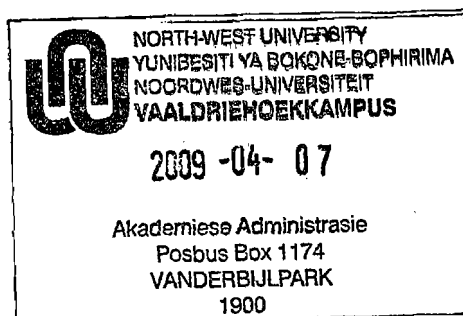


Design and analysis for efficient simulation in petrochemical industry

R.F. Rossouw
20507879

Dissertation submitted in partial fulfilment of the requirements for
the degree *Master of Science* at the Vaal Triangle Campus of the
North-West University

Supervisors: Prof. P.D. Pretorius
Dr. R.L.J. Coetzer



Abstract

Building an industrial simulation model is a very time and cost intensive exercise because these models are large and consist of complicated computer code. Fully understanding the relationships between the inputs and the outputs are not straight forward and therefore utilizing these models only for ad hoc scenario testing would not be cost effective. The methodology of Design and Analysis of Simulation Experiments (DASE) are proposed to explore the design space and pro-actively search for optimization opportunities. The system is represented by the simulation model and the aim is to conduct experiments on the simulation model. The surrogate models (metamodels) are then used in lieu of the original simulation code; facilitating the exploration of the design space, optimization, and reliability analysis.

To explore the methodology of DASE, different designs and approximation models from DASE as well as the Design and Analysis of Computer Experiments (DACE) literature, was evaluated for modeling the overall availability of a chemical reactor plant as a factor of a number of process variables. Both mean square error and maximum absolute error criteria were used to compare different design by model combinations. Response surface models and kriging models are evaluated as approximation models.

The best design by model combination was found to be the Plackett-Burman Design (Screening Phase), Fractional Factorial Design (Interaction Phase) and the Response Surface Model (Approximation Model). Although this result might be specific to this case study, it is provided as a general recommendation for the design and analysis of simulation experiments in industry.

In addition, the response surface model was used to explore the design space of the case study, and to evaluate the risks in the design decisions. The significant factors on plant availability were identified for future pilot plant optimization studies.

An optimum operating region was obtained in the design variables for maximum plant availability. Future research topics are proposed.

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Chapter 1

Introduction

1.1 Problem Setting

Computer Simulation refers to methods for studying a wide variety of models of real world systems by numerical evaluation using software designed to imitate the system's operations or characteristics, often over time. From a practical viewpoint, simulation is the process of designing and constructing a computer model of a real or proposed system for the purpose of conducting numerical experiments to obtain a better understanding of the behavior of that system for a given set of conditions. Although it can be used to study simple systems, the real power of this technique is fully realized when it is used to study complex systems (Kelton et al., 2002b; Kleijnen, 2008a; Law, 2007).

If the relationships that compose the model are simple enough, it may be possible to use mathematical methods to obtain exact information on questions of interest; this is called an analytic solution. However, most real-world systems are too complex to allow realistic models to be evaluated analytically, and these models must be studied by means of simulation. In a simulation a computer model is used to evaluate a model numerically, and data are gathered in order to estimate the desired true characteristics of a model. Simulation is one of the most widely used operations-research and management science techniques (Law, 2007).

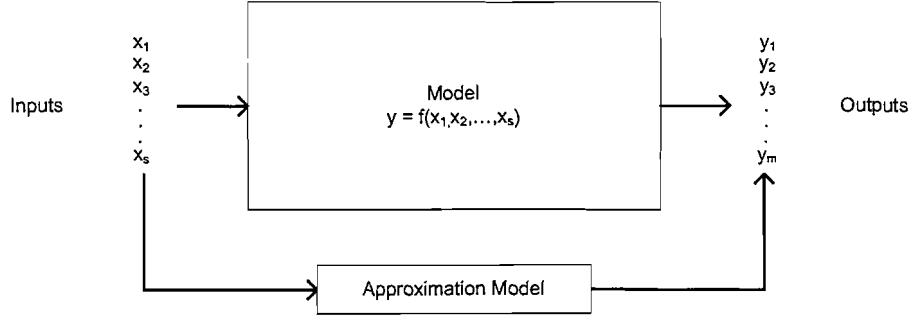


Figure 1.1: Computer model and experiments for an industrial system.

Thinking of the simulation logic and action as being a transformation of inputs into outputs the notion arises that a simulation is just a function, albeit a pretty complicated one that you cannot write down as some empirical formula. But it might be possible to approximate what the simulation does with some simple formula, which could be particularly useful if a large number of input factor combinations are of interest and it takes a long time (hours/days) to run the simulation (Kelton, 1997).

The relationship between the inputs to the system (input variables) $x = (x_1, x_2, \dots, x_s)^T$ and the outputs from the system (responses) $y = (y_1, y_2, \dots, y_m)^T$ can be expressed with the model (1.1).

$$y = f(x_1, x_2, \dots, x_s) \quad (1.1)$$

where f can be any analytical expression, mathematical or fundamental model, or can even be unknown. The computer experiment problem can be illustrated by the model in Figure 1.1. The system is represented by the simulation model and the aim is to conduct experiments on the simulation model (Coetzer and Langley, 2006). The surrogate models (metamodels) are then used in lieu of the original simulation code; facilitating the exploration of the design space, optimization, and reliability analysis. Building approximations for these computer simulations involves (a) choosing an experimental design to sample the computer code in the region of interest, and (b) constructing an approximation model on the observed sample data (Lin et al., 2001).

In experimental design terminology, the input parameters and structural

assumptions composing a model are called factors, and output performance measures are called responses. The decision as to which parameters and structural assumptions are considered fixed aspects of a model and which are experimental factors depends on the goals of the study rather than on the inherent form of the model. Also, in simulation studies there are usually several different responses or performance measures of interest (Law, 2007).

Factors can be either quantitative or qualitative. Quantitative factors naturally assume numerical values, while qualitative factors represent structural assumptions that are naturally quantified (Law, 2007).

Scientific experimental design is a sequential process (Box, 1999; Myers and Montgomery, 1995). The first phase of experimental design in simulation normally is to determine which factors have the greatest effect on a response. This is often called factor screening or sensitivity analysis. Carefully designed experiments are much more efficient than a hit or miss sequence of runs in which a number of alternative configurations are simply tried to observe what happens (Law, 2007).

The screening phase yields a first-order polynomial model with expected value

$$E(y) = \beta_0 + \sum_{j=1}^k \beta_j x_j \quad (1.2)$$

for k factors. In the second phase the first-order polynomial in (1.2) are augmented with two factor interactions, yielding the expected value:

$$E(y) = y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j}^k \sum_{j}^k \beta_{ij} x_i x_j \quad (1.3)$$

Interaction means that the effect of one factor depends on the levels of one or more other factors (Kleijnen, 2008a). Centre points are added to the design to test for curvature (Myers and Montgomery, 1995). Curvature indicates that there exist an optimum in the experimental region, and a possible need for a higher order polynomial model.

If curvature is present in the design region the interaction model in (1.3)

is augmented to a second-order polynomial of the general form:

$$E(y) = y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j}^k \beta_{ij} x_i x_j \quad (1.4)$$

If the goal of the study is prediction, kriging metamodels can be used instead of polynomial models (Kleijnen, 2008a).

The metamodel fitted to the experimental data is used to:

- *Predict* the model response for system configurations that were not simulated.
- Find that combination of input-factor values that *optimizes* a response, using what is called *response-surface methodology* (Law, 2007). This can be either an optimal point, or an optimal region.

The benefit in using an experimental design approach to finding the optimum instead of using one of the commercial “simulation optimizer” programs is two-fold:

1. In most industrial projects the response of interest is not easily computed, and is done outside of the model run by importing the model output into an external software package.
2. An experimental design approach not only indicates an *optimum* value or region, it also provides additional information about the system. For example, a response surface model will provide the estimated coefficients of the factors, and their binary interactions (at least). The response surface model can be used to make predictions of the responses at any combination of the input variables within the experimental region, or to evaluate the change in the predicted response with changes in the design variables.

Design and analysis of computer experiments has received a lot of attention in recent years (Kleijnen, 2008a; Lin, 2003; Lin et al., 2001; Santner et al., 2003; Simpson et al., 1998). The majority of the work is performed on

deterministic computer models in contrast with simulation models. A simulation model is more similar to physical experiments in the sense that the outcome of each experiment is a random value. Therefore, replications are required to estimate experimental error. The simulation model is however still a computer model, and the benefits of design and analysis of computer experiments may be realized in these models as well.

Therefore, in this study experimental designs commonly used in the Design and Analysis of Computer Experiments and Classical Experimental Designs are compared for use in simulation experiments. Different metamodels are also evaluated for the approximation of the input-output relationships.

1.2 Literature Review

1.2.1 Simulation

Computer Simulation refers to methods for studying a wide variety of models of real world systems by numerical evaluation using software designed to imitate the system's operations or characteristics, often over time. A simulation model is a dynamic model that is meant to be solved by means of experimentation (Kelton et al., 2002a; Kleijnen, 2008a).

In a simulation a computer is used to evaluate a model numerically, and data are gathered in order to estimate the desired true characteristics of a model (Law, 2007).

Some advantages of simulation studies are (Law, 2007):

- Most complex, real-world systems with stochastic (random or probabilistic) elements cannot be described by mathematical models, and need simulation.
- Simulation helps one to estimate the performance of an existing system under some projected set of operating conditions.
- Alternative proposed system designs can be compared via simulation to determine which best meets a specific requirement.

-
- In a simulation much better control can be maintained over experimental conditions than would generally be possible when experimenting with the system itself.
 - Simulation allows the study of the system over a long time frame.

There are also a few disadvantages to simulation, for instance (Law, 2007):

- Simulation models are complex programs, and takes a lot of time and skill to write.
- Simulation models are very computing intensive, and a large amount of computer time is required.
- Simulation models do not give an “optimal” solution. Experimentation with the model should be used to find a good solution.
- Each run of a stochastic simulation model produces only estimates of the model’s true characteristics for a particular set of parameters.
- The large volume of numbers produced by a simulation study or the persuasive impact of a realistic animation often creates a tendency to place greater confidence in a study result than is justified.

Shannon (1998) summarizes the steps of a simulation study as:

1. **Problem Definition.** Clearly defining the goals of the study so that the purpose is known, i.e. why are this problem being studied and what questions do the study hope to answer?
2. **Project Planning.** Being sure that sufficient and appropriate personnel, management support, computer hardware and software resources are available to do the job.
3. **System Definition.** Determining the boundaries and restrictions to be used in defining the system (or process) and investigating how the system works.

-
4. **Conceptual Model Formulation.** Developing a preliminary model either graphically (e.g. block diagram or process flow chart) or in pseudo-code to define the components, descriptive variables, and interactions (logic) that constitute the system.
 5. **Preliminary Experimental Design.** Selecting the measures of effectiveness to be used, the factors to be varied, and the levels of those factors to be investigated, i.e. what data need to be gathered from the model, in what form and to what extent.
 6. **Input Data preparation.** Identifying and collecting the input data needed by the model.
 7. **Model Translation.** Formulating the model in an appropriate simulation language.
 8. **Verification and Validation.** Confirming that the model operates the way the analyst intended (debugging) and that the output of the model is believable and representative of the output of the real system.
 9. **Final Experimental Design.** Designing an experiment that will yield the desired information and determining how each of the test runs specified in the experimental design is to be executed.
 10. **Experimentation.** Executing the simulation to generate the desired data and to perform sensitivity analysis.
 11. **Analysis and Interpretation.** Drawing inferences from the data generated by the simulation runs.
 12. **Implementation and Documentation.** Reporting the results, putting the results to use, recording the findings, and documenting the model and its use.

In general, great effort is made by the modeler to make sure that items 1 to 4 are executed correctly. However, the other terms listed above do not receive the same amount of attention. This study will focus on steps 5, 9 and 11.

1.2.2 Design and Analysis of Simulation Experiments

A *simulation model* is a dynamic model that is meant to be solved by experimentation. *Design and Analysis of Simulation Experiments (DASE)* are the field of designing experiments for simulation models and analysing the results (Kleijnen, 2008a).

The essence of a simulation project is running the model and attempting to make sense of the results (Kelton, 2000). Simulation implies that the analysts do not solve their model by mathematical calculus; instead, they try different values for the inputs and parameters of their model in order to learn what happens to the models output (Kleijnen (2008a)). The goals of such a numerical experiment could be:

- Verification and Validation
- Sensitivity Analysis
- Optimization
- Risk Analysis

The process of building, verifying, and validating a simulation model can be arduous, but once it is complete, then it is time to let the model do the work. One extremely effective way of accomplishing this is to use experimental designs to help explore the simulation model. The field of Design of Experiments (DOE) has been around for a long time. Many of the classic experimental designs can be used in simulation studies, thus simulation experiments can be designed in the same way, and analyzed similarly in terms of measuring the effects of the variables and interactions among them. This is primarily due to the random variation found in physical and simulation experiments (Kleijnen, 2008a; Law, 2007).

The environments in which real-world experiments are performed can however also be quite different from the simulation environment. The statistical theory on Design Of Experiments (DOE) was developed for real, non-simulated experiments in agriculture in the 1920s, and in engineering, psychology, etc. since the 1950s. In real experiments it is impractical to

investigate many factors; ten factors seems a maximum. Moreover, it is then hard to experiment with factors that have more than a few values; five values per factor seems the limit. In simulated experiments, however, these restrictions do not apply. Indeed, computer codes may have hundreds of inputs and parameters - each with many values. Consequently, a multitude of scenarios may be simulated. Moreover, simulation is well suited to sequential designs instead of “one shot” designs, because simulation experiments are run on computers that typically produce output sequentially (apart from parallel computers, which are rarely used in practice) whereas agricultural experiments are run during a single growing season. So a change of mindset of simulation experiments is necessary (Kleijnen, 2008a; Law, 2007; Lin et al., 2001; Sanchez, 2007).

Some additional advantageous characteristics of simulation models that distinguish it from physical experimentation are (Law, 2007):

- Factors such as customer arrival rates that are in reality uncontrollable, can be controlled in the model.
- Unlike the situation in physical experiments, the basic source of randomness can be controlled. Thus, variance-reduction techniques such as common random numbers can be used to sharpen the conclusions.
- In most physical experiments it is prudent to randomize treatments and run order to protect against systematic bias contributed by experimental conditions, such as a steady rise in ambient laboratory temperature. Randomizing in simulation experiments is not necessary, assuming the random-number generator is working properly.
- For some physical experiments, it is only possible to make one replication for each combination of factor levels, due to time or cost considerations. Then, to determine whether a particular factor has a statistically significant impact on the response, it is necessary to make the, perhaps questionable, assumption that the response for each factor-level combination has the same variance. However, for many simulation models it is now possible to make multiple replications for each input-factor

combination, resulting in a simple procedure for determining statistical significance.

Some of the special challenges and opportunities when conducting a computer-based simulation experiment rather than physical experiments include (Law, 2007):

- What model configurations should be run?
- How long should the run be?
- How many runs should be made?
- How should the output be interpreted and analyzed?
- What's the most efficient way to make the runs?

A framework specifically geared toward simulation experiments can therefore be beneficial (Kelton, 2000; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007; Sanchez, 2007).

It is important that the simulation analysts pay attention to the design of their experiments. Careful planning, or designing, of simulation experiments is generally a great help, saving time and effort by providing efficient ways to estimate the effects of changes in the model's inputs on its outputs (Kelton, 1997, 1999). A well designed experiment allows the analyst to examine many more factors than would otherwise be possible, while providing insights that cannot be gleaned from trial-and-error approaches or by sampling factors one at a time. For example, if the experimenters keep an input of that simulation model constant, then they cannot estimate the effect of that input on the output (Kleijnen, 2008a; Sanchez, 2007).

Before undertaking a simulation experiment, it is useful to think about why the experiment is needed. Simulation analysts and their clients might seek to (i) develop a basic understanding of a particular simulation model or system, (ii) find robust decisions or policies, or (iii) compare the merits of various decisions or policies. The goal will influence the way the study should be conducted. The design of the experiment is intimately related to

its analysis. An example is analysts assuming that the input has a “linear” effect on the output; i.e. they assume a first-order polynomial approximation or main effects only model. Given this assumption, it suffices to experiment with only two values of that input. Moreover, the analysts may assume that there are (say) $k > 1$ inputs that have main effects only. Then their design requires a relatively small experiment (of order k). For example, changing only one input at a time does give unbiased estimators of all the main effects (Kleijnen, 2008a; Sanchez, 2007).

Computer-based simulation and analysis is used extensively in engineering to predict the performance of a system or product. Design of experiments and statistical approximation techniques such as response surface methodology are becoming widely used in engineering to minimize the computational expense of running such computer analysis (Lin et al., 2001; Sanchez, 2007).

The growing use of computers in design optimization has given rise to considerable research in the design and analysis of computer experiments. The primary research thrusts are to improve:

1. the *efficiency* with which the design space is sampled either by using fewer sample points or seeking better coverage of the design space, and
2. the *accuracy* of the resulting surrogate model by using more complex approximations that are capable of fitting both linear and non-linear functions (Lin et al., 2001).

The “classical” notions of experimental design are irrelevant when it comes to *deterministic* computer experiments, because there are no random error. Also, replication is not necessary since the same response are always obtained for the same input settings (Sahama, 2003). Therefore, sample points should be chosen to fill the design space for (deterministic) computer experiments. Consequently, many researchers advocate the use of “space filling” designs when sampling deterministic computer analysis to treat all regions equally (Lin et al., 2001). Two examples of space filling designs are Latin hypercube sampling and the Uniform design.

Latin hypercubes were the first type of design proposed specifically for deterministic computer experiments (Lin et al., 2001). A Latin hypercube is

a matrix of n by k columns where n is the number of levels being examined and k is the number of design (input) variables. Each of the k columns contains the levels $1, 2, \dots, n$, randomly permuted, and the k columns are matched at random to form the Latin hypercube. Latin hypercubes offer flexible sample sizes while ensuring stratified sampling, i.e., each of the input variables is sampled at n levels. These designs can have relatively small variance when measuring output variance (Lin et al., 2001).

A uniform design provides uniformly scattered design points in the experimental domain. A uniform design is a type of fractional factorial design with an added uniformity property; they have been popularly used since 1980. If the experimental domain is finite, uniform designs are very similar to Latin hypercubes. When the experimental domain is continuous, the fundamental difference between these two designs is that in Latin hypercubes, points are selected at random from cells, whereas in uniform designs, points are selected from the center of cells. Furthermore, a Latin hypercube requires one-dimensional balance of all levels for each factor, while a uniform design requires one-dimensional balance and n -dimensional uniformity. Thus these designs are similar in one-dimension, but they can be very different in higher dimensions (Lin et al., 2001).

Because there is the potential to have many scenarios (factor/level combinations) in search experimentation, very often it is not possible to simulate every single scenario in the time available in order to determine which one meets the target required or provide the optimum result. Consequently, methods need to be found for improving the efficiency of the experimentation process. In broad terms there are three approaches for achieving this (Robinson, 2004):

- *Experimental Design*: identify the experimental factors that are most likely to lead to significant improvements, thereby reducing the total factor/level combinations to be analyzed.
- *Metamodels*: fitting a model to the simulation output (a model of a model). Because the fitted model runs much faster than the simulation, many more factor/level combinations can be investigated.

-
- *Optimization*: performing an efficient search of the factor/level combinations, trying to identify the optimum combination.

When carrying out search experimentation it is often useful to start by identifying the experimental factors that have the greatest impact, that is, give the greatest improvement towards meeting the objectives of the simulation study. For example, is adding more service personnel more effective than increasing the number of automated service points? Does improving machine cycles have more effect than increasing the buffering between machines? The model user can then concentrate on experimenting with the important factors when searching for the optimum or target. There are three ways in which the importance of an experimental factor can be identified (Robinson, 2004):

- *Data Analysis*: by analyzing the data in a model it is sometimes possible to draw conclusions about the likely impact of a change to an experimental factor. For instance, through data analysis a bottleneck process might be identified. Experimental factors that are likely to relieve this bottleneck (e.g. faster cycle time) could then be classified as important. Of course, such analysis does not provide a complete picture in that it cannot take account of the randomness and interconnections in the model.
- *Expert Knowledge*: subject matter experts, for instance, operations staff, often have a good understanding of the system and the factors that are likely to have the greatest impact. It is worth interviewing such people. That said, subject matter experts do not often have a complete understanding of the system. Although they may have a good understanding of isolated sections, their understanding of the total system is unlikely to be complete. If they did have a complete understanding, the simulation study would probably not be required! As a result, care must be taken when relying on the opinions of subject matter experts.
- *Preliminary Experimentation*: changing the levels of experimental factors, running the model and evaluating the effect. Interactive experimentation, if used with caution, may be beneficial in this respect,

although it is important to perform batch experiments to test fully the effect of a change to an experimental factor.

Data analysis and expert knowledge have the advantage that they require less time than preliminary experimentation (Robinson, 2004). Preliminary experimentation, however, provides a more thorough means for investigating the effect of a change to an experimental factor.

Scientific investigation is a sequential process. Statistical experimental design and analysis are deployed to engage in the sequential learning process of data collection, model building, identifying directions of improvement and optimization (Box, 1999; Box and Liu, 1999; Coetzer et al., 2008a; Kleinjen et al., 2005; Myers and Montgomery, 1995; Robinson, 2004).

The investigation process starts with the deployment of an experimental design for the collection of the data. If little or nothing is known about the variables' effects or ranges then a first order or screening design is employed, for identifying the active variables and estimating the effects thereof (Box, 1999; Box and Liu, 1999; Kleinjen et al., 2005; Myers and Montgomery, 1995; Robinson, 2004).

One problem in identifying important experimental factors is that when factors are changed in isolation they may have a very different effect from when they are changed in combination (Robinson, 2004). Such interaction effects are hard to identify except by more formal means. When using informal methods the model user should be aware of possible interaction effects and test them by changing some factors in combination.

A change to an experimental factor may have a significant effect on the simulation output (statistical significance), but this does not necessarily mean that it is an important factor (Robinson, 2004). If the change has limited practical significance (e.g. it is too expensive or breaks safety constraints), it cannot be classified as important. Importance requires both statistical and practical significance (Montgomery, 2005; Myers and Montgomery, 1995; Robinson, 2004).

