# Integrating Computational Simulation into Advanced Separation Engineering: A Teaching Reform under the Emerging Engineering Paradigm

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**Abstract:** Under the emerging engineering education framework driven by digitalization and low-carbon transformation in the chemical industry, this study presents a systematic teaching reform for Advanced Separation Engineering, a core graduate course. Addressing key challenges: fragmented simulation instruction, disconnection between teaching and research, and limited competency development, the reform establishes a three-dimensional pedagogical framework grounded in constructivist learning theory, outcome-based education (OBE), and industry-university collaboration. A four-dimensional strategy was implemented: (1) restructuring the curriculum into multi-scale modules (molecular, equipment, process); (2) designing a three-stage spiral teaching model integrating foundational training, industrial case practice, and research-oriented projects; (3) building an open, shared simulation platform across campus, research lab, and enterprise; and (4) adopting a diversified, competence-oriented assessment system. Over three academic years (2023-2025), the reform engaged 237 chemical engineering postgraduates. Evaluation data demonstrate significant improvements in students' simulation proficiency, engineering design thinking, and independent research capacity. The proposed model offers strong operability and scalability for graduate engineering education reform.

***Keywords*****:** emerging engineering education, advanced separation engineering, computational simulation, postgraduate teaching reform, multi-scale education

## 1. Introduction

The rapid advancement of the global technological revolution and industrial transformation has accelerated the penetration and deep integration of artificial intelligence, big data analytics, and digital twin technologies into the entire value chain of modern process industries. Against the backdrop of global net-zero carbon commitments and China's "dual carbon" strategic goals, the chemical industry is accelerating its transition toward green manufacturing, low-carbon emission reduction, and high-value-added specialty chemicals, which has drastically reshaped talent demand. The market now requires high-level interdisciplinary chemical engineering talents who master both traditional core expertise and cutting-edge digital simulation and intelligent optimization capabilities, and this demand has grown far more rapidly than expected. Consequently, higher engineering education in China is undergoing profound structural adjustments and conceptual updates. The Guidelines for Research and Practice of Emerging Engineering Education Projects issued by the Ministry of Education clearly puts forward the core direction of talent training that focuses on interdisciplinary integration, practical innovation capabilities, and adaptation to future industrial development needs, which provides clear strategic guidance for postgraduate curriculum reform in the field of chemical engineering[1].

Advanced Separation Engineering is an irreplaceable core compulsory course for postgraduate students majoring in Chemical Engineering and Technology, positioning itself as a key bridge connecting basic theoretical research and cutting-edge industrial applications. The course itself has distinct characteristics of strong theoretical rigor, close connection with technological frontiers, and outstanding engineering practicality. In the past decade, with the exponential growth of computing power and the continuous breakthrough of numerical algorithms, computational simulation technology covering multiple scales from molecular dynamics simulation to full-process system modeling has gradually become the core driving force of innovation in the separation technology field. These multi-scale simulation tools enable researchers to achieve full-coverage holistic analysis from microscopic molecular adsorption and diffusion interactions, to mesoscopic equipment internal fluid dynamics, and to macroscopic full-process energy optimization, completely pushing the research and development of separation technology from the traditional trial-and-error paradigm to the modern simulation-driven intelligent R&D paradigm[2].

In recent years, although most chemical engineering colleges in China have gradually introduced mainstream simulation tools such as Aspen Plus and COMSOL into classroom teaching, the depth and systematicness of integration are still obviously insufficient. In most teaching schemes, simulation training is only arranged as scattered and independent software operation practical lessons, which are often disconnected from the explanation of core theoretical knowledge and students' own scientific research practice. Most simulation exercises still rely on idealized and outdated examples in traditional textbooks, and are rarely effectively connected with the cutting-edge research directions of the faculty's research team and the actual technical bottlenecks of cooperative enterprises[3]. In addition, the traditional course evaluation method still focuses on rote memorization of theoretical knowledge, and ignores the assessment of open-ended creative problem-solving ability, which seriously restricts the cultivation of students' independent scientific research ability and systematic engineering thinking[4]. These common pain points and deficiencies in current teaching fully reflect the urgent need for systematic, theory-guided teaching reform that conforms to the concept of emerging engineering education.

