

Original Paper

Application of Uniform Design in Optimization Computations for Chemical Engineering

Huichen Fan¹ & Li He^{1*}

¹ Xinjiang Hetian College, Hotan City, Hotan Region, Xinjiang, China

* Corresponding Author

Received: December 28, 2025 Accepted: February 08, 2026 Online Published: February 25, 2026

doi:10.22158/mmse.v8n1p265 URL: <http://dx.doi.org/10.22158/mmse.v8n1p265>

Abstract

Uniform design is an efficient experimental design method for space filling, with the core goal of rapidly exploring the global optimal solution in chemical and chemical multi parameter complex systems with the minimum number of experiments. This method collects representative data through uniformly dispersed experimental points, effectively supporting the construction of process models and optimization of process parameters. Practical applications have shown that uniform design significantly reduces experimental or computational costs, demonstrating strong practicality in optimizing reaction conditions, developing new material formulations, and analyzing reaction mechanisms. It provides a reliable computational experimental foundation for precise design and intelligent upgrading of chemical processes.

Keywords

Uniform Design, Chemical Engineering Optimization, Process Parameter Optimization, Intelligent Optimization Algorithms

1. Introduction

Chemists and chemical engineers have previously struggled with optimizing chemical processes that are often characterized as high dimensional, non-linear and containing multiple constraints. In general, conventional methods for performing optimizations are constrained to a great degree by large numbers of required experiments, as well as being limited by getting stuck in local optima. The uniform design theory builds upon the use of number theory techniques to create a uniform distribution of points across the parameter space being studied and therefore allows for the greatest benefit to be realized from data produced by any given calculation or experiment. This approach is particularly suited to the realities of both a large number of variables and the associated costs within the disciplines of chemistry and

chemical engineering because it allows researchers to systematically determine and then optimize; the fundamental relationships among process variables and the resulting performance of those processes, with the supreme benefit of minimal resources.

2. Theoretical Foundations of Uniform Design and Its Advantages in Optimization Computation

2.1 Core Concepts and Mathematical Principles of Uniform Design

Uniform design is an experimental design method jointly proposed by scholars Fang Kaitai and Wang Yuan in 1978. Its core idea focuses on evenly distributing experimental points across the entire experimental range, abandoning the excessive pursuit of “neat comparability” in traditional experimental design. It places greater emphasis on the representativeness and coverage of experimental points, as multi-factor, multi-level scenarios are common in practical chemical experiments. Comprehensive experiments are often time-consuming, labor-intensive, and impractical, while uniform design effectively addresses this pain point (Fang, 1968). Its mathematical principles rely on the theory of uniform distribution in number theory, falling within the category of pseudo-Monte Carlo methods. By combining number theory with multivariate statistics, it meticulously designs specialized uniform design tables and supporting tables to guide experimenters in selecting experimental points rationally. This ensures that each level of every factor participates in only one experiment, while guaranteeing that the experimental points of any two factors have only one in each row and column of the planar grid (Wang & Fang, 1981). Such a design can significantly reduce the number of experiments while ensuring the experimental points closely approximate various values of the integrand function. This facilitates subsequent data processing and modeling through simple methods like regression analysis, meeting the practical experimental needs of the chemical engineering field without requiring complex mathematical calculations to achieve scientifically selected experimental points.

2.2 Advantages of Uniform Design Compared to Traditional Experimental Design Methods

The core differences between uniform design and traditional experimental design methods lie in the logic of selecting experimental points and their operational adaptability. In traditional experimental design, orthogonal design and full factorial experiments are widely used. Orthogonal design excessively pursues neat and comparable experimental points, requiring numerous repeated trials to account for interactions among factors, which significantly increases material and time costs in chemical experiments involving multiple factors and levels. Full factorial experiments mandate covering all factor-level combinations, leading to a sharp rise in experimental volume when factors exceed three or levels surpass five, potentially exceeding the practical capacity of experimental conditions. Uniform design abandons the redundant requirement for neat comparability, focusing instead on evenly distributed experimental points. Under identical experimental conditions, it can substantially reduce the number of trials. The key distinctions from the two traditional methods are clearly illustrated in the table below.

