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DEVELOPMENT OF METAMODEL-BASED ROBUST SIMULATION OPTIMIZATION FOR COMPLEX SYSTEMS UNDER UNCERTAINTY

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By

AMIR PARNIANIFARD

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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DEVELOPMENT OF METAMODEL-BASED ROBUST SIMULATION OPTIMIZATION FOR COMPLEX SYSTEMS UNDER UNCERTAINTY

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December 2018

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Computer simulations can help a rapid investigation of various alternative designs to decrease the required time to improve the system. Because of the complexity for analyzing complex systems in way of mathematical formulation, a simulation optimization has been an interest in analyzing and studying the behavior of complex systems in the real world of engineering problems. One of the main difficulties of existing model–based simulation optimization methods is dealing with large number of required simulation evaluation (also called simulation experiments or computer experiments) which causes of costly computational time. In addition, in order to improve the validity of optimal results, uncertainty as a source of variability in the model's output(s) need to be considered while this importance mostly has been ignored in designing of existing simulation optimization models. Under uncertainty, simulation running with stochastic output is complex in terms of computational time and/or cost, therefore the limited number of simulations is desirable. However, the accuracy of simulation result strongly depends on the reality of computer coding and discrepancy between simulation model and actual physical system. Most existing simulation optimization methods need to be improved in such a way to handle conflicting of multiple responses and constraints. This research generally aims to develop the black-box simulation optimization technique to be applicable in stochastic complex systems under effect of uncertainty with the least optimization computational burden (number of simulation experiments). This research develops a new distribution-free method for uncertainty management with unknown distribution of uncertainty. This research also aims to show the applicability and validity of proposed metamodel-based robust simulation optimization method in practical engineering design problems such as direct speed control of DC motor and PID tuning under uncertainty. For this purpose, metamodeling techniques are used for global approximation of complex simulation model. The statistical terminology of Taguchi crossed array design is replaced by global modern metamodels. A distribution-free method is suggested to tackle the lack of information about possible probability distribution of uncertainty scenarios in the model. Results of this research confirmed the validity and applicability of the proposed methodology dealing with practical stochastic complex engineering design problems in three terms; reducing computational time, enhancing flexibility, and improving the applicability. The proposed method can reduce the number of function evaluations for PID tuning under uncertainty to 50 simulation runs compared to more than 1000 function evaluations in common model based method. Compared to classical Ziegler Nichols method, the proposed method shows the better performance which is more than 10% for PID tuning under uncertainty. The proposed distribution–free method applied in economic order quantity problem shows the same accuracy compared to studies in literature whereby this study does not need to estimate distribution of uncertainty.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah.

PEMBANGUNAN PENGOPTIMUMAN SIMULASI TEGUH BERASASKAN METAMODEL UNTUK SISTEM KOMPLEKS DI BAWAH KETIDAKPASTIAN

Oleh

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Simulasi komputer dapat membantu penyiasatan cepat pelbagai reka bentuk alternatif untuk mengurangkan masa yang diperlukan untuk memperbaiki sistem. Oleh kerana kerumitan untuk menganalisis sistem kompleks dalam bentuk rumusan matematik, simulasi pengoptimuman telah menjadi penting dalam menganalisis dan mengkaji tingkah laku sistem kompleks masalah kejuruteraan dalam dunia sebenar. Salah satu kesukaran utama kaedah simulasi pengoptimuman berasaskan model yang sedia ada adalah berurusan dengan sejumlah besar penilaian simulasi yang diperlukan (juga dikenali sebagai eksperimen simulasi atau eksperimen komputer) yang menyebabkan penggunaan masa pengkomputeran yang mahal. Di samping itu, untuk meningkatkan kesahihan keputusan optimum, ketidakpastian sebagai sumber kebolehubahan dalam output model perlu dipertimbangkan, walaupun kepentingan ini kebanyakannya telah diabaikan dalam mereka bentuk model simulasi pengoptimuman yang ada. Di bawah ketidakpastian, simulasi yang dijalankan dengan output stokastik adalah mahal dari segi masa dan / atau kos, oleh itu jumlah simulasi yang terhad adalah wajar. Walau bagaimanapun, ketepatan hasil simulasi sangat bergantung kepada realiti pengekodan komputer dan percanggahan antara model simulasi dan sistem fizikal sebenar. Kebanyakan kaedah simulasi pengoptimuman yang sedia ada perlu diperbaiki sedemikian rupa untuk menangani konflik pelbagai tindak balas dan kekangan. Kajian ini bertujuan untuk membangunkan teknik simulasi pengoptimuman kotak hitam untuk diterapkan dalam sistem kompleks stokastik di bawah kesan ketidakpastian dengan beban pengiraan pengoptimuman paling kurang (bilangan eksperimen simulasi). Penyelidikan ini membangunkan kaedah bebas pengedaran baharu untuk pengurusan ketidakpastian dengan pengagihan ketidakpastian yang tidak diketahui. Kajian ini juga bertujuan untuk menunjukkan kebolehgunaan dan kesahihan kaedah pengoptimuman yang berasaskan metamodel yang dicadangkan dalam masalah reka bentuk kejuruteraan praktikal seperti kawalan kelajuan langsung motor DC dan penalaan PID di