Faced with the above-mentioned multiple prominent contradictions and practical difficulties in conventional teaching implementation, it is urgent to explore a brand-new systematic teaching reform mode which conforms to the core spirit of emerging engineering education, matches the inherent learning law of postgraduate students and makes full use of modern digital simulation technical advantages. Based on this realistic demand, the research team constructs the three-dimensional reform idea of multi-scale integration, research-teaching coordination and competence-oriented cultivation after repeated demonstration and discussion, and launches three-year continuous large-scale practical teaching reform aiming at solving various structural defects of traditional teaching and exploring replicable demonstrative reform path for peer core courses of chemical engineering postgraduate education.

# 2. Theoretical basis and practical deficiencies of traditional teaching

## 2.1 Theoretical foundation for the reform philosophy

The guiding ideology of this teaching reform is based on three mature, widely adopted educational theories: constructivist learning theory, outcome-based education (OBE), and industry-university collaborative education.

Constructivist learning theory posits that effective knowledge acquisition derives from learners' active, autonomous knowledge construction within specific practical contexts, rather than passive teacher-centered indoctrination. Computational simulation tools allow us to construct visual, interactive virtual experimental environments for postgraduate students, transforming abstract separation mechanisms and invisible microscopic mass transfer dynamics into observable simulation outputs and quantitative trends. This framework effectively facilitates deep self-directed learning, providing solid theoretical support for integrating computational simulation with traditional theoretical teaching.

The core tenet of OBE education is to reverse-design course objectives, teaching content, and instructional delivery around the comprehensive capabilities that students are expected to master upon graduation. This reform focuses on cultivating high-order abilities for postgraduate students, including systematic engineering design and independent research innovation, which aligns perfectly with the core design logic of OBE education[5,6].

Industry-university collaborative education emphasizes shared resources and complementary strengths among higher education institutions, research institutes and industrial partners. In this reform, ongoing faculty research projects and real-world industrial optimization cases into daily teaching resources would be integrated. This practice ensures that curriculum content evolves synchronously with cutting-edge industrial technical demands, effectively enhancing the practical relevance and forward-looking nature of postgraduate training[7].

Based on these three theoretical foundations and the core characteristics of the Advanced Separation Engineering curriculum, our research team refined the three-dimensional core connotation of the reform philosophy. (1) Multi-scale integration: This dimension aims to break down the artificial scale barriers that traditionally segregate microscopic, mesoscopic, and macroscopic content in conventional courses. Microscopic molecular simulation tools (e.g., GROMACS, Gaussian), mesoscopic equipment simulation platforms (e.g., COMSOL, Fluent), and macroscopic full-process process simulation software (e.g., Aspen Plus, HYSYS) would be integrated to construct a complete closed-loop teaching chain covering molecular mechanism analysis, equipment performance optimization, and full-process process design. This structure fosters students' holistic, systematic engineering thinking[8]. (2) Research-teaching synergy: a two-way interactive development principle, which transforms faculty frontier research problems into classroom teaching cases, and guides students to apply what they have learned to their own research projects would be implemented. This approach forms a positive, cyclic reinforcement between classroom instruction and academic research. (3) Competence-oriented training: this dimension reverses the long-standing traditional teaching bias that prioritizes rote memorization over practical skill development. Multi-dimensional training objectives centered on three core competencies: simulation proficiency, systematic engineering design capability, and independent research innovation potential would be established. This integrated, three-in-one reform philosophy directly addresses the demand for interdisciplinary innovative talent in the emerging engineering education context, and aligns with the digital, intelligent, and green development trends of the modern separation engineering industry, with clear practical value and contemporary relevance.

### 2.2 Critical limitations of conventional teaching models

While many domestic universities have increasingly recognized the critical value of computational simulation technology as a powerful auxiliary tool for enhancing engineering education quality, a significant gap remains between conventional teaching arrangements and the progressive reform philosophy outlined above. Based on practical investigations and statistical analysis, the key shortcomings in current practice can be categorized into three core aspects.

(1) Fragmented simulation instruction: computational simulation content is typically fragmented and disconnected from the core curriculum. Knowledge related to simulation is often presented as standalone, scattered extracurricular add-ons, rather than being integrated as systematic modules closely aligned with core course teaching objectives. A representative example from our survey of peer institutions illustrates this issue: one domestic university offers an independent elective course focused solely on basic Aspen Plus operation, but this course lacks any substantive connection to the core content of Advanced Separation Engineering. As a result, while students may master basic software operations, they cannot connect these skills to filler structure optimization, internal gas-liquid mass transfer mechanisms, or overall separation efficiency evaluation, leading to fragmented knowledge structures and an incomplete systematic engineering cognitive framework among postgraduate students. This siloed curriculum design is widespread across many domestic institutions and severely hinders the formation of an integrated knowledge system for learners.