Table 1. Comparison between Uniform Design and Mainstream Traditional Experimental Design Methods

Design method	Principles for selecting experimental points	Practical characteristics
Uniform design	Uniform distribution, emphasizing representativeness	Low number of experiments, no need for repeated experiments, suitable for multi factor and multi-level scenarios
orthogonal design	Neat and comparable, while also considering balance	There are many experiments, and it is necessary to set up repeated experiments to adapt to scenarios with few factors and low levels
Comprehensive testing	Covering all level combinations and pursuing comprehensiveness	The number of experiments is extremely high, and the consumption of consumables is time-consuming, making it only suitable for simple experimental scenarios

Table 1 clearly demonstrates the practical advantages of uniform design. In actual chemical engineering experiments, most scenarios involve multiple factors such as reaction temperature, raw material ratios, and reaction time, with each factor requiring multiple gradient levels. The limitations of orthogonal design and comprehensive experiments become increasingly apparent. Uniform design eliminates the need for complex experimental design processes, allowing ordinary experimenters to operate proficiently without specialized training. The selected experimental points can fully cover the experimental range, avoiding redundancy and waste while accurately capturing the intrinsic relationships among factors, making it well-suited for the practical needs of most chemical engineering experiments (Liu & Pang, 1995).

2.3 Analysis of Uniform Design's Suitability for Chemical Engineering Optimization Problems

The core feature of uniform design is abandoning the “orderly and comparable” requirement in orthogonal design, focusing instead on evenly dispersing experimental points across the entire investigation range. This aligns precisely with the practical characteristics of chemical and chemical engineering optimization problems. In many chemical optimization scenarios, numerous factors with wide-ranging levels need to be examined—for instance, in black liquor treatment, parameters such as reaction temperature, oxygen partial pressure, and influent pH must be adjusted simultaneously. Traditional experimental designs would significantly increase the number of trials and costs. Uniform design can cover the entire investigation range without excessive experiments, even without pursuing orderly arrangement of experimental points, yet it effectively captures the influence patterns of various factors on optimization objectives. It is suitable for high-cost, long-cycle experiments in chemical production. Chemical and chemical engineering optimizations often involve nonlinear relationships,

and the uniform distribution of experimental points in uniform design accommodates this characteristic. Combined with conventional regression analysis, it enables the establishment of practical optimization models. Ordinary researchers and frontline technicians can operate it without requiring advanced mathematical theories, lowering the threshold for application.

3. Implementation Methods and Technical Pathways for Uniform Design in Chemical Engineering Optimization

3.1 Experimental Plan Construction and Parameter Space Mapping Based on Uniform Design

In the construction of the experimental scheme, the actual needs of chemical production should be combined. First, the key parameters affecting the effect should be determined according to the specific optimization goals. For example, when preparing nano alumina by the micro lotion method, the reasonable value ranges of aluminum salt concentration, precipitant concentration, and reaction temperature should be determined in combination with the raw material supply and equipment conditions in production. Then, the appropriate number of test levels should be determined according to the common uniform design table and the test cost, so as to avoid excessive level setting increasing reagent and time costs, and also prevent too few levels from omitting key parameter intervals, leading to poor optimization results. Parameter space mapping does not require complex calculation tools. Frontline technicians can convert parameter units in actual production into recognizable codes for uniform design based on their daily operating experience. After mapping is completed, uniform design will automatically generate uniformly distributed test points, which can directly correspond to the operating conditions in actual production and can be put into experimental use without additional adjustments. In practical applications, simple and easy-to-use software such as Minitab can also be used to assist in further improving the accuracy of mapping and reducing human operation errors.