By simulating a limited number of scenarios (factor/level combinations) it is often possible to form an opinion as to the likely outcome of other scenarios

without having to run the simulation (Robinson, 2004). In particular, it may be possible to identify those scenarios that are likely to yield the desired result and those that are unlikely to do so. Through this process the model user forms an understanding of the solution space.

Big simulations usually involves a lot of variables, and the number of variables will have to be paired down to do a workable analysis. For this purpose there are several factor-screening designs to help separate which factors matter and which one's don't (Lin, 2003).

Screening designs commonly used in DASE are Fractional Factorial Designs (Kelton, 2000; Kleijnen, 2008a; Kleinjen et al., 2005; Law, 2007; Sanchez, 2007; Trocine and Malone, 2000), Plackett-Burman designs (Kleijnen, 2008a; Kleinjen et al., 2005; Law, 2007), D-Optimal designs (Kleijnen, 2008a; Law, 2007) and Latin Hypercube Designs (Kleijnen, 2008a; Law, 2007; Sanchez, 2007; Trocine and Malone, 2000). Latin Hypercube Designs and Uniform Designs are commonly used in the screening phase of deterministic computer models (Lin, 2003; Lin et al., 2001; Sacks et al., 1989; Santner et al., 2003).

To perform an experiment with the simulation model, simulation trials are performed at each of a set of settings of x which involve one or more levels of each of the n controllable variables $x_i, i = 1, \dots, n$. The method of least-squares can then be employed to estimate the main effects (β_i) and interactions (β_{ij}) in (1.3). From this analysis, the g most important factors are identified (Lin, 2003).

Usually a center point is included to estimate the curvature effect and whether non-linearity is present in the design range. If curvature is detected, then the design can be augmented with additional design points according to a second-order response surface design (Myers and Montgomery, 1995).

Some of the designs commonly used in the next phase of the scientific investigation process for simulation models are Fractional Factorial designs (Kelton, 1999, 2000; Kleijnen, 2008a; Kleinjen et al., 2005; Law, 2007; Sanchez, 2007), D-Optimal designs (Kleijnen, 2008a; Law, 2007), Latin Hypercube Designs (Kleijnen, 2008a; Kleinjen et al., 2005; Law, 2007; Sanchez, 2007) and Central Composite designs (Barton, 1992, 1994; Kleijnen, 2008a; Kleinjen et al., 2005; Law, 2007). Latin Hypercube Designs and Uniform

Designs are commonly used in the second phase of scientific investigation for deterministic computer models (Lin, 2003; Lin et al., 2001; Sacks et al., 1989; Santner et al., 2003).

A metamodel is a model of a model (Barton, 1992, 1994; Kelton, 2000; Kleijnen et al., 2005; Robinson, 2004), in our case a model of the simulation output. Because the metamodel is normally an analytical model it runs much faster than the simulation. It is therefore, possible to investigate many more scenarios with a metamodel than with the simulation itself. The downside is that the metamodel is an approximation of the simulation output and so the results provided are not as accurate. There is also the overhead of creating the metamodel.

In creating a metamodel a series of results, representing a range of factor/level combinations, must be generated from the simulation (Robinson, 2004). Careful selection of the scenarios to be simulated is important in order to assure the greatest accuracy of the metamodel with the minimum number of simulation runs. This requires appropriate experimental design techniques.

Hood and Welch (1993) discusses the use of response surface methodology and its application in simulation. They assume the model has K continuous parameters $\theta_1, \dots, \theta_K$ and that the performance characteristic of interest are, $C(\theta_1, \dots, \theta_K)$, of the model, which is the expected value of an output random variable, $Y(\theta_1, \dots, \theta_K)$. Exploring the surface of $C(\theta_1, \dots, \theta_K)$ are of interest.

Hood and Welch (1993) describes the “classical” application of experimental design based on standard least squares theory. They assume that $C(\theta_1, \dots, \theta_K)$ is smooth enough so that it can be approximated by either a first or second degree polynomial over the sequence of regions of experimental activity. The methodology is sequential in nature with each successive experiment building on the results and insights of earlier experiments. Thus, it is ideally suited to simulation because of the relative ease with which data can be obtained in the simulation context.

Kriging models are popular models in the design and analysis of deterministic computer experiments. Originally developed for applications in geostatistics, a kriging model postulates a combination of a polynomial model

and departures of the form (1.5),

$$y(x) = f(x) + Z(x) \quad (1.5)$$

where $Z(x)$ is assumed to be a realization of a stochastic process with mean zero and spatial correlation function given by (1.6),

$$Cov[Z(x^i), Z(x^j)] = \sigma^2 \mathbf{R}([R(x^i, x^k)]) \quad (1.6)$$

where σ^2 is the process variance and R is the correlation function. A variety of correlation functions can be chosen; however, the Gaussian correlation function is the most frequently used (Lin et al., 2001). Furthermore, $f_1(x)$ is typically taken as a constant term. Determining the maximum likelihood estimates of the $k\theta$ parameters used to fit the the model is a k -dimensional optimization problem, which can require significant computational time if the sample data set is large. The correlation matrix, $\mathbf{R}$, can also become singular if multiple sample points are spaced close to one another or if the sample points are generated from particular designs (Lin et al., 2001).

Recently a lot of research has been done on using the kriging metamodel in stochastic simulation studies (Jack, 2007; Kleijnen and de Beers, 2004; Kleijnen, 2004, 2008a; Kleijnen et al., 2005; Law, 2007; van Beers and Kleijnen, 2003, 2004).

In simulation, an estimated metamodel can serve several different purposes. Partial derivatives could be taken of the response-surface model to estimate the effect of small changes in the factors on the output response, and any interactions that might be present as modeled would show naturally. The estimated metamodel could also be used as a proxy for the simulation, and to very quickly explore many different input-factor-level combinations without having to run the simulation (Kelton, 2000).

The simple form of a metamodel can reveal the general characteristics of behavior of the more complex simulation model. The insight provided by the simpler metamodel may be used for verification and validation of the complex parent model. It may also be used to identify the system parameters that most affect system performance (i.e. factor screening). Since it uses

fewer computer resources, the metamodel can be run iteratively many times for repeated ‘what if’ evaluation for multi-objective systems for design optimization. This is important when the output of the simulation is a random quantity. Substitution of metamodel code is also an important strategy when the original model is just one component of a complex system model. In this case, the system model may be impractically slow and/or large without using metamodels for some or all of the components (Barton, 1992).

The ultimate goal in using a simulation model is to find input-factor settings that optimize some performance measure. Optimization of nonlinear functions is a hard enough problem in itself, but in a stochastic simulation there is uncertainty in terms of observing the response, as well as other statistical difficulties. One solution is to use the metamodel obtained from the model and optimize this function (Kelton, 1997). This will give an indication of where the best input-factor-combinations might be.

In summary, DASE is needed to improve the efficiency and effectiveness of simulation; i.e. DASE is crucial in the overall process of simulation (Kleijnen, 2008a) .

1.3 Research Objectives and Methodology

In the design and analysis of simulation experiments (DASE) the performance of the Design and Analysis of Computer Experiments and Classical Experiments have not previously been compared in terms of their ability to yield accurate metamodels for simulation models. A case study from the petrochemical industry (Figure 4.1) will be used to assess the relative merit of the different designs by metamodel combinations in terms of maximum absolute error (1.7) and root mean square error criteria (1.8). The design by metamodel choice will be evaluated within all the phases of the classical response surface methodology, i.e. screening, interaction and second order designs (Myers and Montgomery, 1995).

An overview of the methodology that will be used to compare the different combinations are given in Figure 1.2. The second phase will be added to each screening leg, but due to space constraints it is only shown for the D-Optimal

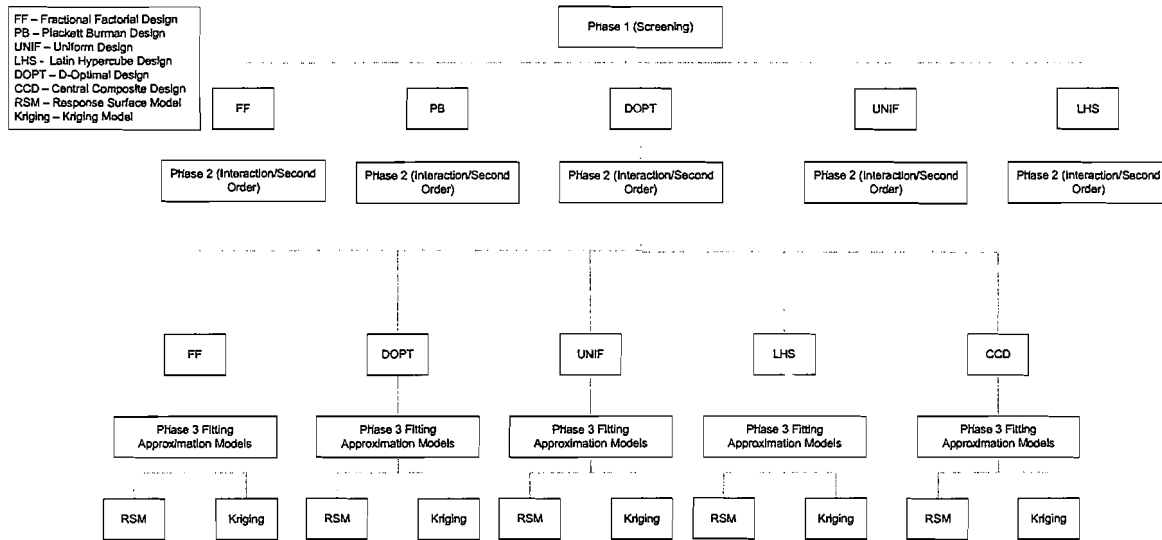


Figure 1.2: Methodology used for comparing different design and approximation model combinations

leg. Therefore, there will be 25 design combinations that will be investigated. The approximation models will be fitted to each of the second phase designs. The Response Surface and Kriging models will therefore be fitted to 25 design combinations. The goal of the study is to determine the best leg(s) of Figure 1.2 for use in simulation experiments.

The study will commence in phases. For the first phase, the screening phase, the following designs will be evaluated to find the significant variables:

- Fractional Factorial Design (Resolution III) (Section 2.2.2).
- Plackett-Burman Design (Section 2.2.3).
- Uniform Design (Section 2.3.2).
- Latin Hypercube Design (Section 2.3.1).
- D-Optimal Design (Section 2.2.5).

In the second phase, the first order model from phase one will be augmented with two factor interactions and second order models if necessary. The following designs will be evaluated:

-
- Fractional Factorial Design (Resolution IV) (Section 2.2.2).
 - Uniform Design (Section 2.3.2).
 - Latin Hypercube Design (Section 2.3.1).
 - D-Optimal Design (Section 2.2.5).
 - Central Composite Design (Section 2.2.4).

These specific designs were chosen to be evaluated because Fractional Factorial Designs, Plackett-Burman Designs, Central Composite Designs, D-Optimal Designs and Latin Hypercube Designs are widely used in the design and analysis of simulation experiments (i.e. Kelton, 1999, 2000; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007; Sanchez, 2007), and Latin Hypercube Designs and Uniform Designs are widely used in the design and analysis of (deterministic) computer experiments (i.e. Fang et al., 2000; Lin, 2003; Lin et al., 2001; Sacks et al., 1989; Santner et al., 2003; Simpson et al., 1998). Also refer to the discussion in Section 1.2.2.

The metamodels that will be implemented are:

- Response Surface (Section 3.2).
- Kriging (Section 3.3).

The comparisons between the different designs and approximation models will be done by sampling additional validation points to assess the accuracy over the region of interest. For each set of validation points, the maximum absolute error (MAX) and root mean square error (RMSE) are computed as:

$$MAX = \max \{ |y_i - \hat{y}_i| \}_{i=1, \dots, n_{error}} \quad (1.7)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n_{error}} (y_i - \hat{y}_i)^2}{n_{error}}} \quad (1.8)$$

where n_{error} is the number of additional validation points. While RMSE provides good estimates of the “global” error over the region of interest, MAX

gives a good estimate of the “local” error by measuring the worst error within the region of interest, where a good approximation will have low RMSE and low MAX values (Lin et al., 2001).

The approximation model from the best overall Phase 1 to Phase 2 to Phase 3 leg will be used to explore the design space for the case study. Specifically the effect of 14 factors on the plant availability for the industrial process depicted in Figure 4.1 will be explored and evaluated.

1.4 Outline of Thesis

The thesis is outlined as follows. In Chapter 2 (Experimental Designs), the experimental designs will be discussed. Specifically the following designs are discussed:

1. 2^k Factorial Designs
2. Fractional Factorial Designs
3. Placket Burman Designs
4. Central Composite Designs
5. Optimal Designs
6. Latin Hypercube Designs
7. Uniform Designs

In Chapter 3 (Approximation models for input-output relationships), the approximation models for input-output relationships will be discussed. Specifically the following approximation models are discussed:

1. Response Surface Models
2. Kriging Models

In Chapter 4 (Case Study), the Case Study will be discussed under the following headings.

-
1. Introduction - A brief overview of the system flowsheet and the factors under investigation will be given.
 2. Screening Experiments - The application of the different screening designs and the corresponding results and Analysis of Variance (ANOVA) tables will be discussed.
 3. Second Phase Experiments - The application of the different designs and approximation models and the corresponding results and ANOVA tables will be discussed.

In Chapter 5 (Results and Practical Application) An overview of the results will be provided as well as the comparison between the different design and approximation model combinations. Some of the insights into the industrial process provided by this experimental study will be discussed.

In Chapter 6 (Conclusions and Future Research), the conclusions from the study and scope for future research are provided.

Chapter 2

Design of experiments for Simulation

2.1 Introduction

In this chapter the designs utilized in the case study are discussed. Some of the more popular designs in the design and analysis for simulation experiments and design and analysis for deterministic computer experiments were chosen to be investigated in this study. The rest of this chapter will be divided in two sections. In the first section the classical designs will be discussed, and in the second section the space filling designs will be discussed.

2.2 Classical Design of Experiments

In this chapter some of the classical designs are discussed. The designs discussed here are some of the designs most commonly used in simulation experiments. Specifically the fractional factorial design (Kelton, 1999, 2000; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007; Sanchez, 2007; Trocine and Malone, 2000), Plackett-Burman designs (Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007), D-Optimal designs (Kleijnen, 2008a; Law, 2007) and Central Composite design (Barton, 1992, 1994; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007) will be discussed.

2.2.1 2^k Factorial Designs

A common strategy to measure the effects of k factors in an experiment is to fix the level of the other $k - 1$ factors at some set of values and make simulation runs at each of two levels of the factor of interest to observe how the response reacts to changes in this single factor. The whole process is then repeated to examine each of the other factors, one at a time. This strategy, which is called the one-factor-at-a-time (OFAT) approach is quite inefficient in terms of the number of simulation runs needed to obtain specific precision. More importantly, it does not allow for the measurement of any interactions; indeed, it assumes that there are no interactions, which is often not the case in simulation applications (Law, 2007).

A much more economical strategy for determining the effects of factors on the response with which interactions can also be measured, called a 2^k factorial, requires that two levels for each factor are chosen. Simulation runs are then performed at each of the 2^k possible factor-level combinations, which are sometimes called *design points*. Usually, a plus sign is associated with the high level of the factor, and a minus sign with the low level. The levels, which should be chosen in consultation with subject-matter experts, should be far enough apart to create a difference in the response, but not so separated that nonsensical configurations are obtained. Because only two levels of the factors are used, the assumption is that the response is approximately linear (or at least monotonic) over the range of the factor. A non-monotonic response can be wrongly identified as having no effect on the response (Law, 2007).

The form of a 2^k factorial design can be compactly represented in tabular form, as in Table 2.1 for $k = 3$. The variable R_i for $i = 1, 2, \dots, 8$ is the value of the response when running the simulation with the i th combination of factor levels. Writing down this array, called the *design matrix*, facilitates calculation of the factor effects and interactions (Law, 2007).

The main effect of factor j , denoted by e_j , is the average change in the response due to moving factor j from its $-$ to its $+$ level while holding all other factors fixed. This average is taken over all combinations of the other factor levels in the design. It is important to realize that a main effect

Table 2.1: Design matrix for a 2^3 factorial design.

Factor Combination (Design Point)	Factor 1	Factor 2	Factor 3	Response
1	-	-	-	R_1
2	+	-	-	R_2
3	-	+	-	R_3
4	+	+	-	R_4
5	-	-	+	R_5
6	+	-	+	R_6
7	-	+	+	R_7
8	+	+	+	R_8

is computed relative to the current design and factor levels only, and it is generally wrong to extrapolate beyond this unless other conditions (e.g. no interactions) are satisfied.

For the 2^3 factorial design in Table 2.1, the main effect of factor 1 is thus

$$e_1 = \frac{(R_2 - R_1) + (R_4 - R_3) + (R_6 - R_5) + (R_8 - R_7)}{4}$$

Note that at design points 1 and 2, factors 2 and 3 remain fixed, as they do at design points 3 and 4, 5 and 6, as well as points 7 and 8. The main effect of factor 2 is

$$e_2 = \frac{(R_3 - R_1) + (R_4 - R_2) + (R_7 - R_5) + (R_8 - R_6)}{4}$$

and that of factor 3 is

$$e_3 = \frac{(R_5 - R_1) + (R_6 - R_2) + (R_7 - R_3) + (R_8 - R_4)}{4}$$

Looking at Table 2.1 and the above examples for the e_j 's leads to an alternative way of defining main effects, as well as a simpler way of computing them. Namely e_j is the difference between the average response when factor j is at its + level and the average response when it is at its - level. Thus, to compute e_j , we simply apply the signs in the "Factor j " column to the corresponding R_i 's, add them up, and divide by 2^{k-1} . For example, in the

2^3 factorial design of Table 2.1,

$$e_2 = \frac{-R_1 - R_2 + R_3 + R_4 - R_5 - R_6 + R_7 + R_8}{4}$$

which is identical to the earlier expression for e_2 .

The main effects measure the average change in the response due to a change in an individual factor, with the average being taken over all possible combinations of the other $k-1$ factors (numbering 2^{k-1}). It could be, though, that the effect of factor j_1 depends in some way on the level of some other factor j_2 , in which case these two factors are said to interact. A measure of interaction is the difference between the average effect of factor j_1 when factor j_2 is at its + level (and all other factors other than j_1 and j_2 are held constant) and the average effect of factor j_1 when factor j_2 is at its - level. By convention one-half of this difference is called the two-factor (two-way) interaction effect and denoted by $e_{j_1 j_2}$. It is also called the $j_1 \times j_2$ interaction. For example, in the design of Table 2.1 we have

$$e_{12} = \frac{1}{2} \left[\frac{(R_4 - R_3) + (R_8 - R_7)}{2} - \frac{(R_2 - R_1) + (R_6 - R_5)}{2} \right]$$

$$e_{13} = \frac{1}{2} \left[\frac{(R_6 - R_5) + (R_8 - R_7)}{2} - \frac{(R_2 - R_1) + (R_4 - R_3)}{2} \right]$$

and

$$e_{23} = \frac{1}{2} \left[\frac{(R_7 - R_5) + (R_8 - R_6)}{2} - \frac{(R_3 - R_1) + (R_4 - R_2)}{2} \right]$$

To observe that the formula for e_{13} , for example, measures the quantity described above, note from the design matrix in Table 2.1 that factor 3 is always at its + level for design points 5, 6, 7, and 8, and that factor 1 moves from its - to its + level between design points 5 and 6 (where all other factors, in this example factor 2, remain fixed at the - level), as well as between design points 7 and 8 (where factor 2 is fixed at its + level). Thus the first fraction inside the square brackets in the above expression for e_{13} is the average effect of moving factor 1 from its - to its + level when factor 3 is

held at its + level. Similarly, the second fraction inside the square brackets is the average effect of moving factor 1 from its – to its + level (design points 1 to 2, and 3 to 4) when factor 3 is held at its – level. The difference in these two factors, then, is the difference in the effect that factor 1 has depending on whether factor 3 is at its + or – level; one half this difference is the definition of the interaction effect between factors 1 and 3 (Law, 2007).

As with the main effects, there is an easier way to compute interaction effects, based on the design matrix. If the above expression for e_{13} is rearranged, for instance, so that the R_i 's appear in increasing order of the i 's, we get

$$e_{13} = \frac{R_1 - R_2 + R_3 - R_4 - R_5 + R_6 - R_7 + R_8}{4}$$

Now if a column labeled “1 × 3” of 8 signs are created by multiplying the i th sign in the Factor 1 column by the i th sign in the Factor 3 column, the new column of signs are precisely the signs of the R_i 's used to form e_{13} ; as with main effects, the divisor is 2^{k-1} . Thus, the interaction effect between factor 1 and 3 can be thought of as the difference between the average response when factor 1 and 3 are at the same (both + or both –) level and the average response when they are at opposite levels. Note that the two-factor interaction effects are completely symmetric; for example $e_{12} = e_{21}$, $e_{23} = e_{32}$, etc.

Although interpretation becomes more difficult, three and higher order interaction effects can be defined and computed, all the way up to k -factor interaction. For example, in the 2^3 factorial design of Table 2.1, the three-factor interaction is one-half the difference between the two-factor interaction effect between factors 1 and 2 when factor 3 is at its + level and the two-factor interaction effect between factors 1 and 2 when factor 3 is at its – level. e_{123} is obtained by multiplying the i th signs from the columns for factors 1, 2, and 3 in Table 2.1 and applying them to the R_i 's; the denominator is once again 2^{k-1} . Three- and higher-factor interaction effects are also symmetric: $e_{123} = e_{132} = e_{213}$, etc.

If two- or higher-factor interactions appear to be present, then the main effect of each factor involved in such a significant interaction cannot be in-

terpreted as simply the effect in general of moving that factor from its $-$ to its $+$ level, since the magnitude and possibly the sign of the change in the response depend on the level of at least one other factor (Box, 1999; Box and Liu, 1999; Kleijnen, 2008a; Law, 2007; Montgomery, 2005).