(2) Disconnection between teaching and research: the long-standing disconnect between classroom teaching and scientific research remains a prominent unresolved issue. According to pre-reform internal questionnaire data, over 60% of enrolled postgraduate students reported that simulation skills learned in conventional classrooms could not be directly applied to their own dissertation research. On the one hand, most teaching cases in traditional courses are derived from outdated, oversimplified textbook models that are disconnected from real-world research scenarios; on the other hand, faculty's cutting-edge research achievements (such as the development of MOF adsorbent materials and the simulation of novel membrane separation processes) have not been systematically transformed into accessible teaching resources, resulting in a persistent disconnect between teaching and research[9]. While previous scholars have proposed improvement strategies such as introducing practical cases and inviting industrial engineers as guest lecturers, most domestic institutions have not yet established a stable, normalized collaborative operational mechanism[10].

(3) Outdated assessment practices: the outdated and homogeneous curriculum assessment system severely constrains the cultivation of postgraduate students' higher-order thinking and abilities. Traditional final evaluation relies primarily on closed-book written examinations, which typically account for over 70% of the total course score, with examination content focused heavily on abstract concept memorization and complex formula derivation. An analysis of past examination papers shows that more than two-thirds of the total score is allocated to formula deduction and definition-based questions, with almost no open-ended engineering design tasks included. Even when practical computer simulation courses are included in individual teaching plans, most practical assignments require students to complete fixed, repetitive operations following pre-detailed steps, with no exploratory open-ended design tasks. This score-driven single-dimensional evaluation model significantly suppresses students' willingness for autonomous exploration and hinders the development of innovative thinking, which contradicts the requirement for cultivating independent research capabilities in postgraduate education.

Overall, the conventional teaching model cannot fully unlock the application potential of modern computational simulation technology, nor can it meet the training objectives for high-level, interdisciplinary, innovative talents in modern chemical engineering postgraduate education. Therefore, systematic structural reform guided by advanced educational philosophy is an inevitable choice to break through current teaching bottlenecks.

## 3. Four-dimensional systematic reform implementation scheme

Targeting the three core drawbacks identified above, teaching reforms across four dimensions are implemented: restructuring the curriculum system, innovating a hierarchical progressive teaching model, constructing a comprehensive practical training platform, and upgrading the diversified assessment system.

### 3.1 Restructuring multi-scale integrated curriculum system

The traditional "theory-first, simulation-later" model was replaced with a three-tiered modular structure. The microscopic module is paired with teaching on molecular separation mechanisms and novel functional separation materials, supported by GROMACS and Gaussian for auxiliary teaching. The mesoscopic module focuses on internal flow field analysis and structural optimization of separation equipment, relying on COMSOL and Fluent for performance simulation. The macroscopic module centers on integrated industrial process design and overall energy consumption optimization, using Aspen Plus and HYSYS as core tools, covering application scenarios from adsorbent screening to complex distillation scheme design.

The total course credit is set at 54 hours, with 16 hours specifically reserved for centralized simulation training to guarantee sufficient practical opportunities. Two frontier topics, AI-assisted process parameter optimization and digital twin real-time monitoring, are newly added. Both modules are developed based on industrial research projects to ensure practical relevance. Meanwhile, the teaching team has compiled customized school-based handouts integrating authentic cases from school-enterprise cooperation and ongoing provincial/ministerial reform projects, realizing the integration of teaching, research, and industrial application.

