

Design-Expert to Streamline Chemical Engineering Experimental Research and Development: Mixed-Method Perspectives

Rishen Roopchand*

Department of Chemical and Materials Engineering, University of South Africa, Johannesburg, 1709, South Africa
roopcr@unisa.ac.za

Naadhira Seedat

Department of Chemical Engineering, University of Pretoria, Pretoria, 0028, South Africa, naadhira.seedat@up.ac.za

Olawumi Oluwafolakemi Sadare

Energy and Bioproducts Research Institute, College of Engineering and Physical Sciences, Aston University, Birmingham B4 7ET, United Kingdom, wumisadare@gmail.com

Kapil Moothi

School of Chemical and Minerals Engineering, North-West University, Potchefstroom, 2250, South Africa, kapil.moothi@nwu.ac.za

Abstract

This paper presents an overview of Design-Expert, a statistical experimental design tool, in optimizing chemical engineering research and development. A mixed-method approach is adopted in the study by using quantitative literature findings of diverse experimental studies incorporating the use of Design-Expert and qualitative findings stemming from a focus group study with four cross-institutional chemical engineering research supervisors. While the quantitative literature studies demonstrate the effectiveness and capabilities of Design-Expert across multiple fields of study, the qualitative study is based on the perspectives, experiences and recommendations of the research supervisors concerning Design-Expert. The qualitative study was structured with five main sections: the integration of Design-Expert into research activities, the effectiveness and outcomes of Design-Expert, management of academic priorities incorporating the use of Design-Expert, research skills and development concerning the training of postgraduate students in applying Design-Expert into their research, and the broader impacts and collaborations facilitated by Design-Expert. Overall, the findings indicate substantial positive findings concerning the productivity and quality of research outcomes incorporating the use of Design-Expert.

Keywords: Design-Expert; Experimental Research; Statistical Experimental Design; Research Optimization; Research and Development

1 Introduction

Chemical engineering academics typically balance four core responsibilities: teaching, research and supervision, community engagement, and academic leadership. Of these, research often receives the greatest emphasis, as it directly influences a university's global ranking and annual government funding. Unlike many other engineering disciplines, chemical engineering research is largely experimental, requiring extensive laboratory or pilot-scale work to generate meaningful results. Supervising numerous experimental projects across undergraduate and postgraduate levels presents logistical challenges, including delays in equipment and materials procurement, scheduling bottlenecks for shared instruments, and prolonged

analysis times. These factors frequently hinder timely project completion. To address such challenges, this paper explores the potential of Design-Expert, a statistical software package widely used for experimental design (DoE), data analysis, and process optimization. The software's intuitive interface and detailed analytical outputs provide valuable insights that can enhance experimental research efficiency. As technological innovation continues to transform pedagogical practices in higher education (Roopchund, 2022; Roopchund & Seedat, 2023), similar innovations in research practice are equally vital. This paper therefore outlines the value of Design-Expert in chemical engineering research, drawing on recent literature and the authors' experiences as chemical engineering academics at a South African university. The discussion highlights specific cases where Design-Expert has supported research progress and completion.

2 Literature Review

2.1 Overview of Design-Expert Optimizations

According to Njoku and Otisi (2023), quadratic models are typically used when dealing with several response factors, while the experimental central composite design (CCD) forms part of the optimization process. Statistically, a CCD is helpful in response surface methodology (RSM), for creating a quadratic model without using a three-level factorial experiment (Bhattacharya, 2021). After performing the designed experiment, iterative linear regression is used to obtain results. Optimizations are done by identifying and improving the independent factors, before RSM can be used to establish relationships between the process variables and their responses.

Overall, design of experiment (DoE) is a statistical approach that involves planning, analyzing, conducting, and interpreting experimental data (Skartland et al., 2011). When dealing with a CCD, a response surface involves a dimensional plot of the experimental results. RSM describes the experimental designs through response surfaces (Skartland et al., 2011). A factor controls an outcome. The output change occurs by manipulating the input factor(s) and can be set at different levels depending on the experimental conditions. These levels could be high, mid, or low (three-level design) or only high and low (two-level design). A response is the result of the experiment's effect, caused by changing the values of the predictors. A model is an equation expressing the relationship between responses and the factors under investigation. The outcome can be represented as a function of the experimental factors.