The standard error of the effect can be used to judge the significance of effects (Montgomery, 2005). The variance of each effect estimate is

$$\begin{aligned} V(\text{effect}) &= V\left(\frac{\text{Contrast}}{n2^{k-1}}\right) \\ &= \frac{1}{(n2^{k-1})^2} V(\text{Contrast}) \end{aligned}$$

Each contrast is a linear combination of 2^k treatment totals, and each consists of n observations. Therefore,

$$V(\text{Contrast}) = n2^k \sigma^2$$

and the variance of an effect is

$$V(\text{effect}) = \frac{1}{(n2^{k-1})^2} n2^k \sigma^2 = \frac{1}{n2^{k-2}} \sigma^2$$

The estimated standard error would be found by taking the square root of this last expression and replacing σ^2 by its estimate S^2 , i.e. the residual mean sum of squares value (Montgomery, 2005):

$$se(\text{Effect}) = \frac{2S}{\sqrt{n2^k}} \quad (2.1)$$

2.2.2 Fractional Factorial Designs

As the number of factors in a 2^k factorial design increases, the number of runs required for a complete replicate of the design rapidly outgrows the resources of most experimenters. For example, a complete replicate of the 2^6 design requires 64 runs. In this design only 6 of the 63 degrees of freedom

correspond to main effects, and only 15 degrees of freedom correspond to two-factor interactions. The remaining 42 degrees of freedom are associated with three-factor and higher interactions (Montgomery, 2005).

If the experimenter can reasonably assume that certain high-order interactions are negligible, information on the main effects and low-order interactions may be obtained by running only a fraction of the complete factorial experiment. These fractional factorial designs are among the most widely used types of designs for product and process design and for process improvement, as well as simulation experiments (Biles, 1979, 1984; Box, 1999; Box and Liu, 1999; Coetzer et al., 2008a; Kelton, 1999, 2000; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007; Montgomery, 2005; Sanchez, 2007; Trocine and Malone, 2000).

A major use of fractional factorials is in screening experiments - experiments in which many factors are considered and the objective is to identify those factors (if any) that have large effects. Screening experiments are usually performed in the early stages of a project when many of the factors initially considered likely have little or no effect on the response. The factors identified as important are then investigated more thoroughly in subsequent experiments (Montgomery, 2005).

The successful use of fractional factorial designs is based on three key ideas (Montgomery, 2005):

1. **The sparsity of effect principle.** When there are several variables, the system or process is likely to be driven primarily by some of the main effects and low-order interactions.
2. **The projection property.** Fractional factorial designs can be projected into stronger (larger) designs in the subset of significant factors.
3. **Sequential experimentation.** It is possible to combine the runs of two (or more) fractional factorials to assemble sequentially a larger design to estimate the factor effects and interactions of interest.

Fractional factorial designs provide a way to get good estimates of the main effects and perhaps two-factor interactions at a fraction of the computa-

tional effort required by a full 2^k factorial design. Basically, a 2^{k-p} fractional factorial design is constructed by choosing a certain subset (of size 2^{k-p}) of all the 2^k possible design points and then running the simulation for only these chosen points. Since only $1/2^p$ of the possible 2^k factor combinations are actually run, it is sometimes referred to as a “half fraction” if $p = 1$, a “quarter fraction” if $p = 2$, and so on. Clearly, it would be beneficial for p to be large from a computational viewpoint, but a larger p may also result in less information from the experiment (Law, 2007).

An important concept in a 2^{k-p} fractional factorial design is the idea of confounding. It is possible in these designs to end up with the exact same algebraic expression for several different effects. For instance, in a 2^{4-1} half fraction, it could be that the formulas for the main effect e_4 and the three-way interaction term e_{123} are identical; that is the main effect e_4 and e_{123} are confounded or aliased. The meaning of this is that the common formula for e_4 and e_{123} is an unbiased estimator for $E(e_4) + E(e_{123})$. e_4 and e_{123} are called aliases of each other, and it is denoted as $e_4 = e_{123}$. If the assumption can be made that $E(e_{123}) = 0$ or is negligible in comparison with $E(e_4)$, then e_4 is an unbiased (or nearly so) estimator of $E(e_4)$. It often happens that higher-way interactions do turn out to be small in comparison with main effects or perhaps two-way interactions, so such an assumption may actually be warranted. Trouble may arise, though, in cases where two-way interactions are confounded with each other; e.g., the formulas for e_{12} and e_{34} could be identical, in which case this common expression is an unbiased estimator for $E(e_{12}) + E(e_{34})$ and it is not that easy to make the assumption that either of the two-way interactions are zero. Worse, a main effect could be confounded with a two-way interaction, which makes the main-effect estimate of limited value if the two-way interaction is present (which cannot be easily determined, because two way interactions are confounded with main effects, with each other, and with higher-way interactions). In general, the higher the value of p , the more pervasive the confounding problem (Law, 2007).

One way to quantify the overall severity of confounding is through the concept of the resolution of a particular 2^{k-p} fractional factorial design. A design is of resolution R if no q -way effect is aliased with another effect

containing less than $R - q$ factors (effects). It is guaranteed that two effects are not confounded with each other if the sum of their “ways” is strictly less than the design’s resolution; for this purpose main effects are regarded as “one-way” effects. The most commonly used fractional factorial designs are resolution III, IV and V (resolutions are denoted by Roman numerals). For instance, in a resolution IV design, no main effect is confounded with any other main effect or with any two-way interaction ($1 + 2 < 4$), but two-way interactions are aliased with each other ($2 + 2 = 4$). Thus, assuming that three-way (and higher-order) interactions are negligible, resolution IV designs allow us to obtain “clear” main-effects estimates. Notationally, the resolution is attached as a subscript: 2_{IV}^{6-1} , 2_V^{5-1} , etc (Law, 2007).

Once the number of factors k and the desired resolution are determined, the design needs to be constructed, i.e., specify p and which 2^{k-p} rows of the full 2^k design matrix to use. The first step is to write out a full 2^{k-p} factorial design matrix in factors $1, 2, \dots, k - p$. This basic design matrix has the required number of rows, namely 2^{k-p} . The remaining p columns (for factors $k - p + 1, \dots, k$) are then determined by “multiplying” certain of the first $k - p$ columns together according to some rules e.g. Montgomery (2005) p. 305.

In the case study a 2_{III}^{14-10} , 14 factor, 16 run design was used in the screening phase (Section 4.2.1). The coded design table for 2_{III}^{14-10} , 14 factor, 16 run design is provided in Table 2.2.

The relevant section in the generator table on page 305 in Montgomery (2005) is reproduced in Table 2.3. The first four columns (A,B,C and D) of the design matrix were created by using a 2^4 factorial design (Section 2.2.1). The remaining columns were obtained by using the generators in Table 2.3. For example, the signs of the coded factors in column E were obtained by multiplying the signs of columns A, B and C. The signs of column F were obtained by multiplying columns A, B and D and so forth.

Table 2.2: Design Table for 2_{III}^{14-10} , 14 factor, 16 run Design

Run Nr.	A	B	C	D	E	F	G	H	J	K	L	M	N	O
1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1
2	1	-1	-1	-1	1	1	1	-1	-1	-1	-1	-1	1	1
3	-1	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1	-1
4	1	1	-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1
5	-1	-1	1	-1	1	-1	1	1	-1	1	-1	1	-1	1
6	1	-1	1	-1	-1	1	-1	1	1	-1	1	-1	-1	1
7	-1	1	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1
8	1	1	1	-1	1	-1	-1	-1	-1	1	1	-1	1	-1
9	-1	-1	-1	1	-1	1	1	1	-1	1	1	-1	1	-1
10	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1
11	-1	1	-1	1	1	-1	1	-1	1	-1	1	-1	-1	1
12	1	1	-1	1	-1	1	-1	-1	-1	1	-1	1	-1	1
13	-1	-1	1	1	1	1	-1	-1	1	1	-1	-1	-1	-1
14	1	-1	1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1
15	-1	1	1	1	-1	-1	-1	1	-1	-1	-1	-1	1	1
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 2.3: Design Generator for 2_{III}^{14-10} design

Number of Factors, k	Fraction	Number of Runs	Design Generators
14	2_{III}^{14-10}	16	$E = ABC$ $F = ABD$ $G = ACD$ $H = BCD$ $J = ABCD$ $K = AB$ $L = AC$ $M = AD$ $N = BC$ $O = BD$

2.2.3 Plackett- Burman Designs

These designs, attributed to Plackett and Burman (1946), are two-level fractional factorial designs for studying $k = N - 1$ variables in N runs, where N is a multiple of 4. If N is a power of 2, these designs are identical to two level fractional factorial designs. However, for $N = 12, 20, 24, 28$ and 36 , the Plackett-Burman designs are sometimes of interest. Specifically these designs cannot be represented as cubes, they are sometimes called non-geometric designs (Lin, 1993; Montgomery, 2005).

The non-geometric Plackett-Burman designs for $N = 12, 20, 24, 28$, and 36 have very messy alias structures. For example, in the 12-run design every main effect is partially aliased with every two-factor not involving itself. For example, the AB interaction is aliased with the nine main effects $C, D, \dots, K$. Furthermore, each main effect is partially aliased with 45 two factor interactions. In the larger designs, the situation is even more complex. These designs must therefore be used very carefully Montgomery (2005) page 319.

In the case study (Section 4) a $N = 20$ run design 19 factor Plackett-Burman design was used in the screening phase. This is the smallest Plackett-Burman design equal to or larger than 14 factors investigated in the case study. After constructing the design columns 15-19 were removed (these columns are not needed because there are only 14 factors present in this study).

Plackett-Burman designs are often used as screening designs in the design and analysis of simulation experiments (Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007).

2.2.4 Central Composite Design

Central composite designs or CCD are the most popular class of designs for fitting response surface models. Generally, the CCD consists of a 2^k factorial (or fractional factorial of resolution V) with n_f runs, $2k$ axial or star runs, and n_c center runs (Montgomery, 2005).

The practical deployment of a CCD often arises through sequential experimentation. That is, a 2^k has been used to fit a first-order model, this

model has exhibited lack of fit, and the axial runs are then added to allow the quadratic terms to be incorporated into the model. The CCD is a very efficient design for fitting the second-order model (Lucas, 1974, 1976). There are two parameters in the design that must be specified: the distance α of the axial runs from the design center and the number of center points n_c (Montgomery, 2005). The choice of these two parameters will now be discussed.

Rotatability

It is important for the second-order model to provide good predictions throughout the region of interest. One way to define “good” is to require that the model have a reasonable consistent and stable variance of the predicted response at points of interest x . The variance of the predicted response at some point x is given by equation 2.2.

$$V[\hat{y}(x)] = \sigma^2 x^T (\mathbf{X}^T \mathbf{X})^{-1} x \quad (2.2)$$

where $\mathbf{X}$ is the $n \times p$ matrix representing the design settings used as well as all the columns necessary to accommodate the assumed model (i.e. (1.2),(1.3) or (1.4)) terms, and x is a vector corresponding to the location in the design space, which is also a function of the model used. Box and Hunter (1957) suggested that a second-order response surface design should be rotatable. This means that $V[\hat{y}(x)]$ is the same at all points x that are the same distance from the design center. That is the variance of predicted responses is constant on spheres. A design with the contours of constant standard deviation of predicted response as concentric circles will leave the variance of $\hat{y}$ unchanged when the design is rotated about the center $(0, 0, \dots, 0)$, hence the name *rotatable* design.

Rotatability is a reasonable basis for the selection of a response surface design. Because the purpose of response surface modeling is optimization and the location of the optimum is unknown prior to running the experiment, thus it makes sense to use a design that provides equal precision of estimation in all directions (Montgomery, 2005).

A central composite design is made rotatable by the choice of α . The value of α for rotatability depends on the number of points in the factorial portion of the design; in fact, $\alpha = (n_f)^{1/4}$ yields a rotatable central composite design where n_f is the number of points used in the factorial portion of the design (Montgomery, 2005).

The Spherical CCD

Rotatability is a spherical property; that is, it makes the most sense as a design criterion when the region of interest is a sphere. However, it is not important to have exact rotatability to have a good design. For a spherical region of interest, the best choice of α from a prediction variance viewpoint for the CCD is to set $\alpha = \sqrt{k}$. This design, called a spherical CCD, puts all the factorial and axial design points on the surface of a sphere of radius $\sqrt{k}$ (Montgomery, 2005). However, this choice of $\sqrt{k}$ is not always practical, i.e. for large k the value of α becomes large, which makes the region of interest impractical. For practical purposes, $\alpha = \sqrt{3}$, is acceptable.

Center Runs of CCD

The choice of α in the CCD is dictated primarily by the region of interest. When this region is a sphere, the design must include center runs to provide reasonable stable variance of the predicted response. Generally three to five center runs are recommended (Draper, 1982; Montgomery, 2005).

Cuboidal Region of Interest

In many situations, the region of interest is cuboidal rather than spherical. In these cases, a useful variation of the central composite design is the face-centered central composite design or the face-centered cube, in which $\alpha = 1$. This design locates the star or axial points on the center of the faces of the cube. This variation of the central composite design is also sometimes used because it requires only three levels of each factor, and in practice it is often difficult to change factor levels. However, note that face-centered central composite designs are not rotatable.

The face-centered cube does not require as many center points as the spherical CCD. In practice, $n_c = 2$ or 3 is sufficient to provide good variance of prediction throughout the experimental region. It should be noted that sometimes more center runs will be employed to give a reasonable estimate of experimental error. For the face-centered cube the standard deviation of predicted response is reasonably uniform over a relatively large portion of the design space (Montgomery, 2005).

Central Composite designs are well known designs in the design and analysis of simulation experiments (Barton, 1992, 1994; Donohue et al., 1993; Kelton, 1999, 2000; Kleijnen, 2008a; Kleijnen et al., 2005; Law, 2007).

2.2.5 D-Optimal Designs

The standard response surface, such as the central composite design, the Box-Behnken design, and their variations (such as the face-centered cube), are widely used because they are quite general and flexible designs. If the experimental region is either a cube or a sphere, typically a standard surface design will be applicable to the problem. However, occasionally an experimenter encounters a situation where a standard response surface design may not be the obvious choice. Computer-generated designs are an alternative to consider in these cases (Montgomery, 2005).

There are three situations where some type of computer-generated design may be appropriate (Montgomery, 2005).

1. **An irregular experimental region.** If the region of interest for the experiment is not a cube or a sphere, standard designs may not be the best choice. Irregular regions of interest occur fairly often. Consider the example in Montgomery (2005) page 439, an experimenter is investigating the properties of a particular adhesive. The adhesive is applied to two parts and then cured at an elevated temperature. The two factors of interest are the amount of adhesives applied and the cure temperature. Over the ranges of these two factors, taken as -1 to $+1$ on the usual coded variable scale, the experimenter knows that if too little adhesive is applied and the cure temperature is too low, the parts

will not bond satisfactorily. In terms of the coded variables, this leads to a constraint on the design variables, say

$$-1.5 \leq x_1 + x_2$$

where x_1 represent the application amount of adhesive and x_2 represents the temperature. Furthermore, if the temperature is too high and too much adhesive is applied, the parts will be either damaged by heat stress or an inadequate bond will result. Thus, there is another constraint on the factor levels

$$x_1 + x_2 \leq 1$$

The constraints effectively remove two corners of the square region, producing an irregular experimental region. There is no standard response surface design that will fit exactly this region.

2. **A nonstandard model.** Usually an experimenter elects a first- or second-order response surface model, realizing that this empirical model is an approximation to the true underlying mechanism. However, sometimes the experimenter may have some special knowledge or insight about the process being studied that may suggest a nonstandard model. For example, the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{112} x_1^2 x_2 + \beta_{1112} x_1^3 x_2 + \epsilon$$

may be of interest. The experimenter would be interested in obtaining an efficient design for fitting this reduced quartic model. As another illustration, sometimes we encounter response surface problems where some of the design factors are categorical variables. There are no standard response surface designs for this situation.

3. **Unusual sample size requirements.** Occasionally, an experimenter

may need to reduce the number of runs required by a standard response surface design. For example, suppose we intend to fit a second-order model in four variables. The central composite design for this situation requires between 28 and 30 runs, depending on the number of center points selected. However, the model has only 15 terms. If the runs are extremely expensive or time-consuming, the experimenter will want a design with fewer trials. Although computer-generated designs can be used for this purpose, there are usually better approaches. For example, a small composite design can be constructed for four factors with 20 runs, including four center points, and a hybrid design with as few as 16 runs is also available. These are generally superior choices to using a computer-generated design to reduce the number of trials (Montgomery, 2005).

Much of the development of computer-generated designs is an outgrowth of work by Kiefer and Wolowitz (1959) in the theory of optimal designs. By an optimal design, it is implied that a design is the “best” with respect to some criterion. Computer programs are required to construct these designs. The usual approach is to specify a model, determine the region of interest, select the number of runs to make, specify the optimality criterion, and then choose the design points from a set of candidate points that the experimenter could consider using. Typically the candidate points are a grid of points spaced over the feasible design region.

There are several popular design optimality criteria. Perhaps the most widely used is the D -optimality criterion. A D -optimal design minimizes

$$|(\mathbf{X}^T \mathbf{X})^{-1}|$$

where $\mathbf{X}$ is the $n \times p$ matrix representing the design settings used as well as all the columns necessary to accommodate the assumed model (i.e. (1.2),(1.3) or (1.4)). It turns out that a D -optimal design minimizes the volume of the joint confidence region on the vector of regression coefficients. A measure of the relative efficiency of design 1 to design 2 according to the D -criterion is given by

$$D_e = \left(\frac{|(\mathbf{X}_2^T \mathbf{X}_2)^{-1}|}{|(\mathbf{X}_1^T \mathbf{X}_1)^{-1}|} \right)^{1/p} \quad (2.3)$$

where $\mathbf{X}_1$ and $\mathbf{X}_2$ are the $\mathbf{X}$ matrices for the two designs and p is the number of model parameters. Central-Composite designs perform very well by the D -efficiency criterion (Lucas, 1974, 1976).

Many of the design construction procedures are based on an exchange algorithm. In the simplest form of this algorithm, a grid of candidate points is selected by the experimenter, and an initial design is selected (perhaps by random) from this set of points. Then the algorithm exchanges points that are in the grid but not in the design with points currently in the design in an effort to improve the selected optimality criterion. Because not every possible design is explicitly evaluated, there is no guarantee that an optimal design has been found, but the exchange procedure usually ensures that a design is “close” to optimal results. Some implementations repeat the design construction process several times, starting from different initial designs, to increase the likelihood that a final design that is very near the optimal will result (Atkinson and Done, 1992).

2.3 Space Filling Designs

From Santner et al. (2003) uncertainty arises in computer experiments because the exact functional form of the relationship between the inputs and response is not known, although the response can be computed at any given input. Any functional models that are used to describe the relationship are only approximations. The discrepancy between the actual response produced by the computer code and the response predicted from the fitted model is model bias.

Because the true relation between the response and inputs is not known, the designs for computer experiments strive to allow any model to be fitted, and to provide information about all portions of the experimental region.

Two “space-filling” designs will be considered in this study.

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1. Designs generated by Latin Hypercube Sampling (Section 2.3.1)
 2. Uniform Designs (Section 2.3.2)

The Latin Hypercube designs are widely used in simulation experiments and deterministic computer experiments (Kleijnen, 2008a; Law, 2007; Lin, 2003; Sacks et al., 1989; Sanchez, 2007; Santner et al., 2003; Trocine and Malone, 2000). Uniform Designs are the most common designs used in deterministic computer experiments (Fang, 2008; Fang et al., 2000; Lin, 2003; Lin et al., 2001; Sacks et al., 1989; Santner et al., 2003).

2.3.1 Latin Hypercube Design

According to Santner et al. (2003) designs generated by Latin hypercube sampling are called Latin hypercube designs (LHD). Consider Latin hypercube (LH) sampling from the unit square $[0, 1]^2$. To obtain a design consisting of n points, divide each axis $[0, 1]$ into the n equally spaced intervals $[0, 1/n), \dots, [(n-1)/n, 1]$. This partitions the unit square into n^2 cells of equal size. Now, fill these cells with the integers $1, 2, \dots, n$ so as to form a Latin square, i.e., an arrangement in which each integer appears exactly once in each row and in each column of this grid of cells. Select one of the integers at random. In each of the n cells containing this integer, select a point at random. The resulting sample of n points is a LHD of size n . The method of choosing the sample ensures that points are (marginally) spread evenly over the values of each input variable. Of course, such a LH sample could select points that are spread evenly along the diagonal of the square. Although the points in such a sample have projections that are evenly spread out over the values of each input variable separately, we would not regard them as evenly spread out over the entire unit square.

Santner et al. (2003) describes a general procedure for obtaining a LH sample of size n from $\mathbf{X} = (X_1, \dots, X_d)$ when $\mathbf{X}$ has independently distributed components. Suppose that a LH sample of size n is to be selected. The domain of each input variable is divided into n intervals. Each interval will be represented in the LH sample. The set of all possible Cartesian products of these intervals constitutes a partitioning of the d -dimensional sample

space into n^d “cells”. A set of n cells is chosen from the n^d population of cells in such a way that the projections of the centers of each of the cells onto each axis are uniformly spread across the axis; then a point is chosen at random in each selected cell.

Santner et al. (2003) construct the LH sample as follows. For $k = 1, \dots, d$, let $F_k(\cdot)$ denote the (marginal) distribution of X_k , the k^{th} component of $\mathbf{X}$ and, for simplicity, assume that $\mathbf{X}_k$ has support $[a_k, b_k]$. The k^{th} axis is divided into n parts, each of which has equal probability, $1/n$, under $F_k(\cdot)$. The division points for the k^{th} axis are

$$F_k^{-1}\left(\frac{1}{n}\right), \dots, F_k^{-1}\left(\frac{n-1}{n}\right).$$

To choose n of the cells so created, let $\mathbf{\Pi} = (\Pi_{jk})$ be an $n \times d$ matrix having columns which are d different randomly selected permutations of $\{1, 2, \dots, n\}$ i.e. (2.4) for $n = 3$ and $d = 2$.

$$\mathbf{\Pi} = \begin{pmatrix} 1 & 1 \\ 2 & 3 \\ 3 & 2 \end{pmatrix} \text{ and } \mathbf{\Pi} = \begin{pmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 1 \end{pmatrix} \quad (2.4)$$

Then the “upper-left hand” coordinates of the j^{th} cell in $\mathfrak{R}^d$ are

$$F_k^{-1}(n^{-1}(\Pi_{jk} - 1)), \quad k = 1, \dots, d,$$

with the convention $F_k^{-1}(0) = a_k$.

