feels easier to understand than just having a normal lecture”*
	Participatory approach	*“encourages everyone participate and this is something that I truly believe that it was helpful”*
Deeper understanding	Critical thinking	*“way of asking questions made me think critically and understand every reason behind every number”*
	Visual	*“I found the reactors part was confusing a bit while studying. but learning in visual way made me understand it better than just trying to imagine it in my head.”*
	Applied	*“It was useful to apply our learning of different reactor types using a simulation and then going through the mathematical meaning behind it.”*
	Underpinning concepts	*“Allowed me to grasp the effect of different variables in terms of the performance equations.”*

‘applied’ form (SG+). Student comments reveal the success of the DSBL approach in facilitating a two-way movement along the SG axis:

> *It was good to the links between the performance equations and real-life changes to the reactors*

> *It was useful to apply our learning of different reactor types using a simulation and then going through the mathematical meaning behind it.*

In the student quotes above, the former represents a movement from SG− (performance equations) to SG+ (real-life changes to the reactors), while the latter comment goes from application (SG+) to the underpinning mathematical equations (SG−). This two-way movement across the SG axis is vital to improving student ability to toggle between the two viewpoints as required. The PBL approach asks students to solve the question or develop an intuition of the answer/trend before engaging with the simulation (SG− to SG+) and once the simulation results are available, the interpretation of the results needs to be done through underpinning concepts, both qualitatively (SD−, SG−) and quantitatively through performance equations (SD+, SG−). And movement in both directions along the SG axis—be it attempting to problem solve or interpret the simulation output—necessitates critical thinking. In terms of semantic density, one aspect of complexity, as mentioned above, was connecting simple qualitative analysis with the more rigorous quantitative calculations. In addition to this, the other layer of complexity built into this DSBL activity was comparative analysis between reactor types (e.g., Q7) and multiple variables in the performance equation (e.g., Q11). This translation across the SD axis is again represented by the ‘deeper understanding’ block in the thematic map, and more explicitly evident in the following student reflections:

> *It gave detail into the reasons for differences in conversion and why certain factors have an effect and others don't.*

> *Allowed me to grasp the effect of different variables in terms of the performance equations.*

Lastly, students also state that the DSBL activity provided a holistic and rounded finish to the reaction engineering teaching. The session is perceived to be ‘synoptic’ in nature [51], where students are challenged to pull together all the concepts taught on the course thus far to critically engage with the computer simulation. Consequently, from a metacognition lens, they see this as a ‘convergence’ of taught knowledge with the activity being an opportunity to ‘summarise’ and ‘recap’ these concepts:

> *The convergence of all 5 weeks knowledge of reaction engineering in 1 particular set of questions.*

> *Good for summarising a lot of what we have been over in lectures.*

> *I can recap the performance equations I have learnt throughout the course.*

6 | Conclusions

The use of DSBL to enhance the educational experience of first-year undergraduate chemical engineering students learning fundamental concepts of reaction engineering was investigated herein. The DSBL activity designed was grounded in a robust pedagogical framework, leveraging LCT to facilitate semantic shifts across the axes of SG and semantic density. This approach enabled students to move between abstract theoretical concepts and concrete applications of varying complexity, fostering a deeper understanding of reaction engineering principles. The findings indicate that students not only enjoyed the DSBL activity but also reported significant improvements in their understanding and confidence of reaction engineering concepts. This aligns with the first research question, demonstrating that the design of DSBL activities can indeed be informed by and integrated with learning theories to enhance educational outcomes.

Furthermore, the analysis of student reflections revealed that the DSBL activity promoted critical thinking and problem-solving skills, as students engaged in iterative code shifting across the semantic plane that required them to apply theoretical knowledge to practical scenarios. As communicated by students, the two-way movement between 'underpinning concepts' and 'application' was facilitated through 'critical thinking', which is consistent with the instructor's expectations during the design of the DSBL activity informed by LCT. Although students are not explicitly made aware of the LCT or its use in activity design, engaging them in metacognition helps verify the alignment of students' self-articulated competency improvement to integration of learning theories for DSBL activity design.

Although the DSBL activity described herein was used as a synthesis activity towards the end of the teaching section on reaction engineering, it would also be of interest to examine the value of embedding DSBL as part of the main teaching approach (coupled to PBL) when each of the reactors are introduced sequentially. In such a case, the synthesis activity could take a different form of DSBL where the emphasis is more on comparative and systems thinking. This could help surface the similarities and differences in terms of shifts accomplished by students across the semantic plane when DSBL is used more than once.

Despite the promising findings, the limitations of the study must not be overlooked. The sample size was relatively small (32 students), and the study was conducted within a single institution, which may limit the generalisability of the results. Although LCT was an elegant fit for this study, its selection was not compared against other alternatives. Exploring the integration of DSBL with other learning theories and pedagogical frameworks could also yield valuable insights into optimising the student learning experience. Additionally, while the study focused on student perceptions and self-reported data, future research could incorporate more formal measures of learning outcomes, such as performance assessments and longitudinal studies, to provide a more comprehensive evaluation of DSBL's effectiveness and integration with learning theories. These limitations notwithstanding, this paper presented a successful case study that bridges the research and implementation gap of grounding DSBL activity design in learning theory and corroborating the beneficial effect of the same through student metacognition.

Conflicts of Interest

The author declares no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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