bawah ketidakpastian. Untuk tujuan ini, teknik metamodel digunakan untuk penganggaran global model simulasi kompleks. Istilah statistik reka bentuk crossed array Taguchi digantikan oleh metamodel moden global. Satu kaedah pengedaran bebas baharu dicadangkan untuk menangani kekurangan maklumat dalam senario ketidakpastian mengenai kemungkinan kebarangkalian taburan dalam model. Keputusan yang diperolehi dalam penyelidikan ini mengesahkan kesahihan dan kebolehgunaan kaedah yang dicadangkan dalam urusan masalah reka bentuk kejuruteraan kompleks stokastik praktikal dalam tiga segi; mengurangkan masa pengiraan, meningkatkan fleksibiliti, dan meningkatkan kebolehgunaan. Kaedah yang dicadangkan dapat mengurangkan bilangan penilaian fungsi untuk penalaan PID di bawah ketidakpastian hingga 50 larian simulasi dibandingkan dengan lebih daripada 1000 penilaian fungsi dalam kaedah berasaskan model biasa. Berbanding kaedah klasik Ziegler Nichols, kaedah yang dicadangkan menunjukkan prestasi yang lebih baik iaitu lebih daripada 10% untuk penalaan PID di bawah ketidakpastian. Kaedah bebas pengagihan yang dicadangkan yang digunakan dalam masalah kuantiti pesanan ekonomi menunjukkan ketepatan yang sama berbanding dengan kajian dalam literatur di mana kajian ini tidak perlu menganggarkan pengagihan ketidakpastian.

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Do not ever take your eyes from the sky
Because God lives
Sew eyes to see God as the sky
keep your head up
do not doubt . . .
God does not hide from you
He is the most interesting.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philoshophy. The members of the Supervisory Committee were as follows:

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Declaration by graduate student

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This is to confirm that:

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LIST OF ABBREVIATIONS

ACO	Ant Colony Optimizer
ANN	Artificial Neural Network
ANOVA	Analysis of Variance
BCI	Bootstrapped Confidence Intervals
CCD	Central Composite Design
DACE	Design and Analysis of Computer Experiments
DASE	Design and Analysis of Simulation Experiments
DC	Direct Current
DOE	Design OF Experiments
EOQ	Economic Order Quantity
EP	Evolutionary Programming
GA	Genetic Algorithm
GRA	Grey Relational Analysis
ISE	Integral Squared Error
LHS	Latin Hypercube Sampling
LTB	Larger The Better
MBRSO	Metamodel Based Robust Simulation Optimization
MIMO	Multi Input Multi Output
NTB	Nominal The Best
OA	Orthogonal Array
PID	Proportional-Integral-Derivative
PR	PR
PSO	Partial Swarm Optimization
RBF	Radial Basis Function
RD	Robust Design
RDO	Robust Design Optimization
RMAE	Relative Maximum Absolute Error
RMSE	Root Mean Square Error
RSM	Response Surface Methodology
SISO	Single Input Single Output
SSE	Sum Square Error
STB	Smaller The Better
STD	Standard Deviation