For $j = 1, \dots, n$, let $\mathcal{X}_{jk}$, $k = 1, \dots, d$, denote the k^{th} component of the j^{th} vector, $\mathcal{X}_j$. Then we define the LH sample to have values

$$\mathcal{X}_{jk} = F_k^{-1}\left(\frac{1}{n}(\Pi_{jk} - 1 + U_{jk})\right),$$

where $\{U_{jk}\}$ are independent and identically distributed $U[0, 1]$ deviates, for $j = 1, \dots, n$ and $k = 1, \dots, d$. In sum, the j^{th} row of $\mathbf{\Pi}$ identifies the cell that $\mathcal{X}_j$ is sampled from, while the corresponding (independently generated) uniform deviates determines the location of $\mathcal{X}_j$ within the sampled cell.

There exists different variations of the standard random Latin Hypercube Design. One such variation is to optimize the location of the $\mathcal{X}_j$ by the maximin criterion (Section 2.3.1).

Maximin Distance Criteria

From Santner et al. (2003), let $\mathcal{D} \subset \mathcal{X} \subset \mathbb{R}^d$ be an arbitrary n -point design consisting of distinct input sites $\{x_1, x_2, \dots, x_n\}$. Let ρ be a metric on $\mathcal{X}$. For example, one important distance measure is the p^{th} order distance between $\mathbf{w}, \mathbf{x} \in \mathcal{X}$ which is defined, for $p \geq 1$, by

$$\rho_p(\mathbf{w}, \mathbf{x}) = \left[\sum_{j=1}^d |\mathbf{w}_j - \mathbf{x}_j|^p \right]^{\frac{1}{p}} \quad (2.5)$$

Rectangular and Euclidean distance are $\rho_p(.,.)$ for $p = 1$ and $p = 2$ respectively.

One measure of the closeness of the points in the set $\mathcal{D}$ is the smallest distance between any two points in $\mathcal{D}$, i.e.,

$$\min_{x_1, x_2 \in \mathcal{D}} \rho_p(x_1, x_2).$$

A design that maximizes this measure is said to be a maximin distance design and denoted by $\mathcal{D}_{Mm}$; thus

$$\min_{x_1, x_2 \in \mathcal{D}_{Mm}} = \max_{\mathcal{D} \subset \mathcal{X}} \min_{x_1, x_2 \in \mathcal{D}} \rho_p(x_1, x_2).$$

In an intuitive sense, $\mathcal{D}_{Mm}$ designs guarantee that no two points in the design are “too close,” and hence the design points are spread over $\mathcal{X}$ (Santner et al., 2003).

2.3.2 Uniform Designs

Introduction

Uniform Designs are the most common design used in deterministic computer experiments (Fang, 2008; Fang et al., 2000; Lin, 2003; Lin et al., 2001; Sacks et al., 1989; Santner et al., 2003).

From Fang et al. (2000), both the Latin hypercube sampling (LHS) and uniform design (UD) are “space filling” experimental designs - the LHS design in a *randomly uniform fashion* and the UD in a *deterministically uniform fashion*. Specifically, if the experimental domain is finite, LHS designs are similar to UD. When the experimental domain is continuous, the fundamental difference between these two designs is that, in LHS designs, points are selected at random from cells, whereas in UD points are selected from the center of cells. Furthermore, an LHS design requires one-dimensional balance of all levels for each factor, but a UD requires one-dimensional balance and d -dimensional uniformity. Thus, these designs are similar in one dimension but can be very different in higher dimensions.

The Koksma-Hlawka inequality gives the upper error bound of the estimate $E(h(x))$:

$$|E(h(x)) - \bar{h}| \leq D(P)V(h), \quad (2.6)$$

where $V(h)$ is a measure of the variation of h and $D(P)$ is the discrepancy of P , a measure of the uniformity of P and $h(x)$ is the output of the experiment. Note that $V(h)$ is independent of the design points. Thus, given a bounded $V(h)$, Inequality (2.6) indicates that, the more uniform a set P points is over the experimental region C^d , the more accurate $\bar{h}$ is as an estimator of $E(h(x))$. Therefore one should choose a set of experimental points with smallest discrepancy among all possible designs for a given number of factors and experimental runs. This is the fundamental idea of UD. Note that UD is robust against changes of the function h for which $V(h)$ remains unchanged. This fact indicates that the UD can provide a good estimate of $E(h(x))$ for a very large class of $h(x)$. The key issue to be addressed then is how to find n points in C^d with minimum discrepancy.

Creating Uniform Designs

Suppose there are d factors of interest over a standard domain C^d . The goal here is to choose a set of n points $P_n = \{x_1, \dots, x_n\} \subset C^d$ such that these points are uniformly scattered on C^d . Let $M(P_n)$ be a measure of the non-uniformity of P_n ; we seek a set P_n^* that minimizes M or, equivalently, maximizes the uniformity over all possible n points on C^d (Fang et al., 2000).

Measures of uniformity

From the Koksma-Hlawka inequality in (2.6), a natural choice of M is the discrepancy $D(P)$. Let $F_n(x)$ be the empirical distribution function of P_n :

$$F_n(x) = \frac{1}{n} \sum_{i=1}^n I\{x_i \leq x\} \quad (2.7)$$

where $I\{\cdot\}$ is the indicator function and all inequalities are understood to be with respect to the component wise order of R^d . Then the L_p discrepancy can be defined as

$$D_p(P^n) = \left[\int_{C^s} |F_n(x) - F(x)|^p dx \right]^{1/p} \quad (2.8)$$

where $F(x)$ is the uniform distribution function of C^d . The popular L_∞ discrepancy obtained by taking $p = \infty$ in (2.8) is called the star discrepancy, or discrepancy for simplicity. This is probably the most commonly used measurement for discrepancy and can be re-expressed as follows:

$$d(p_n) = \sup_{x \in C^d} |F_n(x) - F(x)|. \quad (2.9)$$

The discrepancy has been universally accepted in quasi-Monte Carlo methods and number-theoretic methods. One disadvantage of the discrepancy is that it is expensive to compute. Attempts have been made to evaluate the discrepancy algorithmically (Fang et al. (2000)).

Construction Method

For the case $d = 1$, the UD under D is

$$P_n^* = \left\{ \frac{1}{2n}, \frac{2}{2n}, \dots, \frac{2n-1}{2n} \right\}, \quad (2.10)$$

with $D = 1/2n$. For $d > 1$, the problem of finding a UD is more difficult. One approach is to reduce the domain C^d into a smaller sub-domain $K_d \subset C^d$. Obviously the quality of the K_d UD depends on the quality of candidates K_D .

An $n \times d$ matrix $\mathbf{U}_{n,d} = (u_{ij})$, where each column is a permutation of $\{1, 2, \dots, n\}$, is called a U-type design. Its induced matrix, $\mathbf{X}_{n,d} = (x_{ij})$, is defined as

$$x_{ij} = (u_{ij} - .5)/n, \quad i = 1, \dots, n; j = 1, \dots, d. \quad (2.11)$$

a U-type design $\mathbf{U}_{n,d}$ provides an n -run experimental design for d factors, each having n levels, if the rank of $\mathbf{U}_{n,d}$ is d . The matrix $\mathbf{X}_{n,d}$ can be considered as n points on C^d . Let $\mathcal{U}_{n,d}$ denote the set of all $\mathbf{U}_{n,d}$ and $\chi_{n,d}$ be the set of all $\mathbf{X}_{n,d}$. There is a one-to-one correspondence between $\mathbf{U}_{n,d}$ and $\mathbf{X}_{n,d}$ so that they can be used interchangeably.

From Fang et al. (2000) a U-type design $\mathbf{U}_{n,d}$ with rank d whose induced matrix has the smallest discrepancy over $\chi_{n,d}$ is called a U uniform design and is denoted by $U_n(n^d)$.

The notation $U_n(n^d)$ is purposely chosen to mimic that commonly used for orthogonal designs $L_n(q^d)$, where n is the number of experiments, d the number of factors, and q the number of levels for each factor. The first column of $U_n(n^d)$ can always be taken as $(1, 2, \dots, n)^T$. There are $n! - 2$ possible permutations of $\{1, 2, \dots, n\}$ for the second column, $n! - 2$ choices for the third column, and so on (Fang et al., 2000).

2.3.3 Flexibility of Uniform Design

There are many different uniform designs with different number of runs and factor levels that can be used. A large number of uniform designs are available from the website

Table 2.4: $U_{20}(4^{14})$ Uniform Design

Run Nr.	A	B	C	D	E	F	G	H	J	K	L	M	N	O
1	1	1	4	1	1	1	3	2	2	3	3	4	3	3
2	3	1	1	4	1	2	2	4	2	2	1	3	2	4
3	1	3	2	3	2	1	1	4	4	1	2	1	3	3
4	3	2	4	3	4	2	4	3	2	2	1	1	4	1
5	4	1	4	2	3	1	1	2	1	1	2	2	2	2
6	1	1	1	3	3	3	1	3	3	4	4	3	3	1
7	2	1	2	4	4	3	3	2	4	1	3	2	4	4
8	1	3	2	2	2	4	4	3	1	4	1	2	2	4
9	4	2	3	3	2	4	4	4	4	2	4	3	1	2
10	2	2	3	1	1	4	3	1	3	1	2	1	2	1
11	4	2	2	2	2	2	2	1	4	4	1	4	4	2
12	4	3	1	1	4	4	1	2	2	2	3	4	3	3
13	3	4	4	2	1	3	1	3	3	3	4	2	4	4
14	4	3	2	4	1	3	2	2	1	3	3	1	1	1
15	1	4	4	3	4	3	2	1	3	2	1	3	1	3
16	3	4	1	1	3	1	3	3	4	3	2	2	1	1
17	3	3	3	4	3	1	4	1	3	4	3	4	2	4
18	2	4	3	4	3	4	3	4	1	3	2	4	4	2
19	2	2	3	1	4	2	2	4	2	4	4	1	1	3
20	2	4	1	2	2	2	4	1	1	1	4	3	3	2

<http://www.math.hkbu.edu.hk/UniformDesign/index.html>. In the case study, a $U_{20}(4^{14})$, 14 factor, 4 level, 20 run uniform design was downloaded from the website for the uniform design screening experiments (Section 4.2.3). The downloaded design is provided in Table 2.4.

Chapter 3

Approximation models for input-output relationships

3.1 Introduction

In this chapter the two approximation models utilized in the case study are discussed:

- Response Surface Models (Biles, 1979, 1984; Donohue et al., 1993; Kelton, 1999, 2000; Kleijnen, 2008a; Law, 2007)
- Kriging Models (Jack, 2007; Kleijnen and de Beers, 2004; Kleijnen, 2004, 2008a; Kleijnen et al., 2005; Law, 2007; van Beers and Kleijnen, 2003, 2004).

3.2 Response Surface Models

Response surface methodology, or **RSM**, is a collection of mathematical and statistical techniques useful for the modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimise the response. For example, suppose that a chemical engineer wishes to find the levels of temperature (x_1) and pressure (x_2) that maximize the yield (y) of a process. The process yield is a function of the

levels of temperature and pressure, say

$$y = f(x_1, x_2) + \epsilon$$

where ϵ represents the noise or error observed in the response y . If the expected response is denoted by $E(y) = f(x_1, x_2) = \eta$, then the surface represented by

$$\eta = f(x_1, x_2)$$

is called a response surface (Montgomery, 2005).

The response surface is normally represented graphically, where η is plotted versus the levels x_1 and x_2 . To help visualize the shape of a response surface, the contours of the response surface are often plotted. In the contour plot, lines of constant response are drawn in the x_1, x_2 plane. Each contour corresponds to a particular height of the response surface (Montgomery, 2005).

In most RSM problems, the form of the relationship between the response and the independent variables is unknown. Thus, the first step in RSM is to find a suitable approximation for the true functional relationship between y and the set of independent variables. Usually, a lower-order polynomial in some region of the independent variables is employed. If the response (y) is well modeled by a linear function of the independent variables ($x_i, i = 1, \dots, n$), then the approximating function is the first-order model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \epsilon \quad (3.1)$$

If there is curvature in the system, then a polynomial of higher degree must be used, such as the second-order model

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j}^k \sum_{j=1}^k \beta_{ij} x_i x_j + \epsilon \quad (3.2)$$

Almost all RSM problems use one or both of these models. Obviously, it is unlikely that a polynomial model will be a reasonable approximation of the true functional relationship over the entire space of the independent variables,

but for a relatively small region they usually work quite well (Montgomery, 2005).

Under the assumption of independent and identically distributed errors, the method of least squares (Section 3.2.1) is used to estimate the parameters in the approximation polynomials. Under the assumption of normality the least squares estimates are also the maximum likelihood estimates (Montgomery, 2005). The response surface analysis is then performed using the fitted surface. If the fitted surface is an adequate approximation of the true response function, then analysis of the fitted surface will be approximately equivalent to analysis of the actual system. The model parameters can be estimated most efficiently if proper experimental designs are used to collect the data (Montgomery, 2005).

3.2.1 Least Squares

The method of least squares is typically used to estimate the regression coefficients in a multiple linear regression model. Suppose that $n > k$ observations are available on the response variable, say $y_1, y_2, \dots, y_n$. Along with each observed response y_i , we will have an observation on each regressor variable and let x_{ij} denote the i th observation or level of variable x_j . The data will appear as in Table 3.1. We assume that the error term ϵ in the model has $E(\epsilon) = 0$ and $V(\epsilon) = \sigma^2$ and that $\{\epsilon_i\}$ are uncorrelated random variables. The model equation (3.1) can be written in terms of the observations in Table 3.1 as

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} + \epsilon \\ &= \beta_0 \sum_{j=1}^k \beta_j x_{ij} + \epsilon_i \quad i = 1, 2, \dots, n \end{aligned} \quad (3.3)$$

Succinctly, Equations (3.3), may be written in matrix notation as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad (3.4)$$

Table 3.1: Data for Multiple Linear Regression.

y	x_1	x_2	$\cdots$	x_k
y_1	x_{11}	x_{12}	$\cdots$	x_{1k}
y_2	x_{21}	x_{22}	$\cdots$	x_{2k}
$\vdots$	$\vdots$	$\vdots$	$-$	$\vdots$
y_n	x_{n1}	x_{n2}	$\cdots$	x_{nk}

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \text{ and } \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_k \end{bmatrix}$$

$\mathbf{y}$ is an $(n \times 1)$ vector of the observations, $\mathbf{X}$ is an $(n \times p)$ matrix of levels of independent variables, $\boldsymbol{\beta}$ is a $(p \times 1)$ vector of the regression coefficients, and $\boldsymbol{\epsilon}$ is an $(n \times 1)$ vector of random errors.

The vector of least squares estimators must be found, $\hat{\boldsymbol{\beta}}$, that minimizes

$$L = \sum_{i=1}^n \epsilon_i^2 = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Note that L may be expressed as

$$\begin{aligned} L &= \mathbf{y}^T \mathbf{y} - \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X} \boldsymbol{\beta} \\ &= \mathbf{y}^T \mathbf{y} - 2\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X} \boldsymbol{\beta} \end{aligned} \quad (3.5)$$

because $\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y}$ is a (1×1) matrix, or a scalar, and its transpose $(\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y})^T = \mathbf{y}^T \mathbf{X} \boldsymbol{\beta}$. The least squares estimator must satisfy

$$\left. \frac{\partial L}{\partial \boldsymbol{\beta}} \right|_{\hat{\boldsymbol{\beta}}} = -2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X} \hat{\boldsymbol{\beta}} = \mathbf{0}$$

which simplifies to

$$\mathbf{X}^T \mathbf{X} \hat{\boldsymbol{\beta}} = \mathbf{X}^T \mathbf{y} \quad (3.6)$$

Equation (3.6) is the matrix of the least squares normal equations. To solve the normal equations, multiply both sides of Equation (3.6) by the inverse of $\mathbf{X}^T \mathbf{X}$, assuming it exists. Thus the least squares estimator of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \quad (3.7)$$

Equation (3.6) yields the normal equations. Writing out Equation (3.6) in detail

$$\begin{bmatrix} n & \sum_{i=1}^n x_{i1} & \sum_{i=1}^n x_{i2} & \cdots & \sum_{i=1}^n x_{ik} \\ \sum_{i=1}^n x_{i1} & \sum_{i=1}^n x_{i1}^2 & \sum_{i=1}^n x_{i1}x_{i2} & \cdots & \sum_{i=1}^n x_{i1}x_{ik} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n x_{ik} & \sum_{i=1}^n x_{ik}x_{i1} & \sum_{i=1}^n x_{ik}x_{i2} & \cdots & \sum_{i=1}^n x_{ik}^2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_{i1}y_i \\ \vdots \\ \sum_{i=1}^n x_{ik}y_i \end{bmatrix}$$

is obtained.

In this form it is easy to see that $\mathbf{X}^T \mathbf{X}$ is a $(p \times p)$ symmetric matrix and $\mathbf{X}^T \mathbf{y}$ is a $(p \times 1)$ column vector. Note the special structure of the $\mathbf{X}^T \mathbf{X}$ matrix. The diagonal elements of $\mathbf{X}^T \mathbf{X}$ are the sums of squares of the elements in the column of $\mathbf{X}$, and the off-diagonal elements are the sums of cross-products of the elements in the columns of $\mathbf{X}$. Furthermore, note that the elements of $\mathbf{X}^T \mathbf{y}$ are the sums of cross-products of the columns of $\mathbf{X}$ and the observations $\{y_i\}$ (Montgomery, 2005). The fitted regression model is

$$\hat{\mathbf{y}} = \mathbf{X} \hat{\boldsymbol{\beta}} \quad (3.8)$$

In scalar notation the model is

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^k \hat{\beta}_j x_{ij} \quad i = 1, 2, \dots, n$$

The difference between the actual observations y_i and the corresponding fitted values $\hat{y}_i$ is the residual, say $e_i = y_i - \hat{y}_i$. The $(n \times 1)$ vector of residuals is denoted by

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} \quad (3.9)$$

Equation (3.7) remains the least squares estimate for the parameters in higher order polynomials, where $\mathbf{X}$ is expanded for all the terms in the model.

Response surface models are well established as approximation models in simulation experiments (Biles, 1979, 1984; Donohue et al., 1993; Kelton, 1999, 2000; Kleijnen, 2008a; Law, 2007) as well as in physical experiments (Box and Hunter, 1957; Box, 1999; Box and Liu, 1999; Coetzer et al., 2008a; Draper, 1982; Myers and Montgomery, 1995).

3.3 Kriging Models

From Simpson et al. (1998) kriging postulates a combination of a global model plus departures:

$$y(x) = f(x) + Z(x) \quad (3.10)$$

where $y(x)$ is the unknown function of interest, $f(x)$ is a known (usually polynomial) function of x , and $Z(x)$ is the realization of a stochastic process with mean zero, variance σ^2 , and non-zero covariance. The $f(x)$ term in equation (3.10) is similar to the polynomial model in a response surface and provides a “global” model of the design space. In many cases $f(x)$ is simply taken to be a constant term β .

While $f(x)$ “globally” approximates the design space, $Z(x)$ creates “localized” deviations so that the kriging model interpolates the n_d sampled data points.

The covariance matrix of $Z(x)$ is given by equation (3.11)

$$\text{Cov}[Z(x^i), Z(x^j)] = \sigma^2 \mathbf{R}([R(x^i, x^k)]) \quad (3.11)$$

In Equation (3.11), $\mathbf{R}$ is the correlation matrix, and $R(x^i, x^k)$ is the correlation function between any two of the n_d sampled data points x^i and x^j . $\mathbf{R}$ is a $(n_d \times n_d)$ symmetric matrix with ones along the diagonal. The correlation function $R(x^i, x^k)$ is specified by the user. A Gaussian correlation function is of the form:

$$R(x^i, x^k) = \exp\left[-\sum_{k=1}^{n_{dv}} \theta_k |x_k^i - x_k^j|^2\right] \quad (3.12)$$

where n_{dv} is the number of design variables, θ_k are the unknown correlation parameters used to fit the model, and the x_k^i and x_k^j are the k^{th} components of sample points x^i and x^j .

Predicted estimates, $\hat{y}(x)$ of the response $y(x)$ at untried values of x are given by:

$$\hat{y} = \hat{\beta} + r^T(x) \mathbf{R}^{-1} (y - f\hat{\beta}) \quad (3.13)$$

where y is the column vector of length n_d which contains the sample values of the response, and f is a column vector of length n_d which is filled with ones when $f(x)$ is taken as a constant. In equation (3.13), $r^T(x)$ is the correlation vector of length n_d between an untried x and the sampled data points $\{x^1, \dots, x^{n_d}\}$:

$$r^T(x) = [R(x, x^1), R(x, x^2), \dots, R(x, x^{n_d})]^T \quad (3.14)$$

In Equation (3.13), $\hat{\beta}$ is estimated using Equation (3.15).

$$\hat{\beta} = (f^T \mathbf{R}^{-1} f)^{-1} f^T \mathbf{R}^{-1} y \quad (3.15)$$

The estimate of the variance, σ^2 , between the underlying global model $\hat{\beta}$ and y , is estimated as:

$$\sigma^2 = \frac{(y - f\hat{\beta})^T \mathbf{R}^{-1} (y - f\hat{\beta})}{n_d} \quad (3.16)$$

where $f(x)$ is assumed to be the constant $\hat{\beta}$. The maximum likelihood estimates (i.e., “best guesses”) for the θ_k in equation (3.12) used to fit the model are found by maximising equation (3.17) over $\theta_k > 0$.

$$- \frac{[n_d \ln(\hat{\sigma}^2) + \ln |\mathbf{R}|]}{2} \quad (3.17)$$

Both $\hat{\sigma}^2$ and $|\mathbf{R}|$ are functions of θ_k . While any values of θ_k create an

interpolative model, the best kriging models are found by solving the k -dimensional unconstrained non-linear optimization problem given by equation (3.17) (Simpson et al., 1998).

Kriging models are well established as approximation models in the design and analysis of discrete computer models (Coetzer and Langley, 2006; Sacks et al., 1989; Santner et al., 2003; Simpson et al., 1998). Recently a lot of research has been done on using the kriging metamodel in stochastic simulation studies (Jack, 2007; Kleijnen and de Beers, 2004; Kleijnen, 2004, 2008a; Kleijnen et al., 2005; Law, 2007; van Beers and Kleijnen, 2003, 2004).

Chapter 4

Case Study

4.1 Introduction

In the industrial process studied in this paper, reactions are considered which form main products as well as a range of secondary products. The process takes a chemical feedstock and produces a range of high-valued chemical products for use as commodities in other chemical products. However, the production of polymer is a concern because it may foul the reactor system and necessitates periodic shutdowns for cleaning.

