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RESEARCH ON THE APPLICATION OF MATHEMATICAL MODELING IN CHEMICAL PRODUCTION

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Abstract:

Mathematical modeling has become one of the primary methods in modern chemical production. By using various mathematical computation techniques to simulate complex workflows and systems, and analyzing the production process, mathematical modeling helps optimize production efficiency, improve product quality, and enhance the competitiveness and profitability of enterprises. This article analyzes the basic concepts and roles of mathematical modeling in chemical production, including simulation and modeling. It is hoped that the introduction provided in this article can serve as a reference for chemical enterprises.

Keywords: Mathematical modeling; Chemical production; Simulation; Production process; Chemical engineering; New Engineering

1 The basic concepts and functions of mathematical modeling in chemical production

1.1 Basic knowledge of mathematical modeling

The chemical industry has experienced exponential growth alongside the continuous development of chemical engineering. Driven by factors such as energy, environment, and quality, there is an urgent need for profound reforms and ongoing innovation to enhance the level of industrialization. This increasing industrialization prompts a growing market demand for various types of chemical products, while also raising higher requirements for their production efficiency and quality. Mathematical modeling, as a crucial component of engineering, can describe numerous phenomena in the real world through the use of partial differential equations (PDEs), involving extensive processes of convection, diffusion, reaction (including heat transfer), and fluid dynamics. The demand for constructing virtual prototypes in chemical engineering continues to rise. Linear PDEs, which involve partial derivatives of unknown functions, can often obtain explicit solutions through scientifically sound formulas and methods (such as Fourier series, separation of variables, transformations, superposition, etc.). However, most practical PDEs are nonlinear, significantly increasing the difficulty of obtaining solutions for these nonlinear PDEs, requiring the application of numerical approximations. Both linear Poisson and heat equations are easy to derive analytically but have notable shortcomings in solving uniqueness issues and seeking general solutions. Particularly for the majority of nonlinear chemical engineering equations, solutions to PDEs can be obtained by discretizing the solution domain into a large number of finite elements. Obtaining the complete solution entails generating and solving numerous equations, which may involve multiple arithmetic operations and necessitates the use of diverse software tools to achieve computational capabilities. For instance, the COMSOL Multiphysics software based on PCs is primarily used for solving PDE problems. Currently, the finite element method is widely applied in fields such as structural mechanics, chemical engineering, and electromagnetism. A significant number of problems have been solved using finite element method-based techniques specifically tailored for PDE solutions [1].

1.2 Mathematical Modeling and the New Integration with Chemical Engineering Disciplines

Mathematical modeling is the process of using mathematical language to qualitatively or quantitatively describe real-world problems, and it involves abstracting and simplifying complex issues. Participating in mathematical modeling competitions can broaden university students' research horizons, cultivate a spirit of creativity and cooperation, and significantly enhance their overall quality. At the same time, as a bridge connecting mathematics with other disciplines, the topics for mathematical modeling competitions are generally derived from practical problems in science and engineering, humanities and social sciences, which are appropriately simplified. These topics are highly flexible and applicable. By discussing and analyzing competition problems, collecting data, and proposing new viewpoints, ideas, and solutions that withstand practical testing, students engage in an important pathway to foster innovative thinking. Such competitions typically require participants to complete a paper covering assumptions of the model, model establishment and solving, analysis and validation of the model, and evaluation, improvement, and promotion of the model. The participation process almost simulates the general process of scientific research, promoting university students' abilities to analyze and solve problems, as well as enhancing their abstract thinking. It is of great significance for cultivating university students' ability to integrate knowledge, comprehensive application of computer software, professional paper writing, teamwork, and communication skills. To thoroughly understand and master the field of chemical engineering, it is essential to grasp the knowledge of mathematical modeling, especially the comprehensive application of limit concepts, divergent thinking, and analogy thinking involved in mathematical modeling, which greatly benefits the study of related chemical disciplines [2,3,4,5].