Optimization design seeks to minimize undesired outputs or maximize desired outputs. Often, simple linear and interaction models inadequately represent the nuances of the process. Therefore, response surface designs are used for fitting quadratic models, of which the CCD and Box–Behnken designs (BBD) are most common.

2.2 Diverse Studies using Design-Expert

In the pharmaceutical study of Hooda et al. (2012), Design-Expert was used to optimize gastroretentive ranitidine HCl microspheres. Specifically, the study involved the development and optimization of drug entrapment and bio-adhesion of multi-unit chitosan-based floating system containing Ranitidine HCl by ionotropic gelation for gastroretentive delivery. In this study, the effect of various process variables, including the drug polymer ratio, sodium tripolyphosphate concentration and stirring speed on various physiochemical properties, such as drug entrapment efficiency, particle size and bio-adhesion was optimized using CCD and analyzed using RSM. The observed responses coincided well with the predicted values indicated by the optimization technique.

The chemistry study of Popoola (2019), aimed to investigate activated carbon prepared from walnut shell and rice husk wastes for Cd(II) removal from aqueous solution using artificial neural networks (ANN) and Design-Expert as the design and optimization tools. The results from the two-level factorial DoE indicated a 78.58% Cd(II) sorption efficiency at optimum calcination temperature, calcination time, snail shell-rice husk mixing ratio and magnetite loading of 859.20 °C, 2.32 hours, 2.54 and 5.56 wt% respectively. The calcination

temperature was identified as the most influential factor in adsorbent preparation based on sensitivity analyses. The prepared adsorbent was found to effectively remove Cd(II) from solution to a greater extent than commercial activated carbon with economic viability.

The food technology study of Singh et al. (2020) aimed to optimize the drying of red grapes to raisins using Design-Expert. The grapes were dried using the independent variables of blended oil (1:1 ratio of olive and clove oil) and temperature, generating responses in terms of drying time, acidity, total sugars, ascorbic acid, and phenols. RSM optimization was undertaken in 13 runs. The optimum conditions were 11% blended oil concentration and 63.4°C drying temperature with drying time, acidity, total sugars, ascorbic acid, and phenols of 22.80 hours, 1.26%, 64.2%, 5.60 mg, and 924 mg, respectively. Considering the challenges of maintaining the nutritional quality and shelf stability of fresh harvest, the Design-Expert application in this study was beneficial. Furthermore, statistical modelling can maximise success rates, yielding shelf stable fruits (raisin) that explore the application of oil dehydration to other fruits and vegetables of immense nutrition and shelf stability concerns.

The water treatment study of Shokrollahi et al. (2020) aimed to apply computational fluid dynamics and Design-Expert to optimize potable (drinking) water desalination using membrane distillation. Membrane distillation causes steam to pass from the membrane due to temperature and vapor pressure differences. However, the technology requires development under different operating conditions. Hence, this study investigated the effects of flowrate, temperature, and module length on its performance. Statistical DoE was used to numerically model flux and thermal efficiency. The results showed that increasing flowrate, inlet feed temperature, and decreasing the membrane module's length increased the water flux and thermal efficiency. Numerical flux modelling showed that temperature, module length, and interaction module length-temperature parameters had the most influence on flux and module length, temperature and quadratic relation of module length parameters have the greatest effect on thermal efficiency, respectively.

The pharmaceutical study of Akram and Garud (2021) aimed to prepare a mesalamine nanocarrier system to treat colitis with increased efficacy and targeting. Optimization is critical for understanding nano formulation variables. Hence, statistical DoE using Design-Expert was used to determine the effect of the independent variables (concentrations of chitosan, carboxymethyl inulin, and the drug) on the response variables (particle size and entrapment efficiency of the mesalamine-loaded nanoparticle using BBD). The correlation between the independent and dependent variables was investigated using the generated mathematical equations, contour, and response surface designs. An optimized batch was developed using the ionotropic gel method with selected independent variables and the developed nanoparticles had a particle size of 184.18 nm, zeta potential 26.54 mV, and entrapment efficiency 88.58%. The observed responses were similar to the predicted values. The developed nanoparticles were likely to have a small particle size with positive zeta potential and large extent of drug entrapment. BBD was found to actively optimize the formulation of the drug.