Cleaning is by means of a hot solvent wash process during which the polymer is melted/dissolved in a different solvent to the reaction solvent. If fouling is too severe to be removed in this process, the unit must be opened and mechanically cleaned by means of hydro-blasting.

The flow sheet for both the reaction and hot wash processes is shown in Figure 4.1. It includes:

1. Three parallel equal-sized batch activation reactors, two of which are in operation while the third is being defouled. The product from each activation reactor in operation is sent to a main reactor train. Each activation reactor can feed either of the two main reactor trains (one at a time). A batch charge from the activation reactor to main reactor occurs at constant intervals.
2. Two equal-sized main reactor trains, each consisting of two reactors in

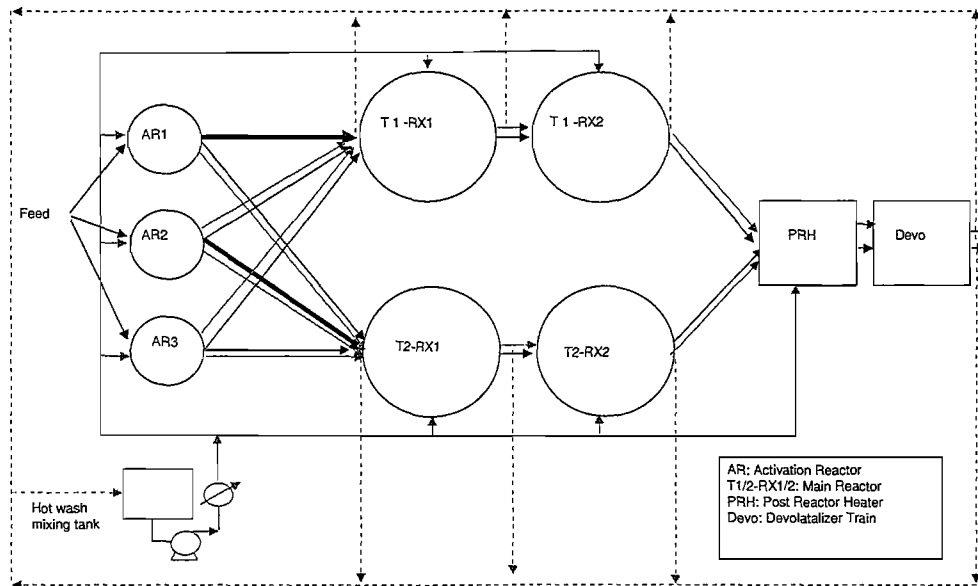


Figure 4.1: Reactor Flow sheet

series. If one of the two main reactors in series needs to be shut down, the other reactor in the train will be shut down and cleaned as well.

3. A spared post-reactor heater plus devolitzation unit. Each post reactor and Devo train services the output of both main reactor trains. If a Devo unit fouls, the associated post reactor heater must also be shut down for cleaning and vice versa

There is one hot wash system which can wash one main reactor train, one activation reactor and one post reactor heater plus Devo unit at a time. It can wash any of these sections separately or all three sections together. Thus it can simultaneously wash sections of the process flow diagram that are in series, but not sections that are in parallel.

The system depicted by the flowsheet in Figure 4.1 was modeled in the Arena stochastic simulation software from Rockwell Software (Kelton et al., 2002b). To carry out a simulation using random inputs such as time to failure, and time to repair, the probability distributions must be specified. Then, given that the input random variables to a simulation model follow particular distributions, the simulation proceeds through time by generating

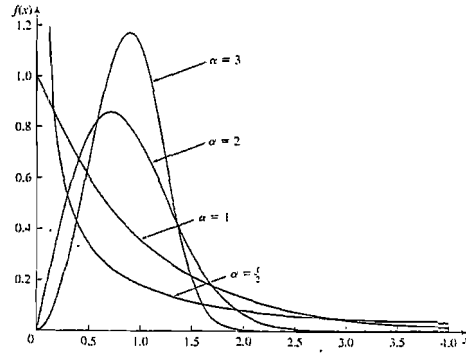


Figure 4.2: Weibull($\alpha,1$) density functions

random values from these distributions (Law, 2007).

The different Probability Distributions used to sample the Time to Failure and Cleaning Time are summarized below:

1. *Time to Failure Activation Reactor*: Weibull distribution.
2. *Time to Failure First main reactor in series*: Weibull distribution.
3. *Time to Failure Second main reactor in series*: Weibull distribution.
4. *Time to Failure Post reactor heater plus Devo unit*: Exponential decay.
5. *Cleaning by means of Hot Wash*: Normal distribution.

In the case of the activation reactor or a main reactor fouling, it is assumed that, on average, one in thirty hot washes will be unsuccessful and that hydro-blasting will be required. A normal probability distribution around the average is assumed. A constant turnaround time for hydro-blasting is assumed. This includes the time taken for attempting and abandoning the hot wash process.

In the case of the post reactor heater or Devo unit fouling, the same probability of a hot wash being unsuccessful and hydro-blasting being needed is assumed.

The reactor's failure distributions are given as Weibull distributions. The Weibull distribution has two parameters α and β . The α parameter is a shape

parameter. If $\alpha = 1$ then the Weibull distribution and the Exponential distribution are the same. The β parameter is a scale parameter. Possible applications of the Weibull distribution are the time to complete some task, time to failure of a piece of equipment; used as a rough model in the absence of data (Law, 2007).

The density function for the Weibull distribution is given by equation 4.1.

$$f(x) = \begin{cases} \alpha\beta^{-\alpha}x^{\alpha-1}e^{-(x/\beta)^\alpha} & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.1)$$

The distribution function of the Weibull function is given by equation 4.2.

$$F(x) = \begin{cases} 1 - e^{-(x/\beta)^\alpha} & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.2)$$

A scale parameter β determines the scale of measurement of the values in the range of the distribution. A change in β compresses or expands the associated distribution without altering its basic form. Also, if the distribution of the random variable X has a scale parameter of 1, then the distribution of the random variable $Y = \beta X$ has a scale parameter β .

A shape parameter α determines, apart from location and scale, the basic form or shape of the distribution with the general family of distributions of interest. Examples of different Weibull density functions are given in Figure 4.2. A change in α generally alters a distribution's properties (e.g., skewness) more fundamentally than a change in location or scale (Law, 2007).

The factors considered in the experimental study, together with their ranges, are depicted in Table 4.1. The definitions are as follows:

- *Hotwash Fail Factor*: Indicates the number of times out of 30 that the hotwash will be unsuccessful and hydro-blasting will be needed.
- *Hydro-blasting Days*: The number of days for hydro-blasting.
- *Hotwash Average*: The hours for the hotwash.

-
- *Hotwash SD*: The standard deviation for the hotwash hours around the average.
 - *Minimum Uptime Activation Reactor*: The minimum uptime for the activation reactor in days.
 - *Shape Parameter (α) for Activation Reactor Uptime*: The shape parameter for the weibull (Equations 4.1 and 4.2) distribution used to approximate the activation reactor uptime.
 - *Scale Parameter (β) for Activation Reactor Uptime*: The scale parameter for the weibull (Equations 4.1 and 4.2) distribution used to approximate the activation reactor uptime.
 - *Main Reactor Fail Factor*: A factor indicating the number of times out of 15 that the main reactor will fail in a shorter time period.
 - *Minimum Uptime Main Reactor*: The minimum uptime for the main reactor in days.
 - *Shape Parameter (α) for Main Reactor Uptime*: The shape parameter for the weibull (Equations 4.1 and 4.2) distribution used to approximate the main reactor uptime.
 - *Scale Parameter (β) for Main Reactor Uptime*: The scale parameter for the weibull (Equations 4.1 and 4.2) distribution used to approximate the activation reactor uptime.
 - *Minimum Uptime Post Reactor/Devo*: The minimum uptime for the Post Reactor/Devo in days.
 - *Mean Uptime Post Reactor/Devo*: The mean uptime for the Post Reactor/Devo in days.
 - *Hotwash Parallel or Series*: Indicates whether the hotwash can treat everything in parallel or only the equipment that are in series. This is a categorical variable, i.e. it can only have discrete values. Series is coded as 0, and parallel as 1.

Table 4.1: Variables and ranges used in phase one of the experimental design process.

Name	Low	High
Hotwash Fail Factor	1	3
Hydroblasting Days	4	6
Hotwash Average	12	36
Hotwash SD	1	3
Minimum Uptime Activation Reactor	2.5	5
Shape Parameter (α) for Activation Reactor Uptime	1	3
Scale Parameter (β) for Activation Reactor Uptime	2	4
Main Reactor Fail Factor	0	2
Minimum Uptime Main Reactor	4	8
Shape Parameter (α) for Main Reactor Uptime	1	3
Scale Parameter (β) for Main Reactor Uptime	2	4
Minimum Uptime Post Reactor/Devo	8	12
Mean Uptime Post Reactor/Devo	13	15
Hotwash Parallel or Series	0	1

The response of interest are the average availability of the plant over a four year period. From the flowchart in Figure 1.2 and it can be observed that at any specific moment in time the overall plant availability can be either 100% (e.g. both trains are on line), 50% (one train is on line) or 0% (both trains are offline). The availability is calculated as the average of all of these states over the four year period.

The Arena stochastic simulation software from Rockwell Software (Kelton et al., 2002b) was used to construct a model for this system. A batch runner was written in Microsoft Excel to facilitate the running of the scenarios needed for the experimentation.

4.2 Phase One - Screening Experiments

It is assumed that if there is an effect there is a cause (Lin, 2003). Engineers are constantly faced with distinguishing between factors which have substantial effects (causal or “active” factors) and those which do not have

a substantial effect (inert or “null” factors). The null factors are then adjusted appropriately to lower the cost; while the active factors are adjusted appropriately to yield better quality. To distinguish between them, a large number of factors can often be listed as possible sources of potential effects. Preliminary investigations may quickly remove some of these “candidate factors”. It is not unusual, however, to find that more than twenty sources of effects exists, and among those factors only a small portion are actually active. The goal here is to apply the Pareto principle of separating the vital few effects from the trivial many. A problem frequently encountered in this area is how to reduce the total number of experiments in such a screening structure. This is particularly important in situations where the cost of an individual run is expensive (e.g., regarding money or time). With powerful statistical software readily available for data analysis, there is no doubt that data collection is the most important part of such a problem (Lin, 2003).

The importance of factors depends on the *experimental domain*. The users should supply information on this domain, including realistic ranges of the individual factors and limits on the admissible factor combinations (e.g., some factor values must add up to 100%). Therefore, in practice, user involvement is crucial for the application of screening methods (Kleijnen, 2008a).

For this study the ranges and variables in Table 4.1 were used. The following designs were evaluated for the screening data collection.

- Fractional Factorial Design (Section 2.2.2).
- Plackett-Burman Design (Section 2.2.3).
- Uniform Design (Section 2.3.2).
- Latin Hypercube Design (Section 2.3.1).
- D-Optimal Design (Section 2.2.5).

Each of the designs will now be discussed, and the summary results presented. For each of the designs one replication of the simulation were performed at each design point. Another approach would have been to replicate

each design point for instance five times and use the average response value in the designs. The reason for using only one replication is that the goal of this study is specifically to assess the most efficient (least amount of model runs) experimental design strategy for simulation experiments. In the screening phase there can literally be hundreds of factors, and adding replications on each design point can prohibitively increase the computer time of the study. Replicated center points are added to the Second Phase (interaction and second order) designs (Section 4.3). This provides protection against curvature from second order effects as well as allow an independent estimate of experimental error to be obtained (Montgomery, 2005).

4.2.1 Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this screening experiment a resolution III design were used. Using a resolution III design the main effect sizes can be evaluated. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 14 variables and ranges (Table 4.1). For 14 variables a 2^{14-10} Fractional Factorial Design in 16 (Resolution III) runs were constructed and analysed using the Design Expert Software (Stat-Ease, 2006). The ANOVA table is provided in Table 7.1, Appendix 7.1. The ANOVA table depicts the significant factors only.

The total degrees of freedom are equal to the total number of experiments minus one for the overall mean, i.e. $16 - 1 = 15$. The degrees of freedom for each of the factors equal to 1 because they are considered as continuous variables.

The degrees of freedom for error are equal to $15 - 8 = 7$. This is important because it affects the experimental error of the results, i.e. the higher the degrees of freedom for error the smaller the experimental error should be. The degrees of freedom for error can be increased by additional replications. The sum of squares of the variables represents the variability in the data that is accounted for by each variable. Therefore, the total variability is indicated by the sum of squares of all the data, which is divided up into the individual sum of squares for the variables and the random error. The F-value is the

mean square for the variable in the model divided by the mean square for error. Thus, the F-value indicates how much is the variability accounted for by the variable greater than the random variability. Obviously, the mean square for the variable must be significantly larger than that of the random error to confirm that the variable has a statistical significant effect on the response. This significance is quantified by the p-value, i.e. the probability of finding an F-value on the F-distribution which is larger than the calculated F-value from the ANOVA. The numerator degrees of freedom are equal to that of the variable, and denominator degrees of freedom are equal to that of the random error for the F-distribution. In practice, a p-value ≤ 0.05 is acceptable for concluding statistical significance, i.e., 95% confidence that the variable has an effect on the response. The significance of the variable is affected by the variability in the data and the number of observations.

4.2.2 Plackett-Burman Design

The Plackett-Burman Designs were discussed in Section 2.2.3. For this screening experiment a 19 factor 20 run Plackett-Burman design was used. This is the smallest Plackett-Burman design equal to or larger than 14 factors. The number of runs for a Plackett-Burman Design must always be a multiple of four. The design was constructed using the Design Expert Software (Stat-Ease, 2006) for the variables and ranges as given in Table 4.1. After constructing the design columns 15-19 were removed (these columns are not needed because there are only 14 factors present in this study). The ANOVA table is provided in Table 7.2, Appendix 7.1.

4.2.3 Uniform Design

The Uniform Designs was discussed in Section 2.3.2. A $U_{20}(4^{14})$, 14 factor, 4 level, 20 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uniform Design Screening Experiments. For the categorical factor “Hotwash Parallel or Series” the levels 1 and 2 were combined to create “Hotwash Series”, coded as 0, and levels 3 and 4 were combined to create “Hotwash

Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.1. The ANOVA table is provided in Table 7.3, Appendix 7.1.

4.2.4 Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. A 14 factor 20 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This creates a Latin hypercube design optimized for the maximin criterion (Section 2.3.1). For the categorical factor “Hotwash Parallel or Series” the levels up to 0.5 were combined to create “Hotwash Series”, coded as 0, and values greater than 0.5 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.1. The ANOVA table is provided in Table 7.4, Appendix 7.1.

4.2.5 D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 15 run D-Optimal design was created and analyzed using the Design Expert Software (Stat-Ease, 2006) for the main effects model and factor ranges in Table 4.1. The ANOVA table is provided in Table 7.5, Appendix 7.1.

4.2.6 Screening Summary

The outputs for all the designs are summarized in Table 4.2. The numbers in the table indicates the relative sizes of the absolute values of the coefficients for the coded factors. This gives an indication of the relative importance of the factors. The values with a * were found to be the significant factors for each design from the ANOVA analysis (i.e. p values < 0.05). If the p value is very small (less than 0.05) then the terms in the model have a significant effect on the response (Stat-Ease, 2006). Also included in the table is the different R-Squared values which give an indication of how good the model represents the data. All the designs have high R-squared values illustrating that the respective models are acceptable. The R-Squared is a measure of the

Table 4.2: Summarized Results from the Screening Experiments.

	Fractional Factorial	Plackett Burman	Doptimal	Uniform	Maximin LHS
HotwashFailFactor	3*	3*	13	3*	3*
HydroblastingDays	5*	6*	5	4*	7
HotwashAverage	1*	1*	1*	1*	1*
HotwashSD	9	12	11	12	9
ActivationReactorMin	7*	13	12	6	14
ActivationReactorAlpha	6*	11	10	9	10
ActivationReactorBeta	11	9	4*	13	11
MainReactorSmallFailFact	8*	5*	3*	8	4*
MainReactorMin	2*	2*	2*	2*	2*
MainReactorAlpha	14	10	6	11	12
MainReactorBeta	4*	7*	8	14	8*
PostReactorMin	13	14	7	7	6*
PostReactorMean	10	8	14	10	13
HotWashParralel	12	4*	9	5*	5*
R-Squared	0.99	0.97	0.97	0.94	0.98
Adj R-Squared	0.98	0.95	0.96	0.92	0.97
Pred R-Squared	0.95	0.92	0.93	0.87	0.94

amount of variation around the mean explained by the model. The Adj R-Squared is a measure of the amount of variation around the mean explained by the model, adjusted for the number of terms in the model. The adjusted R-squared decreases as the number of terms in the model increases if those additional terms don't add value to the model. The Pred R-Squared is a measure of the amount of variation in new data explained by the model. The predicted R-squared and the adjusted R-squared should be within 0.20 of each other. Otherwise there may be a problem with either the data or the model (Stat-Ease, 2006). The p values for the models are also < 0.0001 for all the designs (see the ANOVA tables in Appendix 7.1).

The following can be observed from Table 4.2.

- The order of the first three values are mostly similar, but for the rest of the factors the designs differ.
- The amount of significant variables also differ for all five the designs in this screening study (with four significant factors for the D-Optimal with the least amount of significant factors, to eight significant factors for the resolution III Fractional Factorial Design as the largest amount of significant factors). The differences between the space filling designs (Uniform and Maximin Latin Hypercube designs) and the classical designs (Fractional Factorial, D-Optimal and Plackett-Burman designs) could be due to the fact that the output from stochastic simulation models are not discrete values, and contains variation. Therefore, the classical designs might be more suitable for generating data for stochastic simulation.
- The differences between the Fractional Factorial, D-Optimal and Plackett-Burman designs might be because of the difference in the number of runs, or the factor level combinations chosen for the design.

In the next phase all the designs will be constructed for all the different screening designs and significant factor combinations to evaluate the most efficient screening design.

4.3 Second Phase Experiments

In this phase experimental designs will be evaluated on the sets of variables which were identified as significant in the different screening designs (Phase One). The following designs were used in this phase:

- Fractional Factorial Design (Resolution V) (Section 2.2.2).
- Uniform Design (Section 2.3.2).
- Maximin Latin Hypercube Design (Section 2.3.1).
- D-Optimal Design (Section 2.2.5).
- Central Composite Design (Section 2.2.4).

Given the five designs in the screening phase (Section 4.2) there is therefore 25 design combinations that will be investigated in this section (See Figure 1.2 and discussion in Section 1.3). Each of the five designs mentioned above will be discussed under the heading of each of the screening designs completed (Top level in Figure 1.2).

Normally in the second phase of the sequential design process, interaction designs are used, and the data checked for curvature (Myers and Montgomery, 1995). If curvature is present, a third phase follows where the second order models are fitted. In this study, the curvature were found to be not significant. A Central Composite Design (Section 2.2.4) was however included in this phase, because it is a well known and widely used design.

Both a Response Surface Model (Section 3.2) and a Kriging Model (Section 3.3) were fitted to the data. For the kriging model a constant term for $f(x)$ (Equation (3.10)) and a Gaussian correlation model were used. The Response Surface model was fitted using Design Expert (Stat-Ease, 2006), and for the Kriging Model the DACE package (Lophaven et al., 2002) for Matlab (Mathworks, 2007) was used. For the Response Surface Model both the ANOVA tables and final equation in terms actual factors will be provided. For the kriging model the optimized θ values will be provided. The starting values for all the θ values provided to the optimizer is 0.1. A lower bound of

Table 4.3: Variables and ranges used in the Second Phase for the Fractional Factorial Design.

Name	Low	High
Hotwash Fail Factor	1	3
Hydroblasting Days	4	6
Hotwash Average	12	36
Minimum Uptime Activation Reactor	2.5	5
Shape Parameter (α) for Activation Reactor Uptime	1	3
Main Reactor Fail Factor	0	2
Minimum Uptime Main Reactor	4	8
Scale Parameter (β) for Main Reactor Uptime	2	4

0 and an upper bound of $1e10^9$ for the θ values were used in this study. This effectively leaves the θ values unbounded (Lophaven et al., 2002).

4.3.1 Fractional Factorial Design

The factors in Table 4.3 were found to be significant in the Resolution III Fractional Factorial Design in the Screening Phase (Section 4.2.1). The designs in this section were applied to the factors and ranges in Table 4.3.

Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this experiment a resolution V design was used. Using a resolution V design the main effect and second order interactions can be evaluated. The Design Expert Software (Stat-Ease, 2006) was used to set up a design in the 8 variables and ranges in Table 4.3. A 2^{8-2} Fractional Factorial Design in 64 runs (Resolution V) was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. This provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). 64 Simulation runs were performed. Plant availability is the response of interest. The ANOVA table is provided in Table 7.6, Appendix 7.2. The ANOVA table depicts the significant factors only. The final equation in terms of the actual

factors are provided in Table 4.4. From the ANOVA Table it can be observed that the Sum of Squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between HotwashAverage and MainReactorMin. These two terms also have the largest individual sum of squares. The interaction term is positive (Table 4.4). The MainReactorMin term is positive. This makes intuitive sense, because a larger minimum uptime for the main reactor should increase the availability of the plant. The hotwash average has a negative impact on the plant availability. A larger average time that the hotwash takes will have a negative impact on the availability. One way to visualize the interaction between two terms is by using a contour plot. The contour plot of Hotwash average against the minimum uptime for the main reactor is provided in Figure 4.3. From this plot it is clear that the availability indeed increases in the direction of higher minimum uptime for the main reactor, and lower average time for the hotwash. Some interaction can be detected, but it is also clear that the linear effect is much larger than the interaction effect.

The θ values for the fitted kriging model are provided in Table 4.5. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Uniform Design

The Uniform Designs were discussed in Section 2.3.2. A $U_{48}(4^8)$, 8 factor, 4 level, 48 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uniform Design Experiments. The design was scaled to represent the ranges in Table 4.3. Five center points were added to the design. This provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.7, Appendix 7.2. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.6. Only one interaction term, between HotwashAverage and MainReactorSamllFailFact, is present in this model. The sum of squares

Table 4.4: Response Surface Model Fitted to the Resolution V Fractional Factorial Design Data.