3.2 Model Building, Approximation, and Optimization Strategies

The establishment of optimization models relies on real data obtained from uniform design experiments. First, the experimental data is simply organized to eliminate abnormal data caused by operational errors and instrument errors. Then, the independent and dependent variables of the model are determined based on the constraints of actual production. For example, in the optimization of chemical reaction conversion rates, the independent variables are the reaction temperature, reaction time, and other parameters determined by uniform design, the dependent variable is the actual conversion rate value detected in the experiment. For approximate functions, priority should be given to quadratic polynomials, which are easy to operate and have strong adaptability. Frontline technicians can use ordinary data processing software to complete the fitting of functions and experimental data through basic regression calculations. When optimizing, parameter values should be adjusted around the approximate function to avoid unreasonable parameter combinations that exceed equipment carrying capacity and high raw material consumption. If the fitting effect does not meet the actual production requirements, a small number of uniformly distributed test points can be added to re fit without

repeating all the experiments, which can save time and reduce raw material loss.

3.3 Synergy Between Uniform Design and Computational Intelligence Algorithms (e.g., Genetic Algorithms, Neural Networks)

The collaboration between uniform design, genetic algorithm, and neural network should be in line with the actual operation process of chemical engineering. Uniform design first obtains basic data through a small number of uniformly distributed experiments. These data only need to be organized into a standardized format without complex preprocessing, and can be directly imported into the algorithm running tool. Genetic algorithm is mainly responsible for screening the parameter combinations generated by uniform design. During the screening process, it combines constraints such as raw material supply and equipment load in production to automatically eliminate unreasonable parameter combinations. Then, through gradual iteration, it selects combinations that are closer to the optimal solution, greatly reducing the amount of manual judgment operations. Neural networks are used to mine the hidden nonlinear correlations in uniform design experimental data, compensating for the shortcomings of uniform design in deep data analysis. The training process can be completed with the help of conventional algorithm tools, without the need to manually write complex programs. The trained neural network can quickly predict the effect of new parameter combinations, and then feedback the prediction results to uniform design to guide the parameter settings of subsequent supplementary experiments. Ordinary researchers can proficiently master this collaborative operation method through simple learning.

3.4 Key Steps in Computational Workflow and Result Validation

The calculation process needs to be carried out in an orderly manner based on the experimental plan and collaborative analysis results completed in the previous text. Firstly, the experimental data generated by uniform design and the optimal parameter combination selected by the algorithm are imported into conventional data processing software. The software will complete the correlation calculation between parameters and optimization indicators according to the preset simple calculation logic, without manually inputting complex formulas. Frontline technicians only need to check the accuracy of data input to ensure the smooth progress of the calculation process. After the calculation is completed, it needs to enter the result verification stage. The result verification needs to be carried out using actual experimental methods, selecting the optimal parameter combination obtained from the calculation for multiple repeated experiments. The experimental process strictly follows the operating specifications determined in the previous text to avoid affecting the authenticity of the verification results due to operational differences. The experimental data needs to be compared with the calculated results one by one, with a focus on checking whether the optimization indicators corresponding to the parameter values are consistent. If there is a slight deviation, the parameters can be adjusted according to the actual production situation and verified again. If the deviation is large, it will return to the calculation process to check for data input or algorithm settings. It is not necessary to conduct all experiments again, which not only meets the actual efficiency requirements of chemical production, but

also makes the verification results more practical. Ordinary staff can complete the entire verification process with daily operational experience.

4. Typical Application Domains of Uniform Design in Chemical Engineering Optimization

4.1 Optimization of Chemical Reaction Processes and Process Parameters

Uniform design has practical applications in chemical reaction processes and process parameter optimization, especially suitable for screening reaction conditions under the influence of multiple factors. It can find suitable parameter combinations without conducting a large number of repeated experiments, which is evident in the reaction of turpentine preparation to umbrella hydrocarbons. Turpentine is a common renewable natural chemical raw material in China. Its main component can be converted into p-cymene through catalytic reaction. This product is widely used in daily related fields such as food essence preparation. Pd/C-H₂SO₄ composite catalyst is the key catalytic material for this reaction. The amount of catalyst, acid oil ratio, stirring speed, reaction temperature and reaction time will affect the reaction effect. Uniform design, through reasonable arrangement of experiments and scientific setting of different experimental conditions within the determined range of factors, avoids the tedious process of comprehensive experiments and accurately identifies the inherent connections between various factors. Ultimately, the optimal process conditions suitable for the reaction are screened, allowing turpentine oil to be more efficiently converted into para xylene, adapting to the actual production needs of small and medium-sized spice enterprises, and avoiding the problems of long traditional reaction processes and high equipment requirements (Wang, Chen, Xu et al., 2010).