According to the review of Sopyan et al. (2022), optimized formulation is crucial in pharmaceutical drug development and is completed through lengthy laboratory experiments. Design-Expert can be applied to streamline this process. The review's findings suggest that Design-Expert is widely utilized and effective at reducing the number of trials, time, and costs associated with pharmaceutical formulation development.

In the process optimization study of Njoku and Otisi (2023), CCD was used to optimize Biodiesel yield from the transesterification of methanol and vegetable oil using Design-Expert. This optimization involved conditions of reaction time, methanol to oil ratio, catalyst loading, and reaction temperature. For a randomized experiment at a 95% confidence level, all the factors were found to affect the product's output. A 91% yield was obtained, and operating parameters were optimized at a temperature of 61 °C, methanol to oil ratio of 22.13, and catalyst loading of 3.7 wt%.

2.3 Conclusion of Literature Findings

It is noteworthy that Design-Expert has several diverse applications in pharmacy (Hooda et al., 2012; Akram and Garud, 2021; Sopyan et al., 2022), chemistry (Popoola, 2019), food technology (Singh et al., 2020), water treatment (Shokrollahi et al., 2020), and process optimization (Njoku and Otisi, 2023). Each of these studies reported positive application and optimization capabilities of Design-Expert. In certain studies, the capabilities of Design-Expert were combined with other tools, such as artificial intelligence (Popoola, 2019) and computational fluid dynamics (Shokrollahi et al., 2020). However, despite several experimental (quantitative) studies showcasing the positive features of Design-Expert in the literature, there is a lack of qualitative evidence supporting the use of Design-Expert in research and development. Therefore, this study aims to provide qualitative evidence based on the perspectives of chemical engineering higher education research supervisors.

3 Methodology

The first part of the methodology entailed obtaining quantitative information regarding the use of Design-Expert from the literature. A simple search strategy was employed, which favoured the perspectives of recent and diverse studies. These studies were identified and presented in the literature review to demonstrate a contextualised application basis for Design-Expert, and the way it was integrated into optimization procedures across a range of study areas. The authors' own studies were also included in the literature review. In the second part of the methodology, artificial intelligence was prompted to provide key questions to the research supervisors and authors of this study. The questions were prompted with the aim of identifying the key qualitative themes that enable the effectiveness of Design-Expert to be harnessed by research supervisors to ensure optimal completion of postgraduate research projects- especially against the backdrop of competing academic priorities.

AI-enabled Qualitative Analysis Setup

The following prompts were used to guide the AI software (ChatGPT) to output the qualitative questions used in the qualitative study.

Prompt 1: I am writing a conference paper, titled: "Design-Expert to streamline chemical engineering experimental research and development" are you familiar with the use of Design-Expert in relation to this title/topic?

Prompt 2: Please propose interview questions to ask research supervisors regarding the use and application of Design-Expert in their work/research. Specifically, please provide key questions to the research supervisors to identify the key qualitative themes that enable the effectiveness of Design-Expert to be harnessed by research supervisors to ensure optimal completion of postgraduate research projects- especially against the backdrop of competing academic priorities.

Prompt 3: Please provide a motivation for each section of the questions and indicate what type of themes can be drawn from the question sections.

Based on these prompts, the AI-generated qualitative questions are shown in Table 1.