Availability	=
96.95571	
-3.2233	* HotwashFailFactor
-1.11985	* HydroblastingDays
-0.95398	* HotwashAverage
-0.03061	* ActivationReactorMin
-1.29633	* MainReactorSmallFailFact
1.018319	* MainReactorMin
1.982442	* MainReactorBeta
-0.69066	* HotwashFailFactor * HydroblastingDays
0.050994	* HotwashFailFactor * HotwashAverage
0.294074	* HotwashFailFactor * ActivationReactorMin
0.16719	* HotwashFailFactor * MainReactorMin
0.222951	* HotwashFailFactor * MainReactorBeta
0.029707	* HydroblastingDays * HotwashAverage
0.018121	* HotwashAverage * ActivationReactorMin
-0.03358	* HotwashAverage * MainReactorSmallFailFact
0.036023	* HotwashAverage * MainReactorMin
0.137533	* MainReactorSmallFailFact * MainReactorMin
-0.21766	* MainReactorMin * MainReactorBeta

Table 4.5: θ Values for the Kriging Models for Fractional Factorial Design.

	Fractional Factorial	Uniform	Lhs	Dopt	CCD
HotwashFailFactor	0.1072	0.0330	0.0758	0.0536	0.0785
HydroblastingDays	0.0250	0.0319	0.0189	0.0342	0.0451
HotwashAverage	0.0812	0.0536	0.0574	0.0758	0.2928
ActivationReactorMin	0.0250	0.0297	0.0063	0.0139	0.0595
ActivationReactorAlpha	0.0058	0.0031	0.0250	0.0051	0.0637
MainReactorSmallFailFact	0.0189	0.0225	0.0330	0.0121	0.0555
MainReactorMin	0.0707	0.0406	0.0574	0.0379	0.5098
MainReactorBeta	0.0125	0.0080	0.0189	0.0074	0.0420

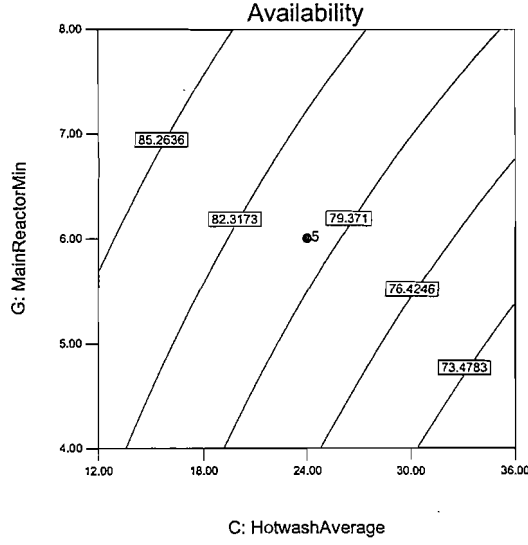


Figure 4.3: Contour Plot Of Hotwash Average Against Minimum Uptime for the Main Reactor for The Fractional Factorial Design

value for this interaction term is small compared to the sum of squares of the linear terms, which indicates that the effect of this interaction on the response is much smaller than the effect of the linear terms. This can be confirmed by looking at the contour plot in Figure 4.4. Availability increases in the direction of decreasing Average Hotwash. At the minimum Average Hotwash the Main Reactor Fail Factor does not have much of an effect on availability. It can also be concluded from this plot that the effect on the availability of the average hotwash time is much bigger than the effect of the main reactor small fail factor. This can be confirmed by looking at the sum of square values in Table 7.7. The sum of square values for hotwash average and minimum uptime for the main reactor are again significantly larger than the values for the other factors.

The θ values for the fitted kriging model are provided in Table 4.5. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Table 4.6: Response Surface Model Fitted to the Uniform Design Data.

Availability	=
88.876093	
-2.6309518	* HotwashFailFactor
-1.9414809	* HydroblastingDays
-0.3907477	* HotwashAverage
0.8664434	* ActivationReactorMin
0.6762777	* MainReactorSmallFailFact
1.751504	* MainReactorMin
1.194288	* MainReactorBeta
-0.078901	* HotwashAverage * MainReactorSmallFailFact

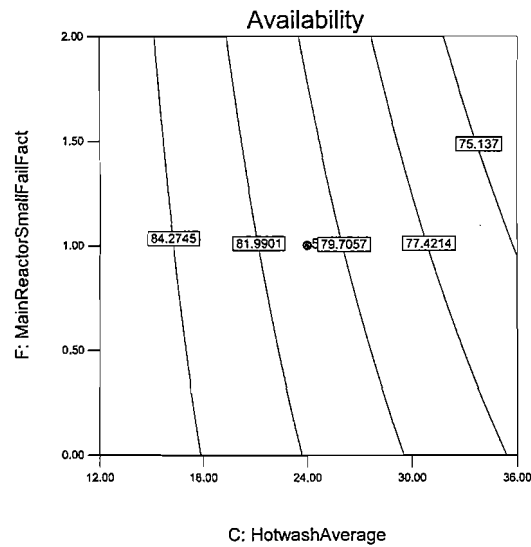


Figure 4.4: Contour Plot Of Hotwash Average Against the Small Fail Factor for the Main Reactor for The Uniform Design

Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. An 8 factor 48 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This creates a Latin hypercube design optimized for the maximin criterion. The design was scaled to represent the ranges in Table 4.3. Five center points were added to the design. This provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.8, Appendix 7.2. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.7. From the ANOVA table it can be observed that the sum of squares of the linear terms are significantly bigger than the sum of squares of the interaction terms. The largest interaction term is between hydroblasting days and minimum uptime for the main reactor. The contour plot for the hydroblasting days against the minimum uptime for the main reactor are provided in Figure 4.5. Plant availability increases in the direction of decreasing hydroblasting days and increasing minimum uptime for the main reactor. The three largest linear effects by sum of squares are the average time to hotwash, the minimum uptime for the main reactor and the hotwash fail factor.

The θ values for the fitted kriging model are provided in Table 4.5. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 42 run D-Optimal design for the main and interaction effects model for the factor ranges in Table 4.3 was created and analyzed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. This provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.9, Appendix 7.2. The ANOVA table depicts the significant factors

Table 4.7: Response Surface Model Fitted to the Maximin Latin Hypercube Design Data.

Availability	=
107.6206	
-2.65307	* HotwashFailFactor
-4.07641	* HydroblastingDays
-0.97994	* HotwashAverage
0.470548	* ActivationReactorMin
-1.11045	* ActivationReactorAlpha
2.013526	* MainReactorSmallFailFact
-3.35224	* MainReactorMin
7.86851	* MainReactorBeta
0.76969	* HydroblastingDays * ActivationReactorAlpha
0.670763	* HydroblastingDays * MainReactorMin
-1.00687	* HydroblastingDays * MainReactorBeta
0.058682	* HotwashAverage * MainReactorMin
0.068648	* HotwashAverage * MainReactorBeta
-0.8886	* ActivationReactorAlpha * MainReactorBeta
-1.08992	* MainReactorSmallFailFact * MainReactorBeta

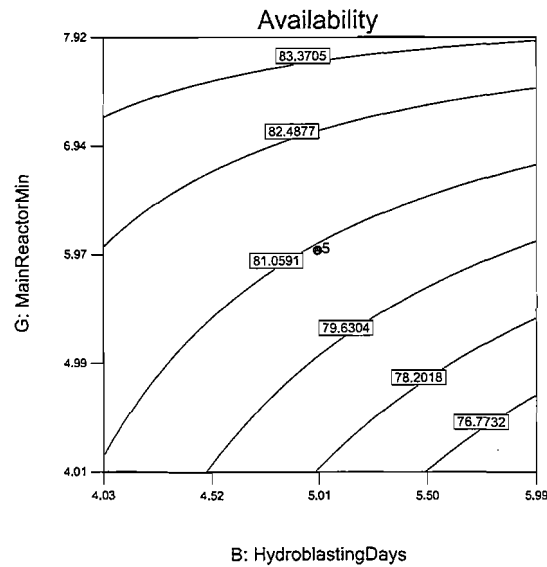


Figure 4.5: Contour Plot Of Hydroblasting Days Against the Minimum Up-time for the Main Reactor for The Latin Hypercube Design

Table 4.8: Response Surface Model Fitted to the D-Optimal Design Data.

Availability	=
99.10795	
-2.68279	* HotwashFailFactor
-1.37287	* HydroblastingDays
-0.93267	* HotwashAverage
-0.98154	* ActivationReactorMin
0.753702	* MainReactorSmallFailFact
0.690362	* MainReactorMin
2.051265	* MainReactorBeta
-0.91728	* HotwashFailFactor * HydroblastingDays
0.065436	* HotwashFailFactor * HotwashAverage
0.408241	* HotwashFailFactor * ActivationReactorMin
0.220395	* HotwashFailFactor * MainReactorMin
0.028895	* HydroblastingDays * HotwashAverage
0.254972	* HydroblastingDays * ActivationReactorMin
-0.31818	* HydroblastingDays * MainReactorSmallFailFact
-0.03303	* HotwashAverage * MainReactorSmallFailFact
0.040284	* HotwashAverage * MainReactorMin
-0.16754	* MainReactorMin * MainReactorBeta

only. The final equation in terms of the actual factors are provided in Table 4.8. From the ANOVA it can be observed that the sum of squares of the linear terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average hotwash time and the main reactor minimum uptime. These two terms also have the largest individual sum of squares. The interaction term is positive (Table 4.8). The contour plot for the average time to hotwash against minimum uptime for the main reactor are given in Figure 4.6. The plant availability increases in the direction of increasing minimum uptime for the main reactor, and decreasing hotwash average. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.5. None of the θ are at the starting value of 0.1, i.e. optimized values were obtained.

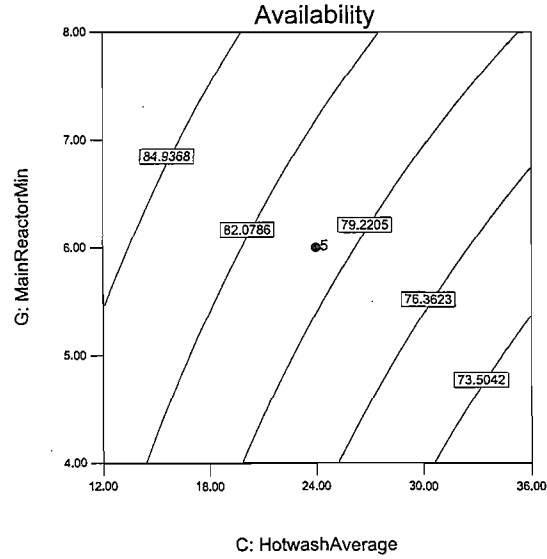


Figure 4.6: Contour Plot Of Hydroblasting Days Against the Minimum Up-time for the Main Reactor for The D-Optimal Design

Central Composite Design

The Central Composite Designs were discussed in Section 2.2.4. For this experiment a resolution V face centered Central Composite Design were used. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 8 variables and ranges in Table 4.3. For 8 variables a 54 run design was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five replications of the center point were added to the design. This provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.10, Appendix 7.2. The ANOVA table depicts the significant factors only. The final equations in terms of the actual factors are provided in Table 4.9. From the ANOVA table it can be observed that sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between average hotwash time and minimum uptime for the main reactor. These two factors also has the largest individual sum of squares. In this equation there is one quadratic term for the alpha parameter for the activation reactor. The sum of

Table 4.9: Response Surface Model Fitted to the Central Composite Design Data.

Availability	=
88.36052	
-2.44609	* HotwashFailFactor
-0.87262	* HydroblastingDays
-0.86045	* HotwashAverage
0.353191	* ActivationReactorMin
3.662175	* ActivationReactorAlpha
-0.86609	* MainReactorSmallFailFact
1.331153	* MainReactorMin
3.079985	* MainReactorBeta
-0.77505	* HotwashFailFactor * HydroblastingDays
0.045666	* HotwashFailFactor * HotwashAverage
0.389908	* HotwashFailFactor * ActivationReactorMin
0.173581	* HotwashFailFactor * MainReactorMin
0.028478	* HydroblastingDays * HotwashAverage
-0.03478	* HotwashAverage * MainReactorSmallFailFact
0.033085	* HotwashAverage * MainReactorMin
0.11239	* ActivationReactorAlpha * MainReactorMin
-0.33313	* MainReactorMin * MainReactorBeta
-1.1	* ActivationReactorAlpha ²

squares of the quadratic term is significantly larger than the sum of squares of the linear term. The quadratic effect is depicted in Figure 4.7, which indicate an optimum value at about median alpha parameter for activation reactor value.

The θ values for the fitted kriging model are provided in Table 4.5. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Summary

The R-Squared values for all the designs discussed in this leg are summarized in Table 4.10. All the designs have high R-squared values illustrating that the respective models are acceptable. The p values for the models are also

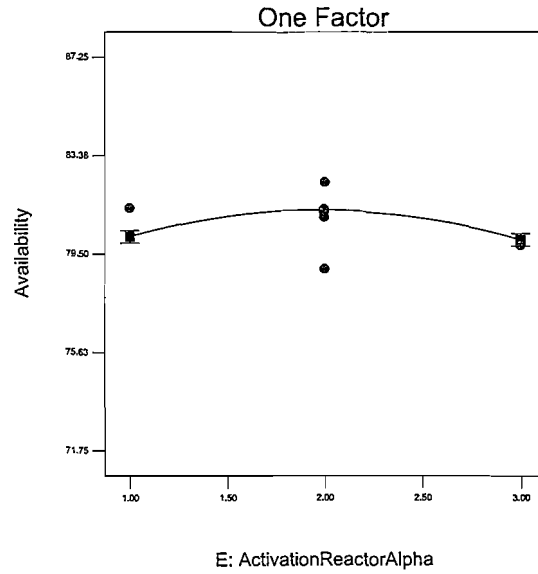


Figure 4.7: Plot Of Activation Reactor Alpha for the Central Composite Design

< 0.0001 for all the designs (see the ANOVA tables in Appendix 7.2) which indicates that the models are significant.

From the ANOVA tables in Appendix 7.2 it can be observed that the hotwash fail factor, average time to hotwash and the minimum uptime for the main reactor consistently are the three factors with the highest sum of square values. It can also be observed that the linear terms generally have significantly larger sum of square values than the interaction terms. Another interesting observation from Table 4.5 is that the highest three θ values were obtained for the hotwash fail factor, average time to hotwash and the minimum uptime for the main reactor, which is in agreement with the results from the response surface models.

Table 4.10: R-Squared values for the designs discussed in for the Fractional Factorial Design.

	R-Squared	Adj R-Squared	Pred R-Squared
Fractional Factorial	0.99	0.99	0.98
Uniform	0.97	0.97	0.96
Latin Hypercube	0.98	0.97	0.95
D-Optimal	0.99	0.98	0.98
Central Composite	0.99	0.99	0.98

Table 4.11: Variables and ranges used in the Second Phase for the Uniform Design Design.

Name	Low	High
Hotwash Fail Factor	1	3
Hydroblasting Days	4	6
Hotwash Average	12	36
Minimum Uptime Main Reactor	4	8
Hotwash Parallel or Series	0	1

4.3.2 Uniform Design

The factors in Table 4.11 were found to be significant from the in the Uniform Design in the Screening Phase (Section 4.2.3). The designs in this section were applied to the factors and ranges in Table 4.11.

Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this experiment a resolution V design was used. Using a resolution V design the main effect and second order interactions can be evaluated. The Design Expert Software (Stat-Ease, 2006) was used to set up a design in the 5 variables and ranges in Table 4.11. A 2^{5-1} Fractional Factorial Design in 16 runs (Resolution V) was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). 5 center points were added to the design. The center point was repeated for both of the levels of the categorical factor “Hotwash Parallel or Series”. The center point provides protection against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.11, Appendix 7.3. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.12. Note that because HotWashParralel is a categoric variable, two equations is obtained. One for Series Hotwash (Coded as 0), and one for Parallel Hotwash (Coded as 1). From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of

Table 4.12: Response Surface Model Fitted to the Fractional Factorial Design Data.

HotWashParralel	0
Availability	=
91.05182	
0.459919	* HotwashFailFactor
0.156968	* HydroblastingDays
-0.71542	* HotwashAverage
0.883881	* MainReactorMin
-0.7193	* HotwashFailFactor * HydroblastingDays
0.042629	* HotwashFailFactor * HotwashAverage
0.033184	* HotwashAverage * MainReactorMin
HotWashParralel	1
Availability	=
94.10304	
0.459919	* HotwashFailFactor
0.156968	* HydroblastingDays
-0.71542	* HotwashAverage
0.883881	* MainReactorMin
-0.7193	* HotwashFailFactor * HydroblastingDays
0.042629	* HotwashFailFactor * HotwashAverage
0.033184	* HotwashAverage * MainReactorMin

the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares. The contour plot of average time to hotwash against minimum uptime for main reactor are provided in Figure 4.8. It can be observed that plant availability increases in the direction of decreasing average time to hotwash, and increasing minimum uptime for the main reactor. The effect of the interaction between the average time to hotwash and the minimum uptime for the main reactor is much smaller than the individual effects.

The θ values for the fitted kriging model are provided in Table 4.13. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

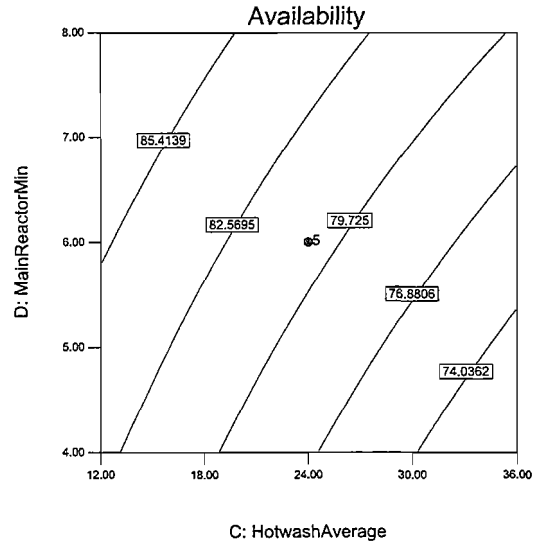


Figure 4.8: Contour Plot Of Hotwash Average Against the Minimum Uptime for the Main Reactor for The Fractional Factorial Design

Table 4.13: θ Values for the Kriging Models for Uniform Design.

	Fractional Factorial	Uniform	Lhs	Dopt	CCD
HotwashFailFactor	0.0138	0.0345	0.0226	0.0138	0.0917
HydroblastingDays	0.0057	0.0336	0.0125	0.0063	0.0748
HotwashAverage	0.2208	0.2264	0.3623	0.1811	0.1713
MainReactorMin	0.0336	0.0762	0.2208	0.0673	0.0525
HotWashParralel	0.0410	0.0088	0.1104	0.0372	0.0347

Uniform Design

The Uniform Designs were discussed in Section 2.3.2. A $U_{20}(4^5)$, 5 factor, 4 level, 20 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uniform Design Experiments. For the categorical factor “Hotwash Parallel or Series” the levels 1 and 2 were combined to create “Hotwash Series”, coded as 0, and levels 3 and 4 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.11. 5 center points were added to the design. The center point was repeated for both of the levels of the categorical factor “Hotwash Parallel or Series”. The ANOVA table is provided in Table 7.12, Appendix 7.3. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.14. Note that because HotWashParallel is a categorical variable, two equations are obtained. One for Series Hotwash (Coded as 0), and one for Parallel Hotwash (Coded as 1). There are no interaction terms present in this model. The average effect of time to hotwash is significantly bigger in terms of the sum of squares than the other factors.

The θ values for the fitted kriging model are provided in Table 4.13. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. A 5 factor, 20 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This creates a Latin hypercube design optimized for the maximin criteria. For the categorical factor “Hotwash Parallel or Series” the levels up to 0.5 were combined to create “Hotwash Series”, coded as 0, and values greater than 0.5 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.11. 5 center points were added to the design. The center point was repeated for both of the levels of the categorical factor “Hotwash Parallel or Series”. The center point provides protection

Table 4.14: Response Surface Model Fitted to the Uniform Design Data.

HotWashParralel	0
Availability	=
95.48	
-2.13	* HotwashFailFactor
-1.61	* HydroblastingDays
-0.45	* HotwashAverage
1.40	* MainReactorMin
HotWashParralel	1
Availability	=
98.283185	
-2.1332352	* HotwashFailFactor
-1.6105522	* HydroblastingDays
-0.4534698	* HotwashAverage
1.3968839	* MainReactorMin

against curvature from second order effects as well as allow an independent estimate of error (Montgomery, 2005). The ANOVA table is provided in Table 7.13, Appendix 7.3. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.15. There are no interaction terms present in this model. The average time to hotwash is significantly bigger in terms of the sum of squares than the other factors.

The θ values for the fitted kriging model are provided in Table 4.13. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 21 run D-Optimal design for the main and interaction effects model for the factor ranges in Table 4.11 was created and analyzed using the Design Expert Software (Stat-Ease, 2006). 5 center points were added to the design. The center point was repeated for both of the levels of the categorical factor “Hotwash Parallel or

Table 4.15: Response Surface Model Fitted to the Latin Hypercube Design Data.

HotWashParralel	0
Availability	=
90.72885	
-2.13456	* HotwashFailFactor
-1.06816	* HydroblastingDays
-0.45805	* HotwashAverage
1.76137	* MainReactorMin
HotWashParralel	1
Availability	=
93.72088	
-2.13456	* HotwashFailFactor
-1.06816	* HydroblastingDays
-0.45805	* HotwashAverage
1.76137	* MainReactorMin

Series". The ANOVA table is provided in Table 7.14, Appendix 7.3. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.16. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also has the largest individual sum of squares values. The interaction term is positive (Table 4.16). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.9. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.13. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Table 4.16: Response Surface Model Fitted to the D-Optimal Design Data.