CHAPTER 1

INTRODUCTION

1.1 Background

Nowadays, developmental processes in engineering world are strongly associated with computer simulations. These computer codes can collect appropriate information about characteristics of engineering problems before actually running the process. Computer simulations can allow for rapid investigation of various alternative designs, so decreasing the required time to improve the system. In addition, most numerical analyses of engineering problems, makes a well-suited use of mathematical programming. Clearly, due to less computation burden, the simulation optimization becomes to find more interest and popularity than other real world optimization methods that be directed in way of mathematical formulation analyzing (Dellino et al., 2014). The main goals of simulation can be defined as first what-if study of model or sensitivity analysis and second is optimization and validation of model (van Beers & Kleijnen, 2003). The essential benefit of simulation is its ability to cover complex processes, either deterministic or random while eliminating mathematical sophistication (Figueira & Almada-Lobo, 2014). In practice, the simulation optimization problem is desirable to consider the possibility of shifting the problem into meaningless due to the existence of even a small uncertainty. Furthermore, due to adding uncertainty into the model, the computational complexity in design problems has increased. The complex analysis and simulation processes are due to the computation burden which caused by the physical or computer testing of data. Metamodels (also called surrogate models) are often used to address such a challenge. Regarding existing of uncertainty in complex and black box simulation models, simulation optimization leads to introduce advanced methods as Metamodel-Based Robust Simulation optimization (MBRSO).

1.2 Problem Statement

Here, four main shortcomings that raised among existing simulation-based optimization methods are highlighted. These gaps are considered throughout developing of metamodel-based robust simulation optimization methodology in this research.

i) Stochastic simulation model due to uncertainty (source of variability in the model)

There are different number of methodologies in optimizing of deterministic simulation (Amaran et al., 2016; Kleijnen, 2017), but there are few number of studies have been done on stochastic or random simulation optimization problems under uncertainty, particularly based on combination of metamodels and robust optimization (Simpson et al., 2001). The main gap for such a scenarios-based methods is that when uncertainty change in its variation region and previous results miss their validation, so the problem needs to be evaluated again by designer (Cao et al., 2015). There is still a gap between theory and practice in optimization under uncertainty, being evident in the fact that robust optimization methods are still not used in many real-world problems (Beyer & Sendhoff, 2007a; Dellino, et al., 2015; Gabrel et al., 2014; Geletu & Li, 2014; Wang & Shan, 2011). Ben-Tal et al. (2009) have claimed that the data of real world optimization problems are uncertain more often and not identified exactly when the problem is being solved. In simulation optimization under uncertainty usually cannot distinguish the exact (deterministic) solution for the black-box system, so the mean and the variance obtained from sampling points (i.e. stochastic or random simulation)(Amaran et al., 2016). In deterministic models, a response of model lacks random error, or in another mean, repeated runs for the same design of input parameters, the same result for the response can be gained from the model. On the other hand, the output in stochastic or random simulation usually follows some probability distribution that may vary around its space. As shown in Figure 1.1, in the stochastic model the running simulation for the same input combination gives different outputs.

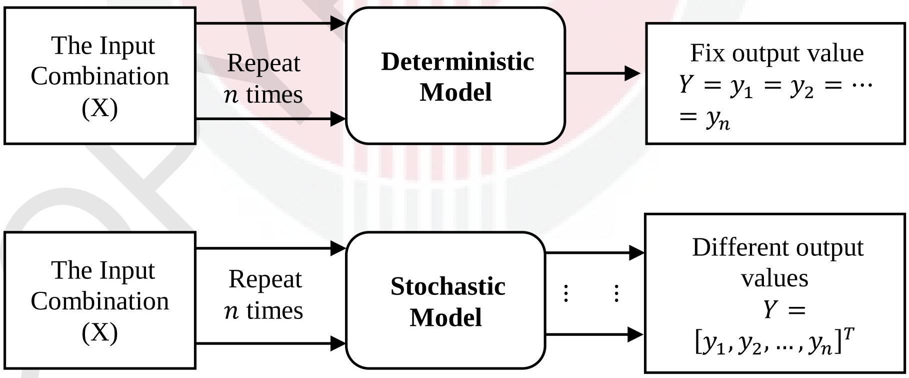

Figure 1.1: Deterministic and stochastic simulation models.