Table 1. Qualitative Interview Questions

Question	Motivation	Themes
Section 1: Integration into Research		

1. How do you incorporate Design-Expert into the planning stages of postgraduate research projects?	Investigating how supervisors integrate Design-Expert into the early stages of research helps to understand the strategic role the software plays. This section also uncovers how it's embedded into the research planning process, which is crucial for aligning resources and timelines.	<ul style="list-style-type: none">• Strategic Planning and Research Workflow• Integration into Experimental Design• Early-Stage Decision-Making and Tool Selection
2. What specific features of Design-Expert do you find most valuable for achieving research objectives?		
Section 2: Effectiveness and Outcomes		
3. In your experience, how has Design-Expert contributed to optimizing experimental design and process efficiency?	Evaluating the effectiveness and tangible outcomes achieved using Design-Expert allows you to determine how impactful the software is in producing high-quality research. This section identifies both qualitative and quantitative benefits that the software brings.	<ul style="list-style-type: none">• Optimization and Process Efficiency• Quality of Research Outcomes• Software's Role in Innovation
4. Can you share examples where Design-Expert directly led to significant improvements in research outcomes?		
Section 3: Managing Academic Priorities		
5. How do you balance the time and effort needed to use Design-Expert effectively with other competing academic responsibilities?	Research supervisors often juggle multiple responsibilities, from teaching to administration. Understanding how they balance their use of Design-Expert amid competing demands highlights whether the software streamlines or complicates project management and supervision.	<ul style="list-style-type: none">• Time Management and Prioritization• Academic Workload and Resource Allocation• Balancing Software Use with Broader Academic Roles
6. What challenges have you encountered when guiding postgraduate students in using Design-Expert, especially when they are managing multiple research tasks?		
Section 4: Skills Development and Training		
7. What training or support do you provide to students to ensure they can fully harness the potential of Design-Expert?	This section explores the learning curve associated with Design-Expert and how supervisors approach skill development among postgraduate students. Effective training can be crucial for maximizing the software's potential in postgraduate research.	<ul style="list-style-type: none">• Training Approaches and Methods• Learning Curve and Usability• Student Competence and Autonomy in Software Use
8. How do you assess whether a student is ready to independently use Design-Expert for their research projects?		
Section 5: Broader Impact and Collaboration		
9. How does the use of Design-Expert influence collaboration between you, your students, and other research teams?	Understanding the role of Design-Expert in collaboration and communication among research teams provides insight into how it facilitates or hinders teamwork.	<ul style="list-style-type: none">• Collaboration and Team Dynamics• Cross-Disciplinary and Cross-Departmental Research

	This section also touches on cross-functional usage and its influence on broader research outcomes.	<ul style="list-style-type: none"> • Communication and Data Sharing
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According to the AI tool, these questions are designed to help uncover the qualitative themes related to the effective use of Design-Expert, including challenges, best practices, and the relationship between software use and academic pressures. Furthermore, the sections and themes provide a structured way to understand the current usage and impact of Design-Expert while offering qualitative insights into its role in balancing the demands of academic supervision with effective research project management.

4 Results and Discussion

Table 2: Qualitative Interview Results from the Supervisors/Researchers

	Supervisor			
	1	2	3	4
Section 1: Integration into Research				
1. How do you incorporate Design-Expert into the planning stages of postgraduate research projects?	When formulating postgraduate research projects, Design-Expert is used to optimize the number of experimental runs in the methodology protocol.	Students use Design-Expert during the conceptual stages in developing the methodology. Design-expert is used to guide the experimental conditions for each run to be conducted with the given variables.	Alignment of research goals and understanding of research constraints; validation of the design through modelling and simulations; experimental plan optimization to maximize data collection with fewer runs; to have a structured approach to data collection, data analysis and data interpretation.	Design-Expert was incorporated into the research by defining the research objectives and hypotheses, identifying the key variables, selecting the appropriate experimental design, and simulating and planning the experiments.
2. What specific features of Design-Expert do you find most valuable for achieving research objectives?	Design-Expert can reduce the number of experimental runs, reducing time and expenses, while outputting high-quality results used to optimize processes.	Composite design	Response Surface Methodology (RSM) allows for optimisation; ANOVA and Regression Analysis allows for statistical reliability and validation.	Design of experiment to systematically investigate the relationships between multiple factors and their effects on a response, optimizing processes or products efficiently.
Section 2: Effectiveness and Outcomes				
3. In your experience, how has Design-Expert contributed to optimizing experimental design and process efficiency?	Design-Expert can reduce the time and expenses needed to conduct laboratory trials, thus improving the overall efficiency of the experimental process.	Design-Expert provides a comprehensive experimental design appropriate for publication and covering all bases for the experimental work to be reliable.	Through optimal design selection, it minimizes the number of experimental runs needed, saving time and resources; optimization tools promptly identify best conditions for desired outcomes.	Design-Expert enables precise identification of key variables and interactions, reducing the number of experimental runs needed, and providing clear insights for process optimization, leading to more effective and resource-efficient research outcomes.

