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Advantages and Applications of Chemical Simulation Software in Chemical Experiment Teaching

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Abstract

This article analyzes the advantages and disadvantages of traditional chemical operation experiments, and compares the advantages of chemical simulation experiments with traditional operation experiments from the aspects of safety, economy, teaching efficiency, data depth, and repeatability. It also discusses the role of chemical simulation experiments in cultivating students' engineering thinking, problem-solving ability, and innovative consciousness. Summarized the specific applications of chemical simulation technology in three core experimental courses: chemical principle experiments, chemical reaction engineering experiments, and chemical separation engineering experiments. It is pointed out that the new mode of modern chemical experimental teaching combining traditional experimental teaching and simulation experimental teaching is an inevitable trend for future development.

Keywords

chemical simulation; Experimental teaching; Principles of Chemical Engineering; Reaction engineering; Separation project; teaching reform

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1. Introduction

Chemical engineering is a science based on experiments, and experimental teaching plays a crucial role in the training of chemical engineering professionals[1]. It is not only a practical verification field for theoretical knowledge, but also an important way to cultivate students' hands-on ability, observation ability, analytical problem-solving ability, and rigorous scientific attitude. Traditional chemical experiment teaching mainly relies on physical experimental devices, where students complete their learning by hands-on operation, observing phenomena, recording and processing data. However, traditional experiments are limited by multiple factors such as equipment cost, footprint, safety, time consumption, and difficulty in demonstrating internal mechanisms, resulting in bottlenecks in teaching effectiveness and coverage[2].

Since the 21st century, the maturity of computer and numerical simulation technology has brought revolutionary changes to chemical experimental teaching[3]. Chemical Process Simulation software and various specialized simulation systems for unit operations, are increasingly widely used in teaching and research in universities[4,5,6]. These software are based on strict principles of thermodynamics, kinetics, and transfer processes, and can simulate real chemical production processes with high accuracy. This article will focus on the application of chemical simulation software in the three core experimental courses, exploring its advantages compared to traditional experiments, its role in cultivating students' comprehensive abilities, in order to provide reference for the reform and innovation of chemical experimental teaching.

2. The advantages and disadvantages of traditional operational experiments

2.1. Advantages

Despite the aforementioned drawbacks, the core value of traditional experiments lies in their "authenticity" and "practicality". It can provide a realistic sense of engineering site that simulation cannot give students; Basic hands-on skills; The ability to handle practical problems; Teamwork and communication skills.

2.2. Disadvantages

Traditional experiments have the following drawbacks: high safety risks; High cost and high resource consumption; Time-consuming; Black box characteristic: Students can only measure import and export parameters, and have no way of knowing the detailed state inside the equipment (such as concentration distribution, reaction progress), making it difficult to deeply understand the process mechanism[7]; Poor repeatability and multiple sources of error. Restricting the opening rate of experiments and failing to achieve talent cultivation goals.

3. The advantages of chemical simulation software compared to traditional operational experiments

3.1. Extremely high security

This is the most prominent advantage of simulation software. Chemical entity experiments often involve high temperature, high pressure, flammable, explosive, toxic substances and operating conditions. Simulation software completely eliminates these security risks, allowing students to try various operations, simulate various accident and fault scenarios, and thus deeply understand the importance of safe operations.

3.2. Significant economic benefits

The hardware cost is low, and the price of a genuine simulation software is much lower than building a complete physical experimental device; Low operating costs, simulation experiments do not require the consumption of water, electricity, steam, or various chemicals, greatly reducing teaching and operating expenses; Low maintenance cost.

3.3. Excellent teaching efficiency and flexibility

Time efficient: Physical experiments often require long preheating, stabilization, sampling, and analysis times, with one experiment often lasting several hours. Simulation experiments almost complete state switching and data output in an "instant", allowing students to explore more working conditions within a limited number of class hours[7].

Infinite space: The software can simulate large and complex process flows that cannot be accommodated in the laboratory, breaking the limitations of space and scale.

Infinite parameters: Students can freely adjust any configurable parameters, from macroscopic operational variables to physical and dynamic parameters, enabling comprehensive exploratory learning, which cannot be achieved with fixed equipment in physical experiments[8].

3.4. Process visualization and data depth

Simulation software provides the ability to "see through" the interior of the device. Students can intuitively see the concentration/temperature distribution inside the tower, the reaction progress inside the reactor, the flow field in the pipeline, etc., transforming abstract theoretical concepts into visual images, greatly deepening their understanding of the essence of the process[9]. Meanwhile, the software can provide massive, continuous, and accurate data points, facilitating in-depth mathematical analysis, model fitting, and optimization research.