4.2 Synthesis of New Materials and Product Formulation Design

Waterborne nano polyacrylate wood coatings are commonly used in daily life as environmental protection coatings. They are characterized by no odor and low pollution, and are suitable for home decoration, furniture painting and other scenarios. However, the compound ratio of nano acrylic copolymer lotion and nano water-based polyurethane dispersion, and the addition amount of nano zinc carbonate and dispersant in the formula will directly affect the hardness, impact resistance and water resistance of the coatings. If the ratio is not correct, the coating film will be easy to crack and fall off when stained with water. Uniform design can sort out the intrinsic relationships between various proportioning factors in a small number of experiments, without testing all combinations one by one like traditional experiments, saving experimental consumables and time costs. It can also accurately screen the best formula that meets daily usage needs. Nano zinc carbonate, as a key additive in coatings, requires a uniformly designed experimental arrangement to fully exert its effect and avoid the situation where nanoparticle aggregation cannot enhance the toughness of the coating. The final formulated coating has fast drying speed, easy application, and coating hardness and water resistance can also meet the basic requirements for daily furniture use (Cao, Zhang, & Liao, 2008). This is also a common application form of uniform design in the optimization of civil new material formulations.

4.3 Optimization of Chemical Analytical Instruments and Testing Conditions

High performance liquid chromatography is a commonly used instrument in chemical analysis, widely used in daily related fields such as traditional Chinese medicine component detection. This instrument is often used to detect the content of paeoniflorin in *Paeonia lactiflora*. As the main active ingredient in *Paeonia lactiflora*, the accuracy of paeoniflorin detection is directly related to the quality control of traditional Chinese medicine products. In the testing conditions of high-performance liquid chromatography, factors such as flow ratio, detection wavelength, and flow rate can all affect the accuracy of paeoniflorin detection. If the conditions are not set properly, problems such as overlapping detection peaks and poor peak shape may occur, making it difficult to accurately determine the content of paeoniflorin. Uniform design can sort out the inherent correlation between these testing conditions within a limited number of experiments, without the need to repeatedly adjust individual conditions like traditional detection, saving detection reagents and time. It can also accurately screen for the best testing conditions suitable for paeoniflorin detection. Under these optimized conditions, high-performance liquid chromatography can clearly display the detection peak of paeoniflorin, avoiding the influence of interference peaks and making the detection of paeoniflorin more accurate. It is suitable for the actual detection needs of traditional Chinese medicine processing plants and small detection institutions. This application form is very common in routine detection of traditional Chinese medicine components and is also a concrete manifestation of uniform design in the field of chemical analysis that is in line with reality (Peng, Lu, & Zhang, 2011).

4.4 Reaction Kinetics Model Identification and Parameter Estimation

Reaction kinetics model is an important way to describe the correlation between reaction rate and influencing factors in chemical production. Ethyl acetate catalyzed hydrolysis reaction is a common chemical reaction in daily life, and its products acetic acid and ethanol are widely used in food, daily chemical and other fields. This reaction commonly uses HZSM-5 zeolite molecular sieve as a catalyst, and the parameter estimation of the reaction kinetics model requires a large amount of experimental data support. Traditional experimental methods require setting up numerous experimental groups to obtain sufficient data, which not only consumes a lot of reagents and time, but also easily leads to parameter estimation bias due to unreasonable distribution of experimental points. Uniform design can reasonably arrange experimental points, obtain effective data that can meet model identification in a small number of experiments, without blindly increasing the number of experimental groups. It can also accurately sort out the correlation between water ester ratio, reaction temperature, catalyst concentration and reaction rate, and thus complete the parameter estimation of the reaction kinetics model. The reaction kinetics model relies on these optimized parameters to better fit the actual reaction situation, avoiding the problem of large errors in traditional parameter estimation and adapting to the actual production modeling needs of small and medium-sized chemical enterprises. It can achieve accurate estimation of model parameters without the need for complex experimental equipment, which is in line with the actual conditions of ordinary chemical production.

