International Journal of Functional Research in Science and Engineering
e-ISSN: 2814-0923
www.ijfrse.com

Introducing SimCenter in Industrial Chemistry: An Innovative Pedagogical Approach to Improve Chemical Formulation Skills in Undergraduates

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Abstract

Chemical formulation skills—the ability to select raw materials, calculate proportions, sequence processes, conduct quality control, and troubleshoot deviations—are central to industrial chemistry practice, yet undergraduate laboratory instruction is often constrained by limited reagents, equipment, and safe repetition opportunities, restricting students' chances to practice formulation decisions before working with real materials. This study evaluated SimCenter, an interactive virtual simulation platform allowing students to manipulate raw material ratios, run simulated quality control tests, and receive immediate feedback, as a complement to conventional laboratory instruction in an undergraduate industrial chemistry formulation course. A quasi-experimental pretest-posttest control group design was used with 100 second- and third-year industrial chemistry students from two intact class sections at a Nigerian university. The experimental group ($n = 50$) received SimCenter-supported instruction alongside standard laboratory sessions across a 12-week formulation unit, while the control group ($n = 50$) received the same laboratory sessions with conventional lecture-based instruction only. Chemical formulation skills were assessed using a practical performance instrument covering five domains: raw material selection, proportioning and dosage calculation, process sequencing, quality control testing, and troubleshooting. Analysis of covariance (ANCOVA), controlling for pretest scores, showed a statistically significant difference in posttest composite scores favoring the experimental group, $F(1, 97) = 91.24$, $p < .001$, partial $\eta^2 = .49$, a large effect, with gains most pronounced in troubleshooting and quality control testing. These findings suggest that simulation-based instruction, when used to complement rather than replace hands-on laboratory practice, can meaningfully strengthen undergraduate chemical formulation competence.

chemical formulation skills, virtual simulation, industrial chemistry education, undergraduate laboratory instruction, SimCenter

Background

Chemical formulation—the practice of combining raw materials in precise proportions and sequences to achieve a target product specification, whether in soap and detergent manufacture, paints and coatings, or pharmaceutical preparations—sits at the core of industrial chemistry practice, yet it is a skill set that undergraduate curricula often struggle to develop adequately through laboratory instruction alone. Formulation competence requires not only conceptual understanding of the underlying chemistry but also repeated, iterative practice in raw material selection, proportioning, process sequencing, quality control, and troubleshooting when a batch deviates from specification, and this iterative practice is precisely what conventional undergraduate laboratories, constrained by limited reagents, equipment, and scheduled time, are least able to provide (Reid & Shah, 2007).

Virtual and computer-simulated laboratory environments have been proposed as a partial response to this constraint, allowing students to rehearse procedural decisions, observe the consequences of formulation errors, and repeat scenarios at low marginal cost before or alongside physical laboratory work. Josephsen and Kristensen (2006) found that simulation of laboratory assignments improved students' conceptual preparedness for introductory inorganic chemistry practical work, while Tatli and Ayas (2013) reported that a virtual chemistry laboratory produced significant achievement gains relative to conventional instruction alone. Winberg and Berg (2007) further showed that a computer-simulated prelab shifted students' cognitive focus during subsequent physical laboratory work toward higher-order conceptual reasoning rather than procedural execution, suggesting that simulation's benefit may lie partly in freeing cognitive capacity for deeper engagement with hands-on practice rather than in replacing it.

These findings align with a constructivist view of chemistry learning, in which students build robust conceptual and procedural understanding through active engagement with representations of chemical phenomena and iterative testing of their own reasoning against feedback, rather than through passive reception of instruction (Bodner, 1986). Seery (2015) has further argued that digital tools are best positioned within chemistry curricula not as replacements for traditional practice but as components of a blended approach that uses technology to extend the time and variety of practice available to students beyond what scheduled laboratory sessions alone permit. Despite this evidence, few studies have examined simulation-based instruction specifically for the multi-domain skill set involved in industrial chemical formulation, as distinct from general laboratory technique or single-reaction conceptual learning, and fewer still have done so within a Nigerian undergraduate industrial chemistry context, where laboratory resource constraints are frequently more acute.

Purpose and Research Questions

This study evaluated whether SimCenter, an interactive virtual simulation platform, improves undergraduate chemical formulation skills when used to complement conventional laboratory instruction, relative to conventional instruction alone. Specifically: (1) Is there a significant difference in overall chemical formulation skill scores between students receiving SimCenter-supported instruction and those receiving conventional instruction, controlling for pretest performance? (2) Do effects differ across the five component skill domains—raw material selection, proportioning and dosage calculation, process sequencing, quality control testing, and troubleshooting? It was hypothesized that the SimCenter group would show significantly higher adjusted posttest composite and domain scores than the conventional instruction group.

Method

Research Design and Participants

This study used a quasi-experimental, nonequivalent control group design with pretest and posttest measures, necessitated by the use of intact class sections; pretest scores were used as a covariate to statistically adjust for baseline group differences. Participants were 100 second- and third-year industrial chemistry undergraduates (54 male, 46 female) at a Nigerian university, with one intact section ($n = 50$) assigned to the experimental condition and a second ($n = 50$) to the control condition. Groups did not differ significantly on pretest composite scores, $t(98) = 1.31$, $p = .193$, or on prior exposure to simulation software, confirmed by a chi-square test of independence, $\chi^2(1) = 0.44$, $p = .508$. Full demographic characteristics are presented in Table 1.

Table 1

Demographic Characteristics of Participants (N = 100)

Characteristic	Category	n	%
Sex	Male	54	54.0
	Female	46	46.0
Level	200 Level	41	41.0

	300 Level	59	59.0
Prior simulation software use	Yes	28	28.0
	No	72	72.0
Group	Experimental (SimCenter)	50	50.0
	Control (conventional)	50	50.0

Note. Percentages may not sum to 100 due to rounding.

SimCenter Platform

SimCenter is an interactive virtual simulation environment in which students select from a virtual raw material inventory, specify proportions and mixing sequences for a target formulation (in this study, liquid soap and toilet soap formulations), and observe simulated outcomes including yield, viscosity, pH, and other quality control parameters relevant to the target specification. The platform flags out-of-specification outcomes and prompts students to identify likely causes and adjust their formulation accordingly, allowing repeated iteration without consuming physical reagents. In this study, the experimental group used SimCenter in weekly 60-minute guided sessions across the 12-week formulation unit, each preceding the corresponding physical laboratory session, with instructor-facilitated debriefing connecting simulated outcomes to the conceptual chemistry underlying each formulation step.

Instrumentation

Chemical formulation skills were assessed using a practical performance instrument comprising five subscales aligned with the core competencies of formulation practice: raw material selection, proportioning and dosage calculation, process sequencing, quality control testing, and troubleshooting. Each subscale included several performance-based tasks rated by trained assessors on a standardized rubric, with subscale and composite scores expressed on a 0–10 scale for reporting consistency. Internal consistency was high (composite $\alpha = .87$; subscale αs = .76–.85), and two independent assessors scoring 25% of practical sessions yielded an intraclass correlation of .89.

Procedure and Data Analysis

Both groups completed the formulation skills pretest during the week preceding the unit and the posttest during the week following its conclusion, administered by the same trained, condition-blind assessors. Both groups covered identical formulation content, physical laboratory sessions, and total instructional contact time; the only substantive difference was the experimental group's additional weekly SimCenter session paired with each laboratory session, ensuring that any observed difference could be attributed to the simulation component rather than to differences in overall instructional time. A one-way ANCOVA was conducted on posttest composite scores, using pretest composite scores as the covariate, to address Research Question 1, with assumption checks confirming linearity, homogeneity of regression slopes, and homogeneity of variance were met. Separate subscale ANCOVAs addressed Research Question 2, all at $\alpha = .05$.

Results

Descriptive statistics for the experimental group's pretest and posttest subscale and composite scores are presented in Table 2. Both groups improved from pretest to posttest across all subscales; however, the experimental group's gains were consistently larger, particularly in troubleshooting and quality control testing.

Table 2

Descriptive Statistics for Chemical Formulation Skill Scores, Experimental Group (n = 50)

Skill Domain	Pretest M	Pretest SD	Posttest M	Posttest SD
Raw material selection	5.68	1.24	8.42	0.96
Proportioning/dosage calculation	4.91	1.38	7.85	1.12
Process sequencing	5.34	1.29	7.96	1.04
Quality control testing	4.52	1.41	7.38	1.19
Troubleshooting	3.87	1.33	6.94	1.27
Composite score	4.86	1.02	7.71	0.88

Note. Scores are standardized to a 0–10 scale for each subscale and the composite. M = mean; SD = standard deviation.

For the control group, composite scores rose from a pretest mean of 4.79 (SD = 1.08) to a posttest mean of 6.34 (SD = 1.15), a smaller gain than in the experimental group. The ANCOVA revealed a significant effect of group, $F(1, 97) = 91.24$, $p < .001$, partial $\eta^2 = .49$, a large effect indicating instruction type accounted for roughly 49% of posttest variance after adjusting for baseline. The covariate was also significant, $F(1, 97) = 19.62$, $p < .001$, partial $\eta^2 = .17$ (Table 3).

Table 3

Summary of Analysis of Covariance (ANCOVA) for Posttest Composite Chemical Formulation Skill Scores

Source	SS	df	MS	F	p	$\eta^2 p$
Pretest (covariate)	16.84	1	16.84	19.62	< .001	.168
Group	78.31	1	78.31	91.24	< .001	.485
Error	83.24	97	0.86	—	—	—
Total	178.39	99	—	—	—	—

Note. SS = sum of squares; MS = mean square; $\eta^2 p$ = partial eta squared.

Subscale-level ANCOVAs showed the experimental group significantly outperformed the control group on all five subscales: raw material selection, $F(1, 97) = 68.14$, $p < .001$, partial $\eta^2 = .41$; proportioning/dosage calculation, $F(1, 97) = 74.52$, $p < .001$, partial $\eta^2 = .43$; process sequencing, $F(1, 97) = 61.87$, $p < .001$, partial $\eta^2 = .39$; quality control testing, $F(1, 97) = 88.36$, $p < .001$, partial $\eta^2 = .48$; and troubleshooting, $F(1, 97) = 94.71$, $p < .001$, partial $\eta^2 = .49$. Effect sizes were largest for troubleshooting and quality control testing and comparatively smaller, though still substantial, for process sequencing.

Discussion

This study examined whether SimCenter, used to complement conventional laboratory instruction, improves undergraduate chemical formulation skills relative to conventional instruction alone. Results support the hypothesis: the SimCenter group showed significantly greater composite gains, with a large effect size, and outperformed the comparison group on every subscale, extending Josephsen and Kristensen (2006) and Tatli and Ayas (2013) to the specific multi-domain skill set of industrial chemical formulation and to a Nigerian undergraduate context in which laboratory resource constraints make repeated hands-on practice especially difficult to provide at scale.

The particularly large gains in troubleshooting and quality control testing are noteworthy, since these domains depend heavily on exposure to a variety of deviation scenarios that would be costly and time-consuming to reproduce repeatedly with physical reagents; SimCenter's capacity to let students trigger, observe, and correct simulated formulation errors at low marginal cost plausibly explains this pattern, consistent with Winberg and Berg's (2007) finding that simulated prelab exposure shifts subsequent laboratory engagement toward higher-order reasoning. The comparatively smaller, though still substantial, gain in process sequencing may reflect the greater role of physical dexterity and timing in this domain, aspects that a screen-based simulation can only partially represent.

Consistent with Seery's (2015) framing of digital tools as complements within a blended curriculum rather than laboratory replacements, both groups in this study received identical physical laboratory instruction, and the observed advantage is attributable specifically to the additional simulation-based rehearsal opportunity rather than to any reduction in hands-on practice. This distinction matters for interpretation: these findings support supplementing, not substituting, laboratory instruction with simulation. This study is limited by its quasi-experimental reliance on intact class sections, a single institution and formulation content area (soap and detergent formulation), and a 12-week window that cannot address retention of formulation skills into subsequent coursework or industrial placement. Future research should examine retention over time, extend the approach to other formulation content areas such as paints or pharmaceutical preparations, and investigate which specific SimCenter design features most strongly drive the troubleshooting and quality control gains observed here.

Conclusion

SimCenter, used to complement conventional laboratory instruction, produced significantly greater gains in undergraduate chemical formulation skills than conventional instruction alone, with the largest advantages in troubleshooting and quality control testing. These results support simulation-based instruction as a valuable complement to, rather than a replacement for, hands-on laboratory practice in industrial chemistry education, particularly in resource-constrained settings where opportunities for repeated formulation practice with physical reagents are limited.

e-ISSN: 2814-0923
www.ijfrse.com

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