3.5. Perfect repeatability and comparability

Physical experiments are difficult to completely replicate due to environmental factors, equipment status, and operational errors. Simulation experiments have perfect repeatability, allowing students to accurately return to any state point for repeated testing or comparison of different schemes[10]. For example, all other conditions can be fixed, and only the reflux ratio can be changed to compare its single impact on product purity. This “control variable” .research method can be most purely reflected in simulation.

4. The role of chemical simulation software in cultivating students’ comprehensive abilities

Chemical simulation software is not only a teaching tool, but also a platform for cultivating abilities, and its role is reflected in multiple aspects.

4.1. Deepen theoretical understanding and establish engineering concepts

Through the interactive mode of “changing parameters and observing results”, students can actively connect abstract theories (such as phase equilibrium, reaction rate, mass transfer efficiency) in courses such as “Chemical Thermodynamics”, “Reaction Engineering”, and “Separation Engineering” with specific engineering phenomena and results, thus constructing a solid engineering concept system[11].

4.2. Cultivate systematic thinking and process integration ability

Complex chemical processes are an organic whole. Simulation software, especially Aspen Plus and other process simulation software, require students to design and analyze the entire process flow from a global perspective, understand the mutual influence and coupling relationship between the units before and after[12]. This greatly cultivates students’ systematic engineering thinking, which is beyond the reach of traditional unit operation experiments.

4.3. Strengthen engineering design and optimization capabilities

The essence of simulation software is a design and optimization tool. Students are no longer passive operators, but active designers. They need to set design specifications (such as product purity requirements) and have the software automatically adjust operating parameters (such as reflux ratio) through iterative calculations to meet the requirements. This process itself is the preliminary engineering design[13]. Further research on parameter sensitivity and optimization has cultivated students’ economic awareness and optimization thinking.

4.4. Inspire innovative thinking and research abilities

A safe and low-cost environment encourages students to engage in “What if”. They can boldly experiment with Novel’s process ideas, operational plans, or extreme conditions, which may lead to the discovery of new phenomena or optimization space, greatly stimulating innovation consciousness and preliminary scientific research capabilities[14].

4.5. Enhance data analysis and problem-solving skills

Faced with a large amount of simulation output data, students need to use mathematical tools and theoretical knowledge to analyze, summarize, and explain, in order to diagnose process problems and propose improvement solutions[15]. This process simulates the complete process of engineers solving practical engineering problems, effectively enhancing their comprehensive literacy in data processing and problem solving.

5. Overview of the Application of Chemical Simulation Software in Three Major Experimental Courses

In addition to the principles of chemical engineering and its experimental courses, chemical unit operation simulation can be used to deepen teaching. Other professional courses in chemical engineering, such as chemical reaction engineering, chemical separation processes, chemical technology, and chemical instrumentation and automation, also have relevant experiments available for operation and learning in simulation software. This chemical engineering major has played a significant role in helping students achieve their graduation project and chemical design competition results.

5.1. Application in Chemical Engineering Principles Experiment

The traditional experimental course of Principles of Chemical Engineering has problems in practical application, such as inconsistency with the course setting and theoretical courses, simple equipment that cannot meet the training requirements, limited class hours that cannot deeply explore the course content, simple and outdated experimental sheets, mainly for verification experiments, and a small number of comprehensive experiments that are difficult to implement. Chemical simulation courses can make up for the shortcomings of experimental courses. Chemical unit operation simulation can not only simulate most of the unit operations in Principles of Chemical Engineering, such as absorption, drying, filtration, distillation, etc., on the computer, strengthen students' understanding of the "three transmission and one reaction" content in Principles of Chemical Engineering courses, but also have advantages that traditional chemical principle experiments do not have. (1) Compared with traditional chemical principle experiments, chemical unit operation simulation software has a larger simulation range, which can simulate various parts such as raw material pretreatment, main unit operations, and product post-processing, and is closer to industrial reality. (2) The simulation process of chemical unit operation is more complete, making it easier to observe and analyze the impact of various operations on experimental results, and the investigation of professional knowledge is more extensive and detailed. (3) It can also simulate processes such as instruments, automatic control, automatic signals, and interlock protection, and is related to operations. It is a strict interactive operation, a comprehensive experiment, rather than a traditional chemical principle experiment that verifies a single principle or implements a unit operation.

5.1.1. Fluid Flow and Transport Machinery Experiment

For centrifugal pumps, it is possible to simulate their start-up, switching, parallel/series operation, and generate characteristic curves (H-Q, N-Q, η - Q curves) without worrying about cavitation or mechanical damage. For example, simulation can clearly demonstrate the occurrence process of "air binding" and "cavitation" phenomena and their impact on pump performance, which is both dangerous and difficult to visually demonstrate in physical experiments.