Having a foundation in mathematical modeling is beneficial for deepening the digestion and application comprehension of theoretical knowledge in chemistry. When studying adsorption thermodynamics in physical chemistry courses, one encounters topics related to determining the type of adsorption (Langmuir, Freundlich, Temkin, etc.) based on adsorption isotherms, thereby inferring the mechanism of adsorption (chemical or physical). However, in actual scientific research, the data obtained from adsorption thermodynamics experiments are often non-continuous points. For example, finding hydrogen storage materials with high stability, fast kinetics, high safety, and low cost is a key issue in the development of hydrogen-oxygen rocket engines. In testing different materials for hydrogen adsorption and storage, drawing adsorption curves is inevitable. To plot adsorption curves and predict their properties, data fitting is essential. Fitting algorithms are an important mathematical model whose core idea is to establish a series of mathematically explicit and concise curves to simplify complex problems. However, the fitting curve does not need to pass through every sample point but only needs to ensure that the error is sufficiently small. For instance, Sun et al. [6] studied the adsorption of heavy metal Cd2+ by KOH-modified biomass carbon adsorbents and performed Langmuir and Freundlich fits on the equilibrium adsorption capacity data at different adsorbent concentrations. To determine the type of adsorption, one needs to examine the R2 value of the fitted curves. The higher the R2 value, the better the fit, thereby inferring the adsorption mechanism. It is evident that even the most basic application of textbook conclusions involves linear fitting, which is one of the most commonly used tools in mathematical modeling and a basic predictive model in machine learning.

Having a foundation in mathematical modeling is beneficial for applying mathematical thinking to solve problems in chemical engineering and chemistry. For example, C4 olefins, as an important chemical raw material, are widely used in the production of chemical products and pharmaceuticals. The B problem of the 2021 National College Student Mathematical Modeling Competition was set against the background of ethanol coupling to produce C4 olefins. It required designing a combination of catalyst components (i.e., Co loading, Co/SiO2, and hydroxyapatite (HAP) feed ratio, ethanol concentration), and exploring the optimal process conditions for ethanol coupling to produce C4 olefins by considering the effects of temperature on the selectivity and yield of C4 olefins. This type of experiment usually appears in undergraduate theses because it involves many variables, and students typically need 2-3 months to complete the related experiments and draw qualitative conclusions from limited data. However, such conclusions are subjective and lack robust data, making them difficult to generalize horizontally or vertically and of limited reference value. But if mathematical modeling methods are used to establish machine learning models, we can derive quantitative relationships between C4 olefin selectivity, ethanol conversion rate, and factors such as temperature, Co/SiO2 and HAP feed ratio, Co loading, and ethanol feed concentration based on a large amount of experimental results. These quantitative data are more reliable than qualitative conclusions drawn from a few experimental results, and the findings are easier to extend to other reactions. Similarly, mathematical modeling can be used to describe the impact of parameters such as feed thermal state, reflux ratio, and operating pressure on energy consumption in distillation columns, clarify the weight of each variable, and thus optimize chemical production design. In the optimization design process, the following steps are usually considered: (1) establish mathematical models for heat and mass balance; (2) perform multivariate regression analysis on variables with energy consumption and production efficiency as objective functions; (3) calculate the sensitivity index of each variable to determine weights; (4) solve the optimization for the objective function; (5) experiment and verify. Li et al. [7] proposed using a multi-objective genetic algorithm to optimize the economic cost and gas emission index of the extractive distillation separation process for the azeotropic mixture of ethyl acetate/ethanol/butanone, with operating pressure and entrainer flow rate as variables. Compared with the original process, the optimized results reduced gas emission costs and operating costs by 20.94% and 10.06%, respectively, and improved thermal efficiency by 8.16%. By comparing the energy consumption of different control structures in the system under disturbances, it was found that the energy consumption of the CS2 structure was lower than that of the CS1 structure. Thus, it is evident that reasonable use of mathematical modeling can guide data analysis in chemical and chemical engineering experiments to some extent and provide a new approach for scientific research.