Except for PR, other types of metamodels like Kriging can hardly support stochastic simulation (Kleijnen, 2017; van Beers & Kleijnen, 2003). In this research, the uncertainty is defined as sources of variability on the model's output that causes obtained optimal results turn to be inferior. The reasons for uncertainty in data are classified in some parts. The first part is to measurement or estimation errors that arise from the impossibility to estimate the exact data on characteristics of physical processes. Second, implementation errors arising from the impossibility to implement an exact solution as it is estimated before.

ii) Complexity of simulation models

Many large scales and detailed simulation models in complex system particularly under uncertainty may be complex to run in terms of time-consuming, computational cost, and resources (Li et al., 2010; Wang & Shan, 2007). Hence, metamodel-based optimization of complex systems is a growing area (Bhosekar & Ierapetritou, 2018; Garud et al., 2017). In this research, complex systems are defined as simulation models with a large computational time or costly running of simulations. In existing model-based methods in the literature, the simulation running (also called simulation experiments or computer experiments) are not time consuming, so a true model (i.e. original simulation model) can be used directly in optimization.

iii) Applicability of metamodel based robust simulation optimization

The robust metamodeling techniques in the framework of engineering design have been used for academically usage more than for practical problems in the real world. Except for inventory management (Jalali & Van Nieuwenhuyse, 2015), the lack of enough research is completely sensible which apply robust metamodeling techniques into different engineering design problems or management science (Barton, 1992; Carson & Maria, 1997; Li et al., 2010; Simpson et al., 2001). Most methods which mentioned in literature just have been tested in theoretical settings of problems, so applying these methods in practical problems and in-depth comparing of their performance can be an interesting area for additional research (Dellino et al., 2009; Jalali & Van Nieuwenhuyse, 2015). There is still a gap between theory and practice in optimization, being evident in the fact that optimization methods are still not used in many real-world problems (Ehrgott et al., 2014). Kleijnen (2009) has emphasized on applying metamodels particularly Kriging in practical random simulation models, which are more complicated than the academic models. Moreover, in simulation optimization methods, the most important parameters of problems such as multi-response (Kleijnen, 2009b; Simpson et al., 2001; Teleb & Azadivar, 1994), constrained system (Fu et al., 2015), different stochastic distribution for uncertain variables (Kleijnen, 2015) need to be attended to be more applicable for practical problems. Different circumstances of real problems in simulation models have been studied by Beyer & Sendhoff (2007a), Gabrel et al. (2014), Geletu & Li (2014), and Wang & Shan (2011). Most methods which mentioned in simulation optimization area, just have been tested in theoretical settings of problems. Thus, applying these methods in practical problems and in-depth comparing of their performance need to be considered (Dellino, 2009; Jalali & Van Nieuwenhuyse, 2015). Kleijnen (2009) has emphasized on applying metamodels particularly Kriging in practical random simulation models, which are more complicated than the academic.

iv) Conflicting multiple objectives and constraints

Another shortcoming is raised when most simulation optimization methods use single variable output, whereas in practice, simulation models may have conflicted multivariable outputs (Kleijnen, 2009b; Simpson et al., 2001; Teleb & Azadivar, 1994). In the real world, a given simulation model has multiple outputs that also called responses or performance criteria (Kleijnen & Mehdad, 2014). Many of proposed approaches in simulation optimization are being developed for application of single objective optimization, while much of engineering design has been structured via multi-objective pattern. In most cases, some or all objectives and constraints are absolute functions of input variables that can be evaluated just by way of computer simulation (Teleb & Azadivar, 1994). Modern simulation optimization models allow for multiple simulation outputs, while choose one output as a goal and keep other remaining outputs as constraints and try to satisfy them (Kleijnen, 2010). Investigating all Pareto optimal solutions is computationally complex and time consuming, because in most cases, Pareto optimal solutions are usually exponentially large (Chinchuluun & Pardalos, 2007). In practice, difficulties arise because of different units of measurement, criteria, and levels of importance among the multiple responses or quality measurements. Moreover, some different methods have been presented which try to tackle the problem of optimizing multiple responses simultaneously (Marler & Arora, 2004; Miettinen, 2012). Chang et al. (2013) have criticized two common methodologies in multi-objective problems. They are combining all individual objective functions into single function by weighted sum method. This cause difficulty to select appropriate and accurate weights in practice. Secondly, all objectives are moved except one into constraint set that need to establish constraint values and increase problem complexity.