HotWashParralel	0
Availability	=
91.95165	
0.449509	* HotwashFailFactor
0.130174	* HydroblastingDays
-0.73237	* HotwashAverage
0.818509	* MainReactorMin
-0.71446	* HotwashFailFactor * HydroblastingDays
0.043839	* HotwashFailFactor * HotwashAverage
0.035	* HotwashAverage * MainReactorMin
HotWashParralel	1
Availability	=
94.66036	
0.449509	* HotwashFailFactor
0.130174	* HydroblastingDays
-0.73237	* HotwashAverage
0.818509	* MainReactorMin
-0.71446	* HotwashFailFactor * HydroblastingDays
0.043839	* HotwashFailFactor * HotwashAverage
0.035	* HotwashAverage * MainReactorMin

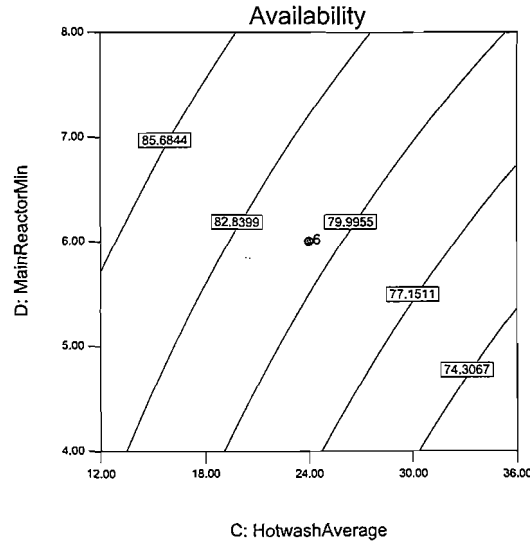


Figure 4.9: Contour Plot Of Hotwash Average Against the Minimum Uptime for the Main Reactor for The D-Optimal Design

Central Composite Design

The Central Composite Designs were discussed in Section 2.2.4. For this experiment a small face centered Central Composite Design were used. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 5 variables and ranges in Table 4.11. For 5 variables a 42 run design was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). The central composite design replicates a 21 run (including 5 center points) 4 factor design for both of the levels of the categorical factor “Hotwash Parallel or Series”. The ANOVA table is provided in Table 7.15, Appendix 7.3. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.17. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to hotwash, and the hotwash fail factor. These two terms also has the largest individual sum of squares values. The interaction term is positive (Table 4.17). The contour plot of average time to hotwash against hotwash fail factor are provided in

Table 4.17: Response Surface Model Fitted to the Central Composite Design Data.

HotWashParralel	0
Availability	=
92.27255	
1.683514	* HotwashFailFactor
0.35881	* HydroblastingDays
-0.70013	* HotwashAverage
0.945262	* MainReactorMin
-1.10881	* HotwashFailFactor * HydroblastingDays
0.052397	* HotwashFailFactor * HotwashAverage
0.023171	* HotwashAverage * MainReactorMin
HotWashParralel	1
Availability	=
89.05878	
2.511087	* HotwashFailFactor
1.155563	* HydroblastingDays
-0.70013	* HotwashAverage
0.945262	* MainReactorMin
-1.10881	* HotwashFailFactor * HydroblastingDays
0.052397	* HotwashFailFactor * HotwashAverage
0.023171	* HotwashAverage * MainReactorMin

Figure 4.10. The plant availability increases in the direction of decreasing average time to hotwash and decreasing hotwash fail factor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.13. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Summary

The R-Squared values for all the designs discussed in this leg are summarized in Table 4.18. The R-Squared is a measure of the amount of variation around the mean explained by the model. All the designs have high R-squared

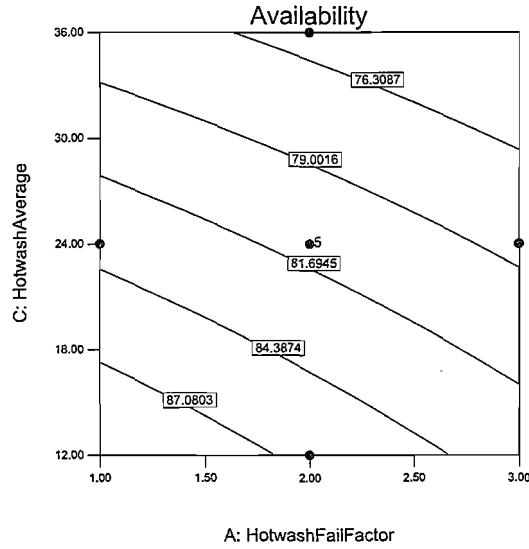


Figure 4.10: Contour Plot Of Hotwash Average Against the Hotwash Fail Factor for The Central Composite Design

values illustrating that the respective models are acceptable. The p value for the models are also < 0.0001 for all the designs (see the ANOVA tables in Appendix 7.3) which indicates that the models are significant.

From the ANOVA tables in Appendix 7.3 it can be observed that the hotwash fail factor, average time to hotwash, minimum uptime for the main reactor, and parallel or series hotwash are consistently the factors with the highest sum of square values. It can also be observed that the linear terms generally have significantly larger sum of square values than the interaction terms.

From Table 4.13 it can be observed that the θ values are significantly larger for the average time to hotwash than for the other factors. The second largest θ values are for the minimum uptime for the main reactor for all the designs, except for the central composite design. For the central composite design the largest θ value is obtained for the hotwash fail factor.

Table 4.18: R-Squared values for the designs discussed in for the Uniform Design.

	R-Squared	Adj R-Squared	Pred R-Squared
Fractional Factorial	0.99	0.98	0.96
Uniform	0.95	0.94	0.91
Latin Hypercube	0.94	0.93	0.90
D-Optimal	0.98	0.97	0.96
Central Composite	0.98	0.98	0.97

Table 4.19: Variables and ranges used in the Second Phase for the Latin Hypercube Design Leg.

Name	Low	High
Hotwash Fail Factor	1	3
Hotwash Average	12	36
Main Reactor Fail Factor	0	2
Minimum Uptime Main Reactor	4	8
Scale Parameter (β) for Main Reactor Uptime	2	4
Minimum Uptime Post Reactor/Devo	8	12
Hotwash Parallel or Series	0	1

4.3.3 Latin Hypercube Design

The factors in Table 4.19 were found to be significant from the in the Latin Hypercube Design in the Screening Phase (Section 4.2.4). The designs in this section are applied to the factors and ranges in Table 4.19.

Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this experiment a resolution VII design was used, because no Resolution V Fractional Factorial Design are available for 7 factors. Using a resolution VII design the main effect and second order interactions can still be evaluated. The Design Expert Software (Stat-Ease, 2006) was used to set up a design in the 7 variables and ranges in Table 4.19. A 2^{7-1} Fractional Factorial Design in 64 runs (Resolution VII) was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table is provided in Table 7.16, Appendix 7.4. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.20. Note that because HotWashParralel is a categoric variable, two equations is obtained. One for Series Hotwash (Coded as 0), and one for Parallel Hotwash (Coded as 1). From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to

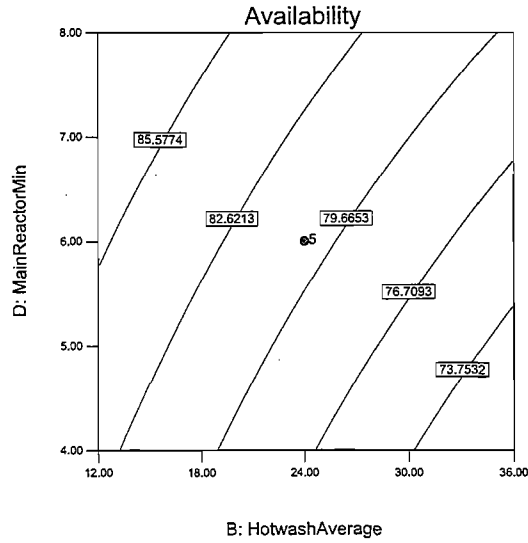


Figure 4.11: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Fractional Factorial Design

hotwash, and the minimum uptime for the main reactor. These two terms also has the largest individual sum of squares values. The interaction term is positive (Table 4.20). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.11. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.21. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Uniform Design

The Uniform Designs were discussed in Section 2.3.2. A $U_{48}(4^7)$, 7 factor, 4 level, 48 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uniform Design Experiments. For the categorical factor “Hotwash Parallel or Series” the levels 1 and 2 were combined to create “Hotwash Series”, coded

Table 4.20: Response Surface Model Fitted to the Fractional Factorial Design Data.

HotWashParralel	0
Availability	=
91.36063	
-4.89343	* HotwashFailFactor
-0.76396	* HotwashAverage
-0.56133	* MainReactorSmallFailFact
1.187926	* MainReactorMin
1.143659	* MainReactorBeta
0.035704	* HotwashFailFactor * HotwashAverage
0.14547	* HotwashFailFactor * MainReactorMin
0.235841	* HotwashFailFactor * MainReactorBeta
-0.02766	* HotwashAverage * MainReactorSmallFailFact
0.033886	* HotwashAverage * MainReactorMin
0.02172	* HotwashAverage * MainReactorBeta
-0.18951	* MainReactorMin * MainReactorBeta
HotWashParralel	1
Availability	=
94.33347	
-3.99277	* HotwashFailFactor
-0.76396	* HotwashAverage
-0.56133	* MainReactorSmallFailFact
0.838263	* MainReactorMin
1.143659	* MainReactorBeta
0.035704	* HotwashFailFactor * HotwashAverage
0.14547	* HotwashFailFactor * MainReactorMin
0.235841	* HotwashFailFactor * MainReactorBeta
-0.02766	* HotwashAverage * MainReactorSmallFailFact
0.033886	* HotwashAverage * MainReactorMin
0.02172	* HotwashAverage * MainReactorBeta
-0.18951	* MainReactorMin * MainReactorBeta

Table 4.21: θ Values for the Kriging Models for Latin Hypercube.

	Fractional Factorial	Uniform	Lhs	Dopt	CCD
HotwashFailFactor	0.0825	0.0707	0.0500	0.0583	0.0764
HotwashAverage	0.2245	0.5138	0.1309	0.1782	0.2425
MainReactorSmallFailFact	0.0303	0.0092	0.0250	0.0116	0.0825
MainReactorMin	0.0445	0.0510	0.1782	0.0561	0.0655
MainReactorBeta	0.0107	0.0087	0.0481	0.0152	0.0583
PostReactorMin	0.0082	0.0008	0.0231	0.0046	0.1414
HotWashParralel	0.0152	0.0749	0.0825	0.0177	0.0303

as 0, and levels 3 and 4 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.19. 5 center points were added to the design. The ANOVA table is provided in Table 7.17, Appendix 7.4. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.20. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.22). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.12. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.21. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. A 7 factor, 48 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This

Table 4.22: Response Surface Model Fitted to the Uniform Design Data.

HotWashParralel	0
Availability	=
97.62156	
-7.07219	* HotwashFailFactor
-0.72948	* HotwashAverage
-0.92976	* MainReactorSmallFailFact
1.253804	* MainReactorMin
1.048075	* MainReactorBeta
-0.60836	* PostReactorMin
0.63524	* HotwashFailFactor * MainReactorBeta
0.259017	* HotwashFailFactor * PostReactorMin
0.043557	* HotwashAverage * MainReactorMin
-0.22395	* MainReactorMin * MainReactorBeta
HotWashParralel	1
Availability	=
98.00026	
-6.03524	* HotwashFailFactor
-0.72948	* HotwashAverage
-0.92976	* MainReactorSmallFailFact
1.253804	* MainReactorMin
1.048075	* MainReactorBeta
-0.60836	* PostReactorMin
0.63524	* HotwashFailFactor * MainReactorBeta
0.259017	* HotwashFailFactor * PostReactorMin
0.043557	* HotwashAverage * MainReactorMin
-0.22395	* MainReactorMin * MainReactorBeta

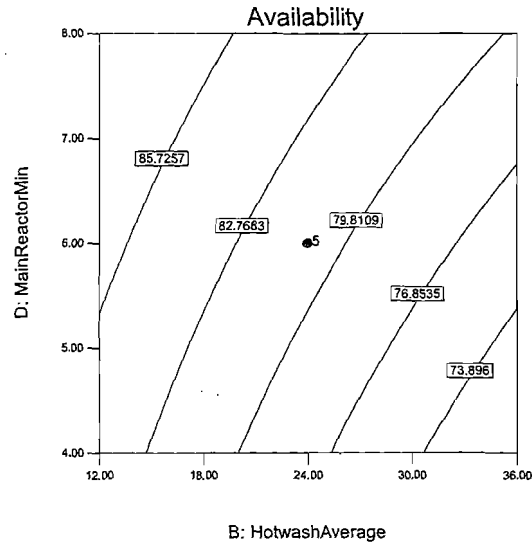


Figure 4.12: Contour Plot Of Hotwash Average Against the Minimum Uptime for the Main Reactor for The Uniform Design

creates a Latin hypercube design optimized for the maximin criteria. For the categorical factor “Hotwash Parallel or Series” the levels up to 0.5 were combined to create “Hotwash Series”, coded as 0, and values greater than 0.5 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.19. Five center points were added to the design. The ANOVA table is provided in Table 7.18, Appendix 7.4. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.23. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest (and only) interaction terms is between the hotwash fail factor, and the minimum uptime for the main reactor. The interaction term is positive (Table 4.23). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.13. The plant availability increases in the direction of decreasing hotwash fail factor and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.21. None

Table 4.23: Response Surface Model Fitted to the Uniform Design Data.

HotWashParralel	0
Availability	=
89.15884	
-6.22964	* HotwashFailFactor
-0.40435	* HotwashAverage
-1.02263	* MainReactorSmallFailFact
0.408042	* MainReactorMin
0.805838	* MainReactorBeta
0.246253	* PostReactorMin
0.645745	* HotwashFailFactor * MainReactorMin
HotWashParralel	1
Availability	=
91.54515	
-6.22964	* HotwashFailFactor
-0.40435	* HotwashAverage
-1.02263	* MainReactorSmallFailFact
0.408042	* MainReactorMin
0.805838	* MainReactorBeta
0.246253	* PostReactorMin
0.645745	* HotwashFailFactor * MainReactorMin

of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 34 run D-Optimal design for the main and interaction effects model for the factor ranges in Table 4.19 was created and analyzed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table is provided in Table 7.19, Appendix 7.4. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.24. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the

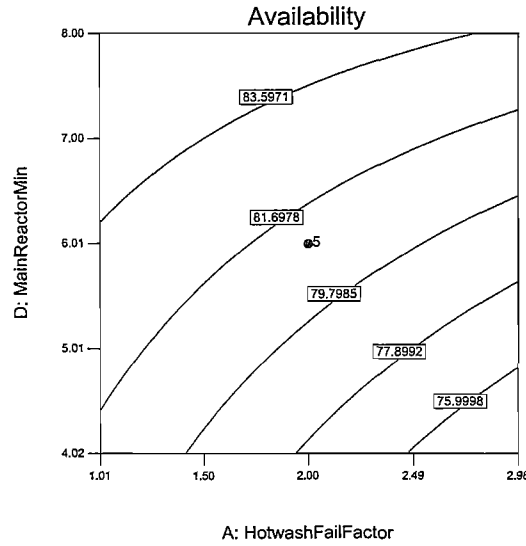


Figure 4.13: Contour Plot Of Hotwash Fail Factor Against the Minimum Uptime for the Main Reactor for The Latin Hypercube Design

sum of squares of the linear terms. The largest interaction term is between the hotwash fail factor and the hotwash parallel terms. The second largest interaction terms is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.24). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.14. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.21. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Central Composite Design

The Central Composite Designs were discussed in Section 2.2.4. For this experiment a minimum Resolution V face centered Central Composite Design

Table 4.24: Response Surface Model Fitted to the D-Optimal Design Data.

HotWashParralel	0
Availability	=
92.5279	
-4.70356	* HotwashFailFactor
-0.58339	* HotwashAverage
1.477392	* MainReactorSmallFailFact
0.26387	* MainReactorMin
0.913913	* MainReactorBeta
0.174606	* PostReactorMin
0.27405	* HotwashFailFactor * MainReactorMin
-0.03323	* HotwashAverage * MainReactorSmallFailFact
0.026647	* HotwashAverage * MainReactorMin
-0.19212	* MainReactorSmallFailFact * PostReactorMin
HotWashParralel	1
Availability	=
91.53657	
-3.12206	* HotwashFailFactor
-0.58339	* HotwashAverage
1.477392	* MainReactorSmallFailFact
0.26387	* MainReactorMin
0.913913	* MainReactorBeta
0.174606	* PostReactorMin
0.27405	* HotwashFailFactor * MainReactorMin
-0.03323	* HotwashAverage * MainReactorSmallFailFact
0.026647	* HotwashAverage * MainReactorMin
-0.19212	* MainReactorSmallFailFact * PostReactorMin

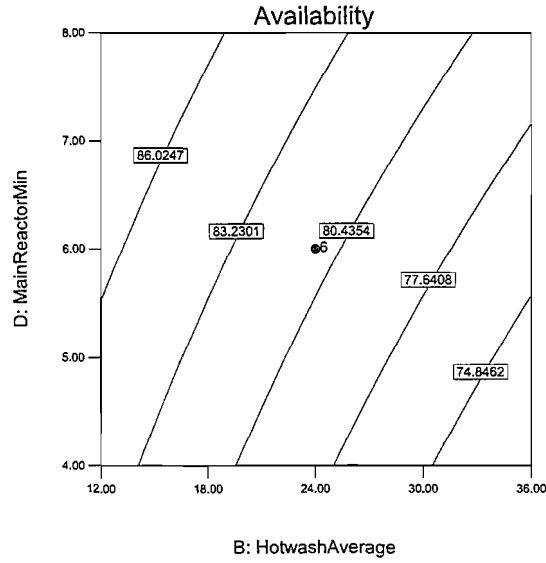


Figure 4.14: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The D-Optimal Design

were used. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 7 variables and ranges in Table 4.19. For 7 variables a 78 run design was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). The central composite design replicates a 39 run (including 5 center points) 6 factor design for both of the levels of the categorical factor “Hotwash Parallel or Series”. The ANOVA table is provided in Table 7.20, Appendix 7.4. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.25. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.25). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.15. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is

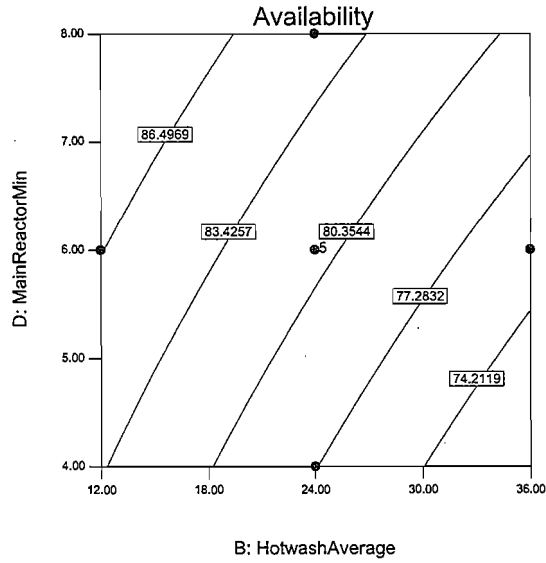


Figure 4.15: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Central Composite Design

evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.21. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Summary

The R-Squared values for all the designs discussed in this leg are summarized in Table 4.26. All the designs have high R-squared values illustrating that the respective models are acceptable. The p value for the models are also < 0.0001 for all the designs (see the ANOVA tables in Appendix 7.4) which indicates that the models are significant.

From the ANOVA tables in Appendix 7.4 it can be observed that the hotwash fail factor, average time to hotwash, minimum uptime for the main reactor, and parallel or series hotwash consistently are the factors with the highest sum of square values. It can also be observed that the linear terms generally have significantly larger sum of square values than the interaction terms.

Table 4.25: Response Surface Model Fitted to the Central Composite Design Data.

HotWashParralel	0
Availability	=
67.7362	
-3.25359	* HotwashFailFactor
-0.67777	* HotwashAverage
-0.9106	* MainReactorSmallFailFact
1.843254	* MainReactorMin
2.554312	* MainReactorBeta
3.314294	* PostReactorMin
0.036156	* HotwashFailFactor * HotwashAverage
-0.02018	* HotwashAverage * MainReactorSmallFailFact
0.026731	* HotwashAverage * MainReactorMin
-0.22315	* MainReactorMin * MainReactorBeta
-0.16005	* PostReactorMin ²
HotWashParralel	1
Availability	=
70.99318	
-2.41533	* HotwashFailFactor
-0.67777	* HotwashAverage
-0.9106	* MainReactorSmallFailFact
1.485222	* MainReactorMin
2.554312	* MainReactorBeta
3.314294	* PostReactorMin
0.036156	* HotwashFailFactor * HotwashAverage
-0.02018	* HotwashAverage * MainReactorSmallFailFact
0.026731	* HotwashAverage * MainReactorMin
-0.22315	* MainReactorMin * MainReactorBeta
-0.16005	* PostReactorMin ²

Table 4.26: R-Squared values for the designs discussed in for the Latin Hypercube Leg.

	R-Squared	Adj R-Squared	Pred R-Squared
Fractional Factorial	0.99	0.99	0.98
Uniform	0.98	0.98	0.97
Latin Hypercube	0.96	0.96	0.95
D-Optimal	0.98	0.98	0.97
Central Composite	0.99	0.99	0.99

From Table 4.21 it can be observed that the θ values are significantly larger for the average time to hotwash than for the other factors for all the designs, except for the maximin latin hypercube design. For the maximin latin hypercube the largest θ value is obtained for the minimum uptime for the main reactor.

Table 4.27: Variables and ranges used in the Second Phase for the D-Optimal Design Leg.

Name	Low	High
Hotwash Average	12	36
Scale Parameter (β) for Activation Reactor Uptime	2	4
Main Reactor Fail Factor	0	2
Minimum Uptime Main Reactor	4	8

4.3.4 D-Optimal Design

The factors in Table 4.27 were found to be significant from the in the D-Optimal Design in the Screening Phase (Section 4.2.5). The designs in this section are based on the factors and ranges in Table 4.27.

Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this experiment a full 2^4 design was used. The Design Expert Software (Stat-Ease, 2006) was used to set up a design in the 4 variables and ranges in Table 4.27. For 4 variables a 2^4 Factorial Design in 16 runs was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table is provided in Table 7.26, Appendix 7.6. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.28. From the ANOVA table it can be observed that the sum of squares of the interaction term are significantly smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.28). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.16. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

Table 4.28: Response Surface Model Fitted to the Fractional Factorial Design Data.

Availabilitiy	=
84.82648	
-0.66353	* HotwashAverage
0.723572	* ActivationReactorBeta
-1.0265	* MainReactorSmallFailFact
1.021977	* MainReactorMin
0.030193	* HotwashAverage * MainReactorMin

Table 4.29: θ Valuev for the Kriging Models for D-Optimal Design.