4.5 Optimization of Energy Chemical and Green Chemical Processes

Biodiesel is a commonly used environmentally friendly energy source in daily life, suitable for household fuel equipment and small heating equipment. Its preparation often uses soybean oil as raw material, which is converted through ester exchange reaction. Sodium hydroxide is commonly used as a catalyst in this reaction. The ratio of methanol to soybean oil, the amount of catalyst used, the reaction temperature, and the reaction time in the reaction all directly affect the preparation effect of biodiesel. If the conditions are not properly controlled, problems such as insufficient conversion of raw materials, insufficient purity of products, and waste of raw materials and reagents may occur. Uniform design can reasonably arrange experimental points and sort out the inherent relationships between various influencing factors in a small number of experiments, without blindly testing all condition combinations like traditional preparation experiments, saving the consumption of raw materials such as soybean oil and methanol, and accurately screening the optimal reaction conditions for the preparation of biodiesel. Under these optimized conditions, soybean oil undergoes ester exchange reaction, which can be fully converted into biodiesel, avoiding the problems of raw material waste and insufficient product purity. It is suitable for the actual production needs of small environmental energy processing plants, without the need for complex production equipment, and meets the practical requirements of green chemical energy conservation and consumption reduction. It is also a common application of uniform design in the field of civil environmental energy (Ma, Liu, Ji et al., 2010).

5. Conclusion

With its unique ability to explore space as a means of establishing a complete methodology from theory to practice in optimization calculations regarding chemical engineering; Uniformly designed processes are both a bridge between experimental design and model optimization as well as an essential computational tool for driving innovation in processes and products. As we move into the future with even more complex chemical systems will come additional opportunities for utilizing data science and machine intelligence to further exploit the capabilities of uniformly designed processes in innovative areas such as green synthesis and smart manufacturing while continuing to assist in developing the chemical industry toward increased efficiency, precision and sustainability.

References

- Cao, Y. J., Zhang, G. Q., & Liao, Z. W. (2008). Application of Uniform Design in Optimizing Conditions for Solubilizing Phosphate Rock Powder Using Nanomaterials. *Journal of South China Agricultural University*, 29(3), 3.
- Fang, K. T. (1980). Uniform Design: Application of Number Theory Methods in Experimental Design. *Acta Mathematicae Applicatae Sinica*, 1980(04), 73-82.
- Liu, W. R., & Pang, S. Q. (1995). Comparison of Orthogonal Designs and Uniform Designs (II). *Mathematical Statistics and Management*, 3.

- Ma, L. C., Liu, D. H., Ji, Y. Q. et al. (2010). Study on Optimal Process Parameters for Biodiesel Production Based on Uniform Design. *Journal of Xi'an Petroleum University: Natural Science Edition*, 25(4), 83-86.
- Peng, X. X., Lu, S. S., & Zhang, Z. W. (2011). Optimization of Paeoniflorin Extraction Process from Paeoniae Radix Rubra Using Mixed Uniform Design Effect Surface Method. *Chinese Pharmacy*, 22(11), 3.
- Wang, L. L., Chen, X. P., Xu, X. et al. (2010). Application of Uniform Design in Direct Preparation of p-Cymene from Turpentine Oil by Liquid-Phase Method. *Food Industry Science and Technology*, 2010(2), 3.
- Wang, Y., & Fang, K. T. (1981). A NOTE ON UNIFORM DISTRIBUTION AND EXPERIMENTAL DESIGN. *A Monthly Journal of Science*, 26(6), 485-485.