4. Can you share examples where Design-Expert directly led to significant improvements in research outcomes?	With limited time to complete my doctoral research during the COVID-19 pandemic, Design-Expert optimized the application of cellulose nanocrystals (CNCs) in green construction material reinforcement. The main publications include: (1) Using cellulose nanocrystals to improve the mechanical properties of fly ash-based geopolymer construction materials (Roopchund et al., 2022) and (2) Cellulose Nanocrystals: Plant Design for Up-scaled Production and Applications in Green Construction Materials (Roopchund, 2021).	An article was submitted to a journal in which Design-Expert or similar software was not used. The reviewers requested that Design-Expert/similar software be used to generate the experimental runs that should be conducted for the article to be considered.	As per the two studies listed: (1) Exploring students' responses to Design-expert in a Chemical Engineering laboratory module (Sadare et al., 2022a) and (2) Parametric optimization of the production of cellulose nanocrystals (CNCs) from South African corncobs via an empirical modelling approach. (Sadare et al., 2022b)	During the production of biodiesel and synthesis of cellulose nanocrystals.
Section 3: Managing Academic Priorities				
5. How do you balance the time and effort needed to use Design-Expert effectively with other competing academic responsibilities?	I integrate Design-Expert into the development of the experimental plan for students' research proposals. Through this integration, there is no separate endeavour/effort to incorporate Design-Expert into my research activities.	Once the principles behind Design-Expert are understood, it does not take much time to perform the simulations.	By focusing on using Design-Expert for key experiments that will significantly impact research outcomes; collaboration with others (working with colleagues or students familiar with the software) gradually enhance proficiency with the software over time.	Design-Expert was used by undergraduate students during the 'Chemical Engineering Laboratory' module. The students were taught how to use the software and were monitored.
6. What challenges have you encountered when guiding postgraduate students in using Design-Expert, especially when they are	Sometimes, it is difficult for postgraduate students to grasp the concept of statistical experimental design using Design-Expert. To alleviate this	The main challenge is providing students with the appropriate training to use Design-Expert. Without the training, students struggle to use the software and rather	Students experience a learning curve and often struggle with using the software while undertaking other research tasks; not completely understanding the	I've encountered challenges in helping postgraduate students grasp the complexity of selecting the appropriate experimental design amidst their multiple research tasks,

managing multiple research tasks?	problem, I developed a guide to help students.	spend time in research tasks they can do.	data interpretation with respect to the software's output and over-reliance on the software without fully grasping the underlying concepts.	and ensuring they fully understand the software's statistical outputs while balancing their time and resources. Additionally, students often struggle with integrating the software's advanced features into their broader research workflow without becoming overwhelmed by the technical details.
Section 4: Skills Development and Training				
7. What training or support do you provide to students to ensure they can fully harness the potential of Design-Expert?	I created a step-by-step guideline (with pictures of each step) to help my postgraduate students manage their statistical experimental designs using Design-Expert.	YouTube videos were provided to students to learn how to use the software. Additionally, an experienced colleague provided guidance to students.	Support via senior students and colleagues to help address individual challenges and materials such as online resources via YouTube and other similar websites.	The students were trained on how to use Design-Expert on the University's learning management system.
8. How do you assess whether a student is ready to independently use Design-Expert for their research projects?	I review the students' initial experimental designs to determine if they are competent in using Design-Expert. I also ensure that the selected factors, responses and ranges are sensible.	This is a difficult question to answer. I believe that every simulation a student runs on Design-Expert should be checked and further evaluated by the subject experts to ensure the results are appropriate.	By assessing the application of the software (observing students' application of Design-Expert in preliminary experiments) one can gauge how students are coping.	The students were given tasks to do to ensure they grasped the concept of Design-Expert. However, they were guided throughout the process of using it.
Section 5: Broader Impact and Collaboration				
9. How does the use of Design-Expert influence collaboration between you, your students, and other research teams?	I find that experimental research can progress at a quicker rate using Design-Expert, implying that more time is created to spend on research publications. Thus,	The collaboration between myself and the student is essential as we analyse the results from the simulations. Collaborations with senior colleagues and/or supervisors are also evident in finalising	Provides a common platform for planning and optimization of experiments.	The students worked in groups. Therefore, Design-Expert facilitates collaboration by providing a common platform for clearly defining experimental designs, sharing data, and analyzing results,