1.3 Research Objectives

The main goal of this thesis is to develop metamodel-based robust simulation optimization methodology in three aspects including i) improving flexibility of models, ii) enhancing applicability, iii) reducing computational complexity. The developed methodology has three main advantages, i) robust against uncertainty and source of variability, ii) simplicity and less computationally cost iii) ease to be applied in practice. Moreover, objectives of this research can be outlined systematically as:

First objective: To develop a distribution-free method applicable in metamodel-based robust simulation optimization.

Second objective: To verify the validity and applicability of metamodel-based robust simulation optimization (one-layer metamodeling).

Third objective: To verify the validity and applicability of metamodel-based robust simulation optimization (two-layer metamodeling).

Fourth objective: To compare the robustness and accuracy of different combination of metamodels and sampling design methods.

Fifth objective: To develop mathematical multi-objective and constrained metamodel-based robust simulation optimization models.

1.4 Scope of the Study

Throughout this study, all numerical test problems and case studies are selected to be small (i.e. one or two decision variables with one or two uncertain variables) or medium in dimension (i.e. three decision variables and two uncertain variables). Considering large dimension of problems (i.e. more than three decision variables or uncertain variables) is out of scope of this research. All problems are complex (i.e. computationally time consuming) so limited number of simulation evaluation is preferred. In addition, considering some subsidiary methods such as adaptive sampling design methods and sequential expected improvement are out of scope of this work. Due to existence of uncertainty (also called noise factors) in the model, deterministic optimization methods such as Genetic Algorithm (GA), Partial Swarm Optimization (PSO), Ant Colony Optimization (ACO) are not involved in optimization procedures. Moreover, due to stochastic framework of simulation optimization in this research, robust design terminology is used in order to minimize the sensitivity of optimization results against sources of variability. Methodologies that are developed in this study can be applied in the class of black-box problems, since it does not need to identify expression or internal structure of the system, but only analyzing output with given list of inputs. As shown in Figure 1.2, this research is considering general framework of black-box simulation model with three types of variables including decision variables (i.e. design variables or input factors), uncertain variables (i.e. noise or environmental factors), and response variables (i.e. output factors).

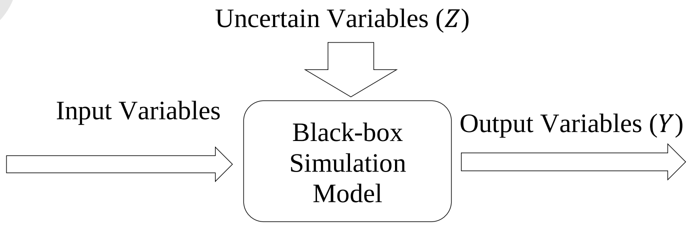

Figure 1.2: A black-box simulation model under uncertainty.

Therefore, any types of process under effect of uncertainty can apply the proposed methodology (i.e. multi-disciplinary application). This research is not limited to specific time or location. Any disciplines of engineering design problems can apply the proposed methods for designing and optimizing of relevant processes such as manufacturing, commercial, management, and different industries like electronic, telecommunication, oil, software, production, and construction.

1.5 Thesis Organization

This thesis is organized based on the style 2 (chapter 2, pages 10-11) of Guide to Thesis Preparation 2013, School of Graduate Studies, Universiti Putra Malaysia. The contents of this thesis are organized in the seven chapters. Thesis objectives and chapters crossing with general methodology of MBRSO is illustrated in Figure 1.3.

This thesis is arranged as followings.

Chapter 2: The main goal of this chapter is to represent a systematic reviewing of literature over subject of study. This chapter also includes discussions about recent development on comprehensive robust design optimization methods and metamodel based simulation optimization. In addition, the systematic review has been conducted among various types of optimization methods for black-box and complex simulation models under uncertainty.

Chapter 3: Throughout this chapter, the sequence steps of one-layer metamodeling technique on MBRSO methodology are explained. This chapter also proposing a novel method for simulation optimization when the probability distribution of uncertain variables is unknown. The proposed method uses the Taguchi robust terminology and the crossed array design when its statistical techniques are replaced by design and analysis of computer experiments and Kriging. At the end, two different case studies are provided to show the applicability and validity of MBRSO methodology with one layer-metamodeling technique with known and unknown probability distribution of uncertainty.