In summary, mathematical modeling is a process that applies mathematical methods and techniques to solve complex practical problems. For students majoring in chemical engineering, learning mathematical modeling can help understand, analyze, and optimize chemical production processes, cultivate innovation and engineering practice abilities, improve academic research skills, and promote the cross-application of interdisciplinary knowledge [8].

1.3 Shortcomings in Mathematical Modeling Education

Mathematical modeling thinking can train university students' problem-solving approaches, and mathematical modeling competitions can significantly improve their overall quality. However, it is undeniable that there are still some deficiencies in the current mathematical modeling education in China. For instance, students' innovative thinking has not been fully unleashed. When faced with real mathematical modeling problems, students need to establish appropriate mathematical models. In fact, mathematical modeling problems usually do not have just one solution. Students should practice more flexible problems regularly, as this can not only improve their problem-solving abilities but also enhance their confidence when facing difficult problems.

Additionally, some students lack the ability to apply knowledge practically. Facing familiar types of problems, they dare not use their professional knowledge and instead mechanically apply mathematical models without integrating mathematical modeling thinking into other subjects. The fundamental solution to this problem is to incorporate mathematical modeling thinking into the study of professional courses, linking what is learned with real-world problems. However, this method has low feasibility: first, it is challenging to popularize mathematical modeling thinking, as some students are not good at mathematics; second, teachers have their areas of expertise and may not be able to study the detailed content of mathematical modeling[9].

2 The application significance of mathematical modeling in the chemical production process.

2.1 Promoting the sustainable development of modern chemical enterprises.

In the research and equipment manufacturing of chemical processes, the combined use of mathematical methods and computer technology has become an important pathway for the development of modern chemical engineering. Rising energy prices and environmental regulations present significant challenges to chemical production, with product pricing and quality facing global market competition. This has led to substantial changes in the chemical industry. To align with the concept of energy-efficient development, optimization techniques have emerged as a primary engineering approach to describe these conditions. They provide technical support for the design and operational optimization of chemical plants, better accommodating diverse constraints in chemical production. While enhancing production efficiency, these techniques also aim to reduce costs [10]. Computer-integrated manufacturing seeks to effectively implement optimal operating conditions. The complexity of problems solved by optimization techniques has expanded, necessitating the use of computer software that incorporates improvement technologies. Additionally, as chemical companies continue to expand their business types and scales in recent years, some chemical products still face imbalances in supply and demand, with most products being oversupplied. This has spurred the development of fine chemicals and contract chemical manufacturing. The pharmaceutical raw materials market faces increasingly fierce competition, requiring the cultivation of independent competitive advantages to secure more effective orders. Essentially, this involves perfecting and innovating the synthesis process development [11]. Long-term breakthrough developments in production processes need to be based on existing technologies, combining cost-effective, safe, and stable raw materials with scientifically sound mathematical modeling to simplify production processes. This improves the quality and recovery rate of certain stages, seeking simple and efficient physical and chemical treatment methods to reduce waste emissions.

2.2 Accommodating the growth demands of advanced chemical industries.

In chemical production management and new product development, the application of computer network-based mathematical modeling is essential to meet the development needs of modern chemical enterprises. A competitive advantage for future chemical companies lies in their ability to adapt to international market demands through robust global supply chain management. This capability allows for the production of both generic and specialized products, tailored to diverse global customer needs, providing targeted personalized services [12]. Additionally, it enables rapid adaptation to market demand changes, facilitating the research and optimization of production processes and chemical products. For instance, utilizing mathematical modeling in biotechnology can enhance the quality and efficiency of producing both general and specialized products. This necessitates that mathematical education in chemical engineering schools integrates with the chemical specialty, stays current with advancements, and effectively applies mathematical modeling in chemical production [13].