	Fractional Factorial	Uniform	Lhs	Dopt	CCD
HotwashAverage	0.3564	0.2245	0.0749	0.3564	0.1808
ActivationReactorBeta	0.0250	0.0118	0.0452	0.0250	0.0958
MainReactorSmallFailFact	0.0070	0.0125	0.0273	0.0070	0.0493
MainReactorMin	0.0500	0.3364	0.2709	0.0500	0.0805

The θ values for the fitted kriging model are provided in Table 4.29. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Uniform Design

The Uniform Designs were discussed in Section 2.3.2. A $U_{20}(4^4)$, 4 factor, 4 level, 20 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uniform Design Experiments. For the categorical factor “Hotwash Parallel or Series” the levels 1 and 2 were combined to create “Hotwash Series”, coded as 0, and levels 3 and 4 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.27. Five center points were added to the design. The ANOVA table is provided in Table 7.27, Appendix 7.6. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.30. No interaction terms are present in this model. The largest factors in terms of sum of squares are the average time to hotwash, and the minimum

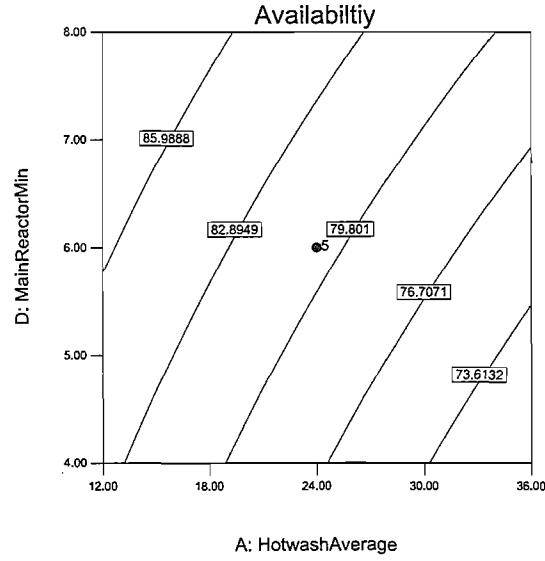


Figure 4.16: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Fractional Factorial Design

Table 4.30: Response Surface Model Fitted to the Uniform Design Data.

Availability	=
80.24153	
-0.47175	* HotwashAverage
0.597277	* ActivationReactorBeta
-1.30074	* MainReactorSmallFailFact
1.908769	* MainReactorMin

uptime for the main reactor. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor.

The θ values for the fitted kriging model are provided in Table 4.29. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Table 4.31: Response Surface Model Fitted to the Latin Hypercube Design Data.

Availabilitiy	=
81.85653	
-0.47407	* HotwashAverage
0.717627	* ActivationReactorBeta
-1.12213	* MainReactorSmallFailFact
1.59682	* MainReactorMin

Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. A 4 factor, 20 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This creates a Latin hypercube design optimized for the maximin criteria. The design was scaled to represent the ranges in Table 4.27. Five center points were added to the design. The ANOVA table is provided in Table 7.28, Appendix 7.6. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.31. No interaction terms are present in this model. The largest factors in terms of sum of squares are the average time to hotwash, and the minimum uptime for the main reactor. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor.

The θ values for the fitted kriging model are provided in Table 4.29. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 16 run D-Optimal design for the main and interaction effects model for the factor ranges in Table 4.27 was created and analyzed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table

Table 4.32: Response Surface Model Fitted to the D-Optimal Design Data.

Availabilitiy	=
84.91651	
-0.66353	* HotwashAverage
0.723572	* ActivationReactorBeta
-1.0265	* MainReactorSmallFailFact
1.021977	* MainReactorMin
0.030193	* HotwashAverage * MainReactorMin

is provided in Table 7.29, Appendix 7.6. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.32. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.32). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.17. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.29. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Central Composite Design

The Central Composite Designs were discussed in Section 2.2.4. For this experiment a small face centered Central Composite Design was used. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 4 variables and ranges in Table 4.27. For 4 variables a 21 run design was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table

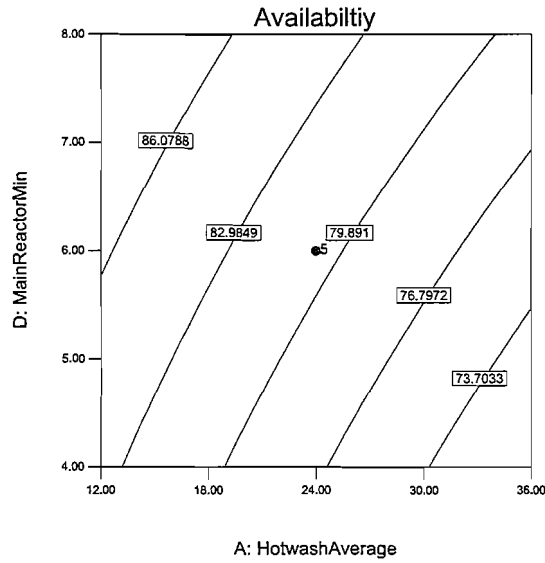


Figure 4.17: Contour Plot Of Hotwash Average Against the Minimum Uptime for the Main Reactor for The D-Optimal Design

is provided in Table 7.30, Appendix 7.6. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.33. No interaction terms are present in this model. The largest factors in terms of sum of squares are the average time to hotwash, and the minimum uptime for the main reactor. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor.

The θ values for the fitted kriging model are provided in Table 4.29. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Summary

The R-Squared values for all the designs discussed in this leg are summarized in Table 4.34. All the designs have high R-squared values illustrating that the respective models are acceptable. The p value for the models are also < 0.0001 for all the designs (see the ANOVA tables in Appendix 7.6) which indicates that the models are significant.

Table 4.33: Response Surface Model Fitted to the Central Composite Design Data.

Availabilitiy	=
81.856526	
-0.474072	* HotwashAverage
0.7176267	* ActivationReactorBeta
-1.1221254	* MainReactorSmallFailFact
1.5968198	* MainReactorMin

Table 4.34: R-Squared values for the designs discussed in for the D-Optimal Leg.

	R-Squared	Adj R-Squared	Pred R-Squared
Fractional Factorial	0.99	0.98	0.98
Uniform	0.97	0.97	0.96
Latin Hypercube	0.96	0.96	0.95
D-Optimal	0.99	0.98	0.98
Central Composite	0.97	0.97	0.96

From the ANOVA tables in Appendix 7.6 it can be observed that the average time to hotwash, and minimum uptime for the main reactor consistently are the factors with the highest sum of square values. It can also be observed that the linear terms generally have significantly larger sum of square values than the interaction terms.

From Table 4.29 it can be observed that the θ values are significantly larger for the average time to hotwash than for the other factors for all the designs, except for the uniform design. For the uniform design the largest θ value is obtained for the minimum uptime for the main reactor.

Table 4.35: Variables and ranges used in the Second Phase for the Plackett-Burman Design Leg.

Name	Low	High
Hotwash Fail Factor	1	3
Hydroblasting Days	4	6
Hotwash Average	12	36
Main Reactor Fail Factor	0	2
Minimum Uptime Main Reactor	4	8
Scale Parameter (β) for Main Reactor Uptime	2	4
Hotwash Parallel or Series	0	1

4.3.5 Plackett-Burman

The factors in Table 4.35 were found to be significant from the Plackett-Burman design in the Screening Phase (Section 4.2.2). The designs in this section are based on the factors and ranges in Table 4.35.

Fractional Factorial Design

The Fractional Factorial Designs were discussed in Section 2.2.2. For this experiment a resolution VII design was used, because no Resolution V Fractional Factorial Design are available for 7 factors. Using a resolution VII design the main effects and second order interactions can still be evaluated. The Design Expert Software (Stat-Ease, 2006) was used to set up a design in the 7 variables and ranges in Table 4.35. For 7 variables a 2^{7-1} Fractional Factorial Design in 64 runs (Resolution VII) was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The center point was repeated for both of the levels of the categorical factor “Hotwash Parallel or Series”. The ANOVA table is provided in Table 7.21, Appendix 7.5. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.36. Note that because HotWashParralel is a categorical variable, two equations are obtained. One for Series Hotwash (Coded as 0), and one for Parallel Hotwash (Coded as 1). From the ANOVA table it can be observed that the sum of squares of the interaction term are significantly

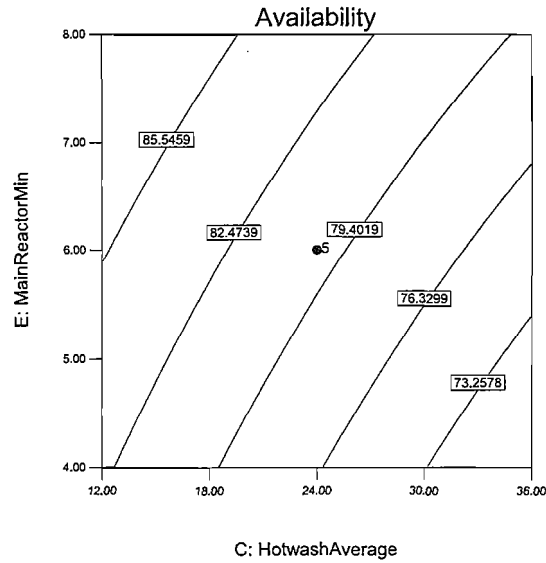


Figure 4.18: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Fractional Factorial Design

smaller than the sum of squares of the linear terms. The largest interaction terms is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.36). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.18. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.37. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Uniform Design

The Uniform Designs were discussed in Section 2.3.2. A $U_{48}(4^7)$, 7 factor, 4 level, 48 run uniform design was downloaded from the website <http://www.math.hkbu.edu.hk/UniformDesign/index.html> for the Uni-

Table 4.36: Response Surface Model Fitted to the Fractional Factorial Design Data.

HotWashParralel	0
Availability	=
89.08986	
-0.83866	* HotwashFailFactor
-0.85466	* HydroblastingDays
-0.72114	* HotwashAverage
-1.20139	* MainReactorSmallFailFact
1.849825	* MainReactorMin
2.608921	* MainReactorBeta
-0.49076	* HotwashFailFactor * HydroblastingDays
0.035224	* HotwashFailFactor * HotwashAverage
0.030927	* HotwashAverage * MainReactorMin
-0.25827	* MainReactorMin * MainReactorBeta
HotWashParralel	1
Availability	=
87.22467	
0.085295	* HotwashFailFactor
0.233336	* HydroblastingDays
-0.72114	* HotwashAverage
-1.20139	* MainReactorSmallFailFact
1.478649	* MainReactorMin
2.608921	* MainReactorBeta
-0.49076	* HotwashFailFactor * HydroblastingDays
0.035224	* HotwashFailFactor * HotwashAverage
0.030927	* HotwashAverage * MainReactorMin
-0.25827	* MainReactorMin * MainReactorBeta

Table 4.37: θ Values for the Kriging Models for Plackett-Burman Design.

	Fractional Factorial	Uniform	Lhs	Dopt	CCD
HotwashFailFactor	0.0583	0.0962	0.1587	0.0184	0.1470
HydroblastingDays	0.0429	0.0794	0.0882	0.0085	0.0583
HotwashAverage	0.1260	0.3849	0.2775	0.0463	0.2722
MainReactorSmallFailFact	0.0092	0.0116	0.2311	0.0054	0.0735
MainReactorMin	0.0630	0.1039	0.0386	0.5040	0.0520
MainReactorBeta	0.0146	0.0764	0.0642	0.0170	0.0707
HotWashParralel	0.0583	0.3429	0.1133	0.0184	0.0540

form Design Experiments. The design was scaled to represent the ranges in Table 4.35. For the categorical factor “Hotwash Parallel or Series” the levels 1 and 2 were combined to create “Hotwash Series”, coded as 0, and levels 3 and 4 were combined to create “Hotwash Parallel” coded as 1. Five center points were added to the design. The ANOVA table is provided in Table 7.22, Appendix 7.5. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.38. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.38). The contour plot of average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.19. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.37. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Table 4.38: Response Surface Model Fitted to the Uniform Design Data.

HotWashParralel	0
Availability	=
75.79199	
5.193429	* HotwashFailFactor
1.901617	* HydroblastingDays
-0.57305	* HotwashAverage
-0.76026	* MainReactorSmallFailFact
-1.01976	* MainReactorMin
4.761282	* MainReactorBeta
-1.39503	* HotwashFailFactor * HydroblastingDays
0.097711	* HotwashAverage * MainReactorMin
-0.12559	* HotwashAverage * MainReactorBeta
HotWashParralel	1
Availability	=
84.50658	
5.193429	* HotwashFailFactor
1.901617	* HydroblastingDays
-0.57305	* HotwashAverage
-0.76026	* MainReactorSmallFailFact
-1.01976	* MainReactorMin
2.93782	* MainReactorBeta
-1.39503	* HotwashFailFactor * HydroblastingDays
0.097711	* HotwashAverage * MainReactorMin
-0.12559	* HotwashAverage * MainReactorBeta

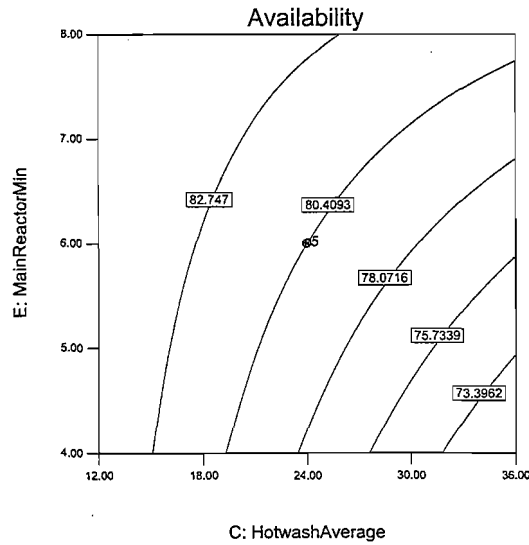


Figure 4.19: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Uniform Design

Latin Hypercube Design

The Latin Hypercube Designs were discussed in Section 2.3.1. A 7 factor 48 run Latin hypercube was created in R (R Development Core Team, 2008) using the function `maximinLHS` in the `lhs` package (Carnell, 2006). This creates a Latin hypercube design optimized for the maximin criteria. For the categorical factor “Hotwash Parallel or Series” the levels up to 0.5 were combined to create “Hotwash Series”, coded as 0, and values greater than 0.5 were combined to create “Hotwash Parallel” coded as 1. The design was scaled to represent the ranges in Table 4.35. Five center points were added to the design. The ANOVA table is provided in Table 7.23, Appendix 7.5. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors is provided in Table 4.39. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the hydroblasting days and the hotwash parallel terms.

The θ values for the fitted kriging model are provided in Table 4.37. None

Table 4.39: Response Surface Model Fitted to the Latin Hypercube Design Data.

HotWashParralel	0
Availability	=
100.8434	
-2.50878	* HotwashFailFactor
-2.22546	* HydroblastingDays
-0.45455	* HotwashAverage
1.22038	* MainReactorMin
HotWashParralel	1
Availability	=
89.81669	
-2.50878	* HotwashFailFactor
0.352479	* HydroblastingDays
-0.45455	* HotwashAverage
1.22038	* MainReactorMin

of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

D-Optimal Design

The D-Optimal Designs were discussed in Section 2.2.5. A 34 run D-Optimal design for the main and interaction effects model for the factor ranges in Table 4.35 was created and analyzed using the Design Expert Software (Stat-Ease, 2006). Five center points were added to the design. The ANOVA table is provided in Table 7.24, Appendix 7.5. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.40. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.40). The contour plot of

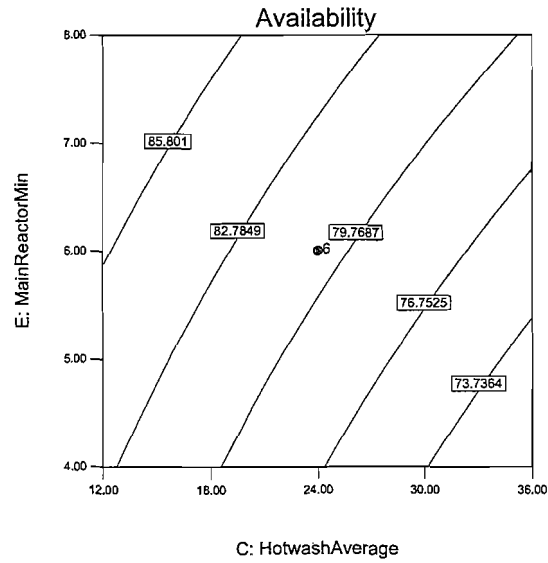


Figure 4.20: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The D-Optimal Design

average time to hotwash against minimum uptime for the main reactor are provided in Figure 4.20. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.37. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Central Composite Design

The Central Composite Designs were discussed in Section 2.2.4. For this experiment a minimum Resolution V face centered Central Composite Design were used. The Design Expert Software (Stat-Ease, 2006) were used to set up a design in the 7 variables and ranges in Table 4.35. For 7 variables a 78 run design was constructed and analysed using the Design Expert Software (Stat-Ease, 2006). The central composite design replicates a 39 run (including 5 center points) 6 factor design for both of the levels of the categorical

Table 4.40: Response Surface Model Fitted to the D-Optimal Design Data.

HotWashParralel	0
Availability	=
96.74765	
-4.4761	* HotwashFailFactor
-1.68826	* HydroblastingDays
-0.72359	* HotwashAverage
-1.22787	* MainReactorSmallFailFact
1.146591	* MainReactorMin
2.395587	* MainReactorBeta
0.03765	* HotwashFailFactor * HotwashAverage
0.264416	* HotwashFailFactor * MainReactorMin
0.032332	* HotwashAverage * MainReactorMin
-0.21765	* MainReactorMin * MainReactorBeta
HotWashParralel	1
Availability	=
97.35636	
-4.4761	* HotwashFailFactor
-0.64822	* HydroblastingDays
-0.72359	* HotwashAverage
-1.22787	* MainReactorSmallFailFact
0.635248	* MainReactorMin
2.395587	* MainReactorBeta
0.03765	* HotwashFailFactor * HotwashAverage
0.264416	* HotwashFailFactor * MainReactorMin
0.032332	* HotwashAverage * MainReactorMin
-0.21765	* MainReactorMin * MainReactorBeta

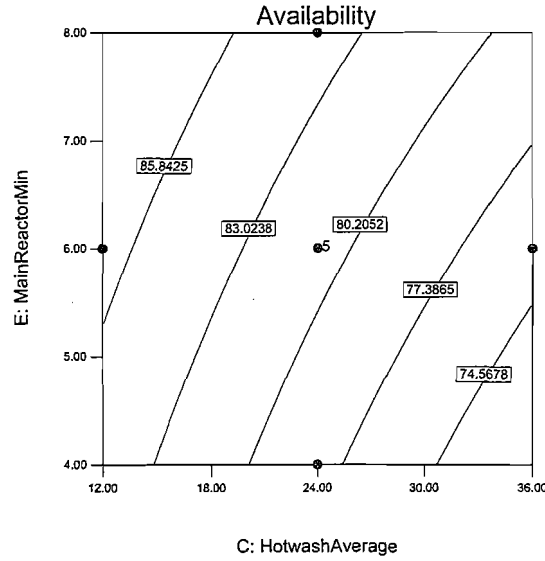


Figure 4.21: Contour Plot Of Hotwash Average Against the Minimum Up-time for the Main Reactor for The Central Composite Design

factor “Hotwash Parallel or Series”. The ANOVA table is provided in Table 7.25, Appendix 7.5. The ANOVA table depicts the significant factors only. The final equation in terms of the actual factors are provided in Table 4.41. From the ANOVA table it can be observed that the sum of squares of the interaction terms are significantly smaller than the sum of squares of the linear terms. The largest interaction term is between the average time to hotwash, and the minimum uptime for the main reactor. These two terms also have the largest individual sum of squares values. The interaction term is positive (Table 4.41). The contour plot of average time to hotwash against minimum uptime for the main reactor is provided in Figure 4.21. The plant availability increases in the direction of decreasing average time to hotwash and increasing minimum uptime for the main reactor. Some interaction is evident, but it is small compared to the effect of the two individual factors.

The θ values for the fitted kriging model are provided in Table 4.37. None of the θ values are at the starting value of 0.1, i.e. optimized values were obtained.

Table 4.41: Response Surface Model Fitted to the Fractional Factorial Design Data.

HotWashParralel	0
Availability	=
87.82554	
-0.08308	* HotwashFailFactor
-0.34735	* HydroblastingDays
-0.81331	* HotwashAverage
0.589992	* MainReactorSmallFailFact
1.110545	* MainReactorMin
4.320281	* MainReactorBeta
-0.60735	* HotwashFailFactor * HydroblastingDays
0.034207	* HotwashFailFactor * HotwashAverage
-0.03052	* HotwashAverage * MainReactorSmallFailFact
0.035951	* HotwashAverage * MainReactorMin
0.033248	* HotwashAverage * MainReactorBeta
-0.33594	* MainReactorSmallFailFact * MainReactorBeta
-0.16839	* MainReactorMin * MainReactorBeta
-0.43525	* MainReactorBeta ²
HotWashParralel	1
Availability	=
83.4447	
0.817523	* HotwashFailFactor
0.705681	* HydroblastingDays
-0.81331	* HotwashAverage
0.589992	* MainReactorSmallFailFact
1.110545	* MainReactorMin
4.320281	* MainReactorBeta
-0.60735	* HotwashFailFactor * HydroblastingDays
0.034207	* HotwashFailFactor * HotwashAverage
-0.03052	* HotwashAverage * MainReactorSmallFailFact
0.035951	* HotwashAverage * MainReactorMin
0.033248	* HotwashAverage * MainReactorBeta
-0.33594	* MainReactorSmallFailFact * MainReactorBeta
-0.16839	* MainReactorMin * MainReactorBeta
-0.43525	* MainReactorBeta ²

Table 4.42: R-Squared values for the designs discussed in for the Plackett-Burman Leg.

	R-Squared	Adj R-Squared	Pred R-Squared
Fractional Factorial	0.98	0.98	0.97
Uniform	0.83	0.79	0.69
Latin Hypercube	0.86	0.84	0.81
D-Optimal	0.98	0.98	0.96
Central Composite	0.98	0.98	0.96

Summary

The R-Squared values for all the designs discussed in this leg are summarized in Table 4.26. All the designs have high R-squared values illustrating that the respective models are acceptable. The p value for the models are also < 0.0001 for all the designs (see the ANOVA tables in Appendix 7.5) which indicates that the models are significant.

From the ANOVA tables in Appendix 7.5 it can be observed that the average time to hotwash, and minimum uptime for the main reactor consistently are the factors with the highest sum of square values. It can also be observed that the linear terms generally have significantly larger sum of square values than the interaction terms.

From Table 4