Chapter 4: This chapter aims to show the applicability and validity of MBRSO according two-layer metamodeling technique to reduce the computational complexity of robust tuning and analyzing the sensitivity of PID controller under uncertainty in physical load parameters. In this study, two-layer Kriging metamodeling technique is combined with Taguchi viewpoint on robust design to construct robust optimization model in the class of dual response. Randomness in uncertainty to design simulation experiments is analyzed through bootstrapped Kriging metamodels by computing confidence regions. Results confirm better performance in terms of expected Integral Squared Error (ISE) and robustness against both environmental disturbances and uncertainty in load parameters compared to traditional Ziegler-Nichols method and Grey Relational Analysis (GRA).

	Chapter 3		Chapter 4	Chapter 5	Chapter 6
	Objective 1	**Objective 2**	**Objective 3**	**Objective 4**	**Objective 5**
Start					
Identify problem characterization	EOQ inventory control problem under uncertainty	Direct speed control of DC motor under uncertainty	Robust optimal design of PID controller under uncertainty	5 mathematical test problem and EOQ inventory problem under uncertainty	Mixture Production problem under uncertainty
Choose the appropriate strategy	Distribution-free metamodel-based robust simulation optimization (one-layer metamodeling)	One-layer metamodeling technique on metamodel-based robust simulation optimization	Two-layer metamodeling technique on Metamodel-based robust simulation optimization	One-layer metamodeling technique on metamodel-based robust simulation optimization	Metamodel-based multi-objective constrained robust optimization
Design and run simulation experiments (computer base)	Latin Hypercube Sampling (LHS)	LHS	LHS	- LHS-randomized - LHS-Maximin - LHS-Correlation - Orthogonal array	Central Composite Design (CCD)
Fit metamodel on experiment results	Kriging	Kriging	Kriging	- Polynomial regression - Kriging - Radial Basis Function (RBF)	Polynomial regression
Validate metamodel	Leave-one out cross validation	Leave-one out cross validation	Leave-one out cross validation	Root Mean Square Error (RMSE)	R-Square
No Metamodel can fit the model? Yes					
Robust design optimization via metamodeling	Robust dual surface design	Four different forms of robust dual surface design	Robust dual surface design	Robust dual surface design	Taguchi quality loss function
Solve the model	Grid search method-Estimate Pareto frontier	Grid search method-Estimate Pareto frontier	Grid search method-Estimate Pareto frontier	Grid search method-Estimate Pareto frontier	Two mathematical programing models
Sensitivity analysis	Distribution-free bootstrapping method	--	Bootstrapping method	--	--
Yes No Results satisfy model requirements					
Finish					

Figure 1.3: Research objectives and general procedure of MBRSO.

Chapter 5: In this chapter, a systematic comparative study is implemented to evaluate the performance of three common metamodels namely PR, Kriging, and RBF. The required experiments are designed by different space-filling methods including the Orthogonal Array (OA) design and three forms of Latin Hypercube Sampling (LHS) such as randomized, maximin, and correlation approaches. Although, the impact of sample size on the performance of metamodels in robust optimization results are investigated. All methods are analyzed using five two-dimensional test problems and one engineering problem while all of them are considered in two forms that are complex (with a small sample size) and semi-complex (with a large sample size). Uncertainty is in all problems as a source of variability, so all test problems are conducted in the format of robust optimization in the class of dual response surface in order to estimate robust Pareto frontier. The performances of methods are studied in two terms of accuracy and robustness.

Chapter 6: In this chapter, a novel multi-objective robust optimization model is introduced to investigate the best levels of design variables. The primary objective is to minimize the production cost while increasing robustness and performance. The response surface methodology is utilized as a common approximation model to fit the relationship between responses and design variables in the worst-case scenario of uncertainty. The target mean ratio α is applied to ensure the quality of the process by providing the robustness for all types of quality characteristics and with a trade-off between variability and deviance from the ideal point. The L_p metric method is used to integrate all objectives in one overall function. In order to estimate target value of the quality loss by considering production tolerances, the process capability ratio (C_{pm}) is applied. At the end, a numerical chemical mixture problem is served to show the applicability of the proposed method.

Chapter 7: This thesis is concluded in Chapter 7, while main trends and gaps of proposed approaches are discussed. In this chapter, the important points of the study are highlighted and different suggestions for future research are directed.

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LIST OF PUBLICATIONS

❖ **Published (or In Press)**

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