2.3 Mathematical Modeling and “Principles of Chemical Engineering”.

In the course of “Principles of Chemical Engineering” there are generally two types of mathematical engineering analysis methods: dimensional analysis and mathematical modeling. Dimensional analysis uses the principle of dimensional consistency and the π theorem to analyze the relationships between output results and various parameters or groups based on experimental data. For example, in the process of convective heat transfer, the derivation of the Nusselt number for forced convection heat transfer in a circular straight tube employs this method. Mathematical modeling involves describing and constructing models using mathematical language based on the physical characteristics of chemical processes, then verifying the models and calculating parameters based on experimental output results. Each of these methods has its advantages and disadvantages. Dimensional analysis studies processes through experimental results and experience, which requires significant effort and can be used when there is limited understanding of the chemical process. If issues arise during the analysis process, it can result in substantial errors. In contrast, mathematical modeling involves making reasonable simplifications to real-world problems when there is a basic understanding of the chemical process, analyzing certain variables in conjunction with physical models, requiring less effort but demanding that technicians have a deep understanding of the chemical process. The constructed models should not be overly simplified to the point of losing accuracy. Comparing these two engineering analysis methods, mathematical modeling is undoubtedly more scientifically reasonable [14].

In the analysis of the gravitational settling process of solid particles in “Principles of Chemical Engineering” let me briefly introduce the general process of mathematical modeling. The first step is model assumptions. Based on the shape of the solid particles, we classify them into spherical and non-spherical particles. For non-spherical particles, we assume that they can be modified using the volume equivalent diameter and shape factor and treated as spherical particles. This simplification reduces the complexity of the analysis significantly. Next is model analysis, where we identify the forces acting on the solid particles during their gravitational settling, namely gravity, buoyancy, and sedimentation resistance. According to physical analysis, the net force is zero at uniform settling velocity. Finally, in model solving, by combining these three forces, we can determine the settling velocity. While chemical engineering courses may involve some degree of mathematical modeling thinking, relying solely on non-specialized courses to learn this skill is far from sufficient. Such knowledge is not systematic and inadequate for addressing practical issues in production. Chemical engineering students should conduct more scientific and in-depth research into mathematical modeling to enhance their professional learning capabilities [9].

3 Application of Mathematical Modeling in Chemical Production

3.1 Optimizing the Raw Material Ratio in Chemical Production Using Mathematical Modeling.

Most chemical production raw materials are extracted from petroleum, coal, biomass, and minerals. Based on different life characteristics, these materials are categorized into organic and inorganic types. Different raw materials, when reasonably proportioned and designed, can produce superior chemical products that facilitate industrial development and daily life. The design of raw material ratios directly affects product quality, and wasteful use of raw materials leads to significant resource loss. Many experts and scholars have introduced mathematical modeling theory into the chemical production process, using mathematical modeling to simulate and design the raw material ratios for chemical production. They treat the required raw material ratios as mathematical parameters to construct a mathematical model of chemical production. Through simulation design, they analyze the impact of changes in the content of certain raw materials on product quality and performance. After multiple simulation designs, the raw material ratios for chemical products are optimized. This approach not only reduces waste of raw materials needed for production but also enhances the quality and performance of chemical products, effectively addressing the rising costs of energy and raw materials. In summary, chemical enterprises utilizing mathematical modeling can more precisely control the raw material ratios and content, effectively manage production costs, and significantly increase economic benefits [15].

3.2 Optimizing Chemical Product Production Processes Using Mathematical Modeling.

As society progresses, the variety of chemical products has gradually increased, and their production technologies and processes have become increasingly complex. To address this, many chemical enterprises utilize mathematical modeling to optimize production processes and workflows, thereby further enhancing production efficiency. When producing chemical products, companies can use mathematical modeling to construct product manufacturing processes, analyze by products at each stage, and optimize through simulation and prediction methods. This improves the design of unreasonable aspects in the production process, making the entire workflow more streamlined and efficient. Additionally, chemical enterprises can leverage mathematical modeling and computer information technology to manage and control production processes, making them more intelligent and digital [15].