5.1.2. Heat transfer experiment

It can simulate the operation of various heat exchangers (such as sleeve type, tube type, plate type). Students are able to adjust the flow rate and inlet temperature of cold and hot fluids, and study their effects on heat transfer rate, average temperature difference, and total heat transfer coefficient K[16]. The software can simulate the advantages and disadvantages of different flow arrangements such as counterflow and parallel flow, and can break through equipment limitations to simulate heat transfer behavior under extreme working conditions (such as extremely high/low flow rate, temperature), which may not be achievable for physical equipment due to safety or material reasons.

5.1.3. Mass transfer and tower equipment experiments

Distillation, absorption and other tower equipment operations are the key and difficult points of chemical engineering principle experiments. Simulation software can establish a complete tower model, and students can observe the temperature, concentration distribution, gas-liquid flow rate changes on each tray in the tower in real time by changing many parameters such as feed position, feed state (q value), reflux ratio, tower kettle heating steam volume, and operating pressure, as well as the final impact on the purity of products at the top and bottom of the tower[17]. This kind of visualization of the "black box" process inside the tower cannot be provided by any physical experiment.

5.2. Application in Chemical Reaction Engineering Experiments

Chemical reaction engineering experiments focus on the determination of reaction kinetics and the design, operation, and optimization of reactors.

5.2.1. Reaction kinetics research

The simulation software is equipped with various reaction kinetics models (such as power-law model, Langmuir Hinshelwood model, etc.). Students can simulate the reaction process under different temperature, pressure, and concentration conditions, quickly fit the kinetic parameters (reaction order, activation energy, etc.) through the data processing function of the software, and compare them with theoretical values[18]. This avoids the errors and workload caused by frequent sampling and analysis in physical experiments.

5.2.2. Reactor operation and optimization

It can simulate the dynamic and steady-state operation of various reactors (batch reactor CSTR, continuous stirred tank reactor CSTR, laminar flow reactor PFR, fixed bed reactor, etc.). Students can explore the following:

CSTR: Study the effects of residence time and feed concentration on conversion rate and selectivity.

PFR: Compare with CSTR to understand the impact of backmixing on reaction results.

Fixed bed reactor: Simulate the effects of catalyst loading, particle size, and feed air velocity on the reaction, and even simulate the dynamic changes of catalyst deactivation process[19].

5.2.3. Thermal stability and parameter sensitivity analysis

This is a huge advantage of simulation software. It can simulate the “flying temperature” phenomenon of the reactor, study the influence of coolant flow rate and temperature on the thermal stability of the reactor, and find a safe operating range[20]. This is highly dangerous in physical experiments and is usually prohibited or only demonstrated by teachers.

5.3. Application in Chemical Separation Engineering Experiments

Separation engineering experiments are more complex, often involving the separation of multiple components and non ideal systems.

5.3.1. Design and optimization of complex distillation sequences

For multi-component mixtures (such as hydrocarbon mixtures), separation requires a sequence composed of multiple columns. Simulation software can easily build and simulate the entire separation sequence. Students can evaluate the energy consumption, equipment investment, and product yield of different separation sequences, thereby learning how to select the optimal process from an economic and technical perspective[21]. It is almost impossible to build such a complex multi tower linkage device in a physical laboratory.

5.3.2. Simulation of special distillation

It can simulate special separation processes such as azeotropic distillation, extraction distillation, and reactive distillation. Students can add entrainers and study the effects of their dosage and feeding position on breaking the azeotropic point; It can simulate the optimization of solvent ratio in extraction distillation[22]. These experiments have complex equipment, high drug consumption, and extremely long time consumption in reality, while simulations provide efficient research methods.

5.3.3. Simulation of other separation processes

In addition to distillation, absorption, extraction, crystallization, membrane separation, and other processes can also be simulated.

6. Conclusion

Chemical simulation software and traditional operational experiments are not mutually exclusive or either or relationships, but a community with complementary advantages and mutual benefits.

Chemical simulation software, with its unique advantages of safety, economy, efficiency, depth, and flexibility, perfectly compensates for the shortcomings of traditional experiments in demonstrating process mechanisms, exploring complex systems and hazardous conditions, and plays an irreplaceable role in cultivating students’ advanced abilities such as engineering thinking, system design, optimization, and innovation. Traditional operational experiments have fundamental value in cultivating students’ practical skills, engineering site awareness, fault handling ability, and teamwork skills.

Therefore, the future direction of chemical experiment teaching reform is inevitably to build a diversified and multi-level teaching system that combines traditional experiments and simulation experiments. Through this organic integration, simulation experiments and traditional experiments support and verify each other, jointly building a complete chemical engineering practical ability training chain from basic skills to high-level thinking, from unit operation to system integration, thus cultivating more excellent chemical engineering and technical talents with solid theoretical foundations, strong practical skills, and outstanding innovative thinking for society.

Disclosure statement

The author declares no conflict of interest.

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