## 3.2 Establishing a three-stage spiral, research-teaching integrated teaching mode

The semester is divided into three progressive stages to achieve ability upgrading from basic operation to independent innovative research. Stage 1 (Weeks 1-4): Basic simulation training, the core goal is to help students master basic operational specifications and verify classic theoretical knowledge through visualization. Teachers demonstrate typical ethanol-water rectification modeling on Aspen Plus, then students complete independent modeling to compare theoretical and simulated results, lowering the learning threshold for students with heterogeneous backgrounds. Stage 2 (Weeks 5-9): Comprehensive engineering simulation training, to improve practical industrial analysis ability, a real ethyl acetate recycling optimization project from a domestic pharmaceutical enterprise is introduced as the training task. Students complete the full workflow including parameter estimation, process framework construction, energy consumption calculation and economic evaluation, tightly connecting classroom learning to real industrial demands. Stage 3 (Week 10 to the end of semester): Independent innovative research practice, students select cross-scale topics aligned with their own dissertation direction (e.g., CO2 capture porous material development, pervaporation membrane structure optimization), complete full research from microscopic adsorption energy calculation to macroscopic process integration, and submit a formal research report for in-class defense. Outstanding works are recommended for national and provincial postgraduate innovation competitions to stimulate research enthusiasm.

## 3.3 Building a tripartite open shared practical training platform

By integrating scattered teaching resources, idle research computing equipment and industrial off-site resources, a three interconnected shared platforms to address the long-standing problems of insufficient resources and isolated equipment in traditional teaching was constructed.

Campus-level centralized teaching platform: Based on the university's virtual simulation experiment center, equipped with fully authorized mainstream software and standardized operation guides to meet the routine teaching demand for large groups of postgraduates.

Advanced research-oriented simulation platform: Relying on the Institute of Low-Carbon Technology Application, this platform opens high-performance GPU parallel computing servers to support large-scale complex molecular simulation for high-level innovative projects.

Off-campus industrial platform: Co-established with leading chemical enterprises in Shaanxi Province, which regularly provides real-time on-site production data and industrial optimization tasks, and invites senior engineers to deliver thematic lectures and project tutoring. The three interconnected platforms achieve seamless transition from basic skill training to advanced research and industrial application.

## 3.4 Optimizing a competency-oriented, diversified assessment system

The original single closed-book final examination was completely replaced by a multi-dimensional weighted assessment mechanism combining whole-process formative evaluation and final open-design examination. The specific weight allocation is: 10% for daily classroom performance and literature reading report; 20% for routine simulation task completion and operation assessment; 20% for industrial case simulation report and economic analysis; 20% for independent research project quality and in-class defense; 30% for the final cross-scale open design assignment.

The final examination adopts a dual-track design: fixed compulsory topics assess core theoretical knowledge and basic skills, while optional self-designed topics allow students to develop personalized research schemes based on their own research interests, fully satisfying the differentiated cultivation requirements for postgraduates in diversified research fields.

## 4. Empirical analysis of three-year teaching reform effects

The four-dimensional comprehensive reform scheme formulated in this study has been continuously implemented in full-scale teaching practice over three complete academic years (2023-2025), covering a total of 237 postgraduate students from the School of Chemical Engineering, Northwest University. To systematically evaluate the effectiveness of the reform, the research team collected multi-dimensional teaching evaluation data through standardized questionnaire surveys, in-depth offline semi-structured interviews with students, and long-term tracking of academic performance. Core quantitative indicators are presented in two structured tables for concise and intuitive display, and the following discussion focuses on in-depth analysis of the reform outcomes, avoiding redundant repetition of raw data.

**Table 1. Comparison of students' ability before and after reform**

| Inspection index | Pre-reform | Post-reform |
|---|---|---|
| Proportion of students completing full-process independent modeling | 41% | 89% |
| Feasible optimization proposals in VOCs project | 30% | 61% |

**Table 2. Statistical results of postgraduate satisfaction questionnaire**

| Survey content | Recognition rate |
|---|---|
| Total satisfaction | 93.5% |
| Close to scientific research capability and dissertation preparation | 90.3% |
| Simulation training improves personal research efficiency | 88.7% |
| Three-stage progressive teaching mode is reasonable | 94.1% |
| Will recommend the course to lower-grade students | 85.6% |

As summarized in Table 1, a significant improvement in students' core engineering practice competencies was observed after the reform: The proportion of students capable of independently completing multi-scale process modeling and simulation increased from 41% to 89%. The percentage of feasible optimization proposals in VOCs project rose from 30% to 61%. The significant growth in students' independent modeling and problem-solving ability fully verifies the effectiveness of the constructed hierarchical progressive multi-scale simulation training system, confirming that the reform can effectively bridge the gap between theoretical teaching and practical engineering requirements.