3.3 Optimizing the Chemical Production Process Using Mathematical Modeling.

The modeling procedure has the advantage of being simpler than establishing a mathematical model. Applying mathematical models to investigate flow in porous media involves processes with 2 reactants and 1 product. The corresponding substances obtained after completing the reaction are injected into the product in a stable porous medium catalytic bed, combining the main pipeline with the injection tube. The specific construction process generally includes: First, complete the construction of the corresponding geometric model and define regions with different characteristics to reasonably reduce the experimental workload; second, for the already feasible physical design, the application model can also be used through selectable simulation processes to complete relevant design functions, such as designing material properties and boundary conditions. For various application module physical designs, any form that can be set to constant can be used. For fluid parameter transmission systems on porous beds, they generally include free fluid parameter zones and porous media zones, etc., which can be described in detail using the Brinkman equation. The simulation of different material transfers can also be done through flow methods; third, the grid system in the polygonal modeling program is composed of a large number of triangles or other forms of materials, and according to the defined physical space size, it constitutes the corresponding network to describe this system; fourth, select and apply solution procedures. If various solution processes such as linear or nonlinear parameters, transient, adaptive, etc., have been carried out in the model environment, then take the transient solution process as an example. On the basis of the pre-selected solution procedure and generated solution process, complete the diffusion-type solution processes such as Brinkman, gas convection phenomena, etc., in two stages according to the sequence. When necessary, the program can also calculate the entire process simultaneously, thereby reducing possible errors due to atmospheric pressure changes during the reaction process [15].

4 Emergency Management Evaluation of Chemical Industrial Parks Based on Fuzzy Mathematical Models.

In recent years, the rapid development of chemical industrial parks has led to an increasing variety and quantity of chemicals, with concentrated hazard sources posing significant safety risks. This necessitates efficient risk evaluation in chemical industrial parks to effectively reduce safety risks. One important aspect is emergency management evaluation, which is a crucial component of safety management and risk assessment. This paper takes the emergency management system of a certain chemical industrial park as the research subject. Based on existing research results and on-site investigations of the park, it comprehensively considers various types of emergencies (including pre-incident, during-incident, and post-incident phases). By integrating fuzzy mathematical models and the Analytic Hierarchy Process (AHP), the evaluation process of the emergency management level system is realized. The ultimate goal is to achieve a comprehensive judgment of the emergency management level and identify deficiencies and loopholes in emergency management, providing references for further improvements [16].

5 Other Simulations.

This simulation process is still in its preliminary stages. It can also simulate the flow momentum conservation of fuel cells, energy conservation in heat exchangers, mass transfer in static laminar mixers, electrochemical effects, etc. For example, in tumor electrochemical therapy, it can be used for scientifically reasonable design of microfluidic devices for electric field mixing and detailed inspection of electrophoresis and chromatography effects, among others. Many studies require simulation of mass transfer and fluid flow, coupled with physical fields such as electromagnetic or structural mechanics. The COMSOL Multiphysics mathematical modeling software lays a solid foundation for research on problems involving the simultaneous coupling of multiple physical fields [17].

6 Conclusion

The essence of mathematical modeling is to use mathematical methods to solve real-world problems. The application of mathematical modeling in chemical production can effectively improve chemical production technology and processes, especially in terms of raw material utilization and product quality control. The specific working mechanisms of chemical processes are generally easy to grasp and understand, but determining the optimal parameters, such as raw material quantities and proportions, reactor types and specifications, optimal rates, and reaction conditions, involves a large amount of engineering work. Under traditional models, this often requires repeated trials and practical experience to effectively address related issues. This method also increases practical application costs due to the establishment and testing of large-scale prototype equipment. Using mathematical modeling can significantly improve work efficiency and enhance process technology.

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