	collaborations can be made more fruitful.	the experimental design obtained from Design-Expert. However, I do not feel that it has led to collaborations with other research teams.		which enhances communication, ensures consistency across research teams, and accelerates the decision-making process, leading to more cohesive and coordinated research.
10. In your opinion, what qualitative factors determine the successful application of Design-Expert in completing research projects on time?	Firstly, students' overall confidence and command in undertaking their experimental trials. Secondly, the ease and pace of conducting experimental trials. Finally, students' ability to use the Design-Expert outputs (such as the three-dimensional response surface models) to create high-quality research outputs.	It refines the number of experimental runs that must be completed to produce valid and reliable data, including base and reference runs. Without the use of Design-Expert the number of experimental runs is not defined and may have to continually be added, which wastes time and resources.	It allows for effective planning by facilitating a clear experimental design with corresponding objectives.	Qualitative factors like the user's familiarity with the software, clarity of the research objectives, team members' ability to communicate and collaborate effectively, and the ability to incorporate software-generated insights into practical decision-making throughout the project, in my opinion, determine the successful application of Design-Expert in completing research projects on time.

Supervisors widely recognized Design-Expert as a valuable tool for optimizing research methodologies, particularly in planning and defining experimental conditions. It enables efficient data collection with fewer runs, saving time and resources. Its RSM and ANOVA features allow detailed analysis of factor–response relationships, supporting process optimization. Overall, the supervisors viewed Design-Expert as highly relevant to chemical engineering research. In reflecting on their experiences, supervisors noted that Design-Expert improved experimental efficiency, ensured reliable data, and increased the likelihood of publication. Its optimization capabilities helped identify optimal conditions and visualize variable interactions. For example, Supervisor 1 used Design-Expert during the COVID-19 pandemic to complete doctoral research on cellulose nanocrystals, resulting in a published article (Roopchund et al., 2022). Supervisor 2 applied it following reviewer feedback to refine experimental design, while Supervisors 3 and 4 published studies on biodiesel and CNC production using the software (Sadare et al., 2022a; 2022b). Collectively, these experiences demonstrate Design-Expert's effectiveness in streamlining experimental planning and execution.

Regarding integration, supervisors emphasized introducing Design-Expert early in postgraduate research to build proficiency. Supervisor 4 further recommended exposing undergraduates to the tool to reduce learning barriers later. Although students often struggle initially with interpreting outputs, supervisors agreed that Design-Expert enhances research quality and innovation. To support student learning, supervisors employed diverse strategies, including step-by-step guides, online tutorials, peer training, and institutional learning resources. Regular feedback and practical exercises reinforced

understanding and autonomy. While some supervisors felt Design-Expert mainly improved individual efficiency, others found it encouraged collaborative experimentation and shared problem-solving. Successful application depended on confidence, effective planning, clear objectives, and familiarity with the software. Overall, Design-Expert was viewed as a powerful enabler of efficient, collaborative, and high-quality research.

5 Conclusions

This study indicated the applicability and optimization abilities of Design-Expert in Chemical Engineering research, as qualitatively documented by cross-institutional research supervisors. While the underlying concepts and statistical terms comprising Design-Expert may not be easily grasped by first-time student users, research supervisors are encouraged to provide resources, tools, and training to their students, to guide them through the application of Design-Expert in their studies. Based on the qualitative findings, Design-Expert was found to optimize the time, resources, and costs associated with experimental research. Hence, the authors recommend the use and application of Design-Expert in engineering and related experimental research. Considering the workload of academic staff members, Design-Expert was found to be a valuable tool in streamlining experimental research.

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