Correspondingly, the satisfaction survey results presented in Table 2 show that the overall satisfaction rate of participating postgraduate students exceeded 93%, with more than 90% of students reporting that the reform had a "significant positive impact" on their scientific research capability and dissertation preparation. This indicates that the reform has been widely recognized by students, and effectively improves the learning experience of the course.

In addition to the above quantitative evaluation indicators, the reform practice has also produced extensive regional demonstration effects. Over the past three years, the teaching team has received more than ten visits and academic exchanges from teaching teams of domestic universities including Xi'an Jiaotong University, East China University of Science and Technology, and Chang'an University, covering activities such as special seminars, open class observations, and shared platform on-site visits. The customized teaching cases and practical training handouts have been shared openly with more than 5 domestic universities carrying out similar reforms, providing a replicable reference model for postgraduate teaching reform in chemical engineering in the region.

## 5. Discussion on existing deficiencies and future optimization prospect

Notwithstanding the encouraging outcomes achieved in teaching quality and postgraduate competency cultivation through three years of continuous reform practice, there remain several unaddressed limitations in the current daily teaching arrangement that require targeted improvements in subsequent long-term teaching optimization.

(1) Cross-scale data integration, the coupling depth of multi-scale simulation calculation requires further enhancement. At present, simulation tasks across different scales still operate independently without an efficient data transmission interface. In the next stage of curriculum upgrading, the teaching team plans to introduce professional cross-scale parameter coupling technology, to achieve truly coordinated co-simulation that enables seamless data transfer from microscopic molecular parameter output to macroscopic process model input.

(2) Expansion of industry partnerships: the coverage of school-enterprise cooperative partners needs continuous expansion. Currently, partner enterprises are mainly concentrated in traditional fine chemical and separation manufacturing

industries within Shaanxi Province. In future development, the team will actively explore long-term cooperative resources with domestic new-energy and environmental protection enterprises, to continuously enrich the authentic industrial case repository for classroom teaching.

(3) Personalized learning support: a refined personalized tutoring system is not yet fully established. The research team plans to develop an exclusive competency portrait evaluation system for each student, which can generate customized targeted learning path recommendations based on individual research directions and specific ability weaknesses of each postgraduate.

After the continuous improvement of the current reform scheme, the mature and stable reform framework characterized by "multi-scale integration, research-teaching coordination, and competency orientation" will be gradually extended to other core postgraduate courses, including Reaction Engineering and Process System Engineering. The popularization will follow a three-phase implementation roadmap: Complete the revision of the curriculum framework in the first academic year; Finish case matching and teacher trial teaching in the second academic year; Launch full-scale formal teaching implementation in the third academic year. Through this phased promotion, the formation of serialized branded curriculum reform achievements is targeted, and a positive contribution to the high-quality cultivation of outstanding innovative advanced talents in chemical engineering under the background of emerging engineering education will be achieved.

## 6. Conclusion

Against the overall construction background of emerging engineering education, this paper focuses on the core requirement of cultivating high-level compound innovative talents. Aiming at the prominent practical teaching difficulties of the postgraduate core course Advanced Separation Engineering, this paper proposes and systematically implements a three-dimensional reform guideline featuring multi-scale integration, research-teaching coordination, and ability-oriented cultivation. Comprehensive targeted reform is carried out across four key dimensions: restructuring of the curriculum system, upgrading of the hierarchical teaching mode, construction of a shared practical training platform, and optimization of the diversified assessment mechanism. A brand-new innovative teaching ecosystem is established, which realizes the deep integration of theoretical knowledge learning and practical engineering training, the two-way cyclic promotion of classroom teaching and academic research, and the whole-process development of ability-centered talent cultivation.

Three-year large-scale continuous teaching practice, summarized in the quantitative tables of this study, fully demonstrates that the proposed systematic reform effectively addresses long-standing prominent teaching problems, including fragmented simulation content, serious separation between teaching and research, and the rigid single final assessment system. As a result, postgraduates' digital engineering literacy and independent innovative research capability have been comprehensively improved. With reliable operability and high replicable promotion value, the summarized reform framework provides valuable practical reference experience for the digital transformation of core postgraduate courses in domestic chemical engineering disciplines.

In future long-term teaching practice, the teaching team will adhere to the student-centered, ability-oriented core educational principle, and continuously iterate and optimize the detailed curriculum design, so as to build a high-quality reform benchmark for core postgraduate courses in chemical engineering for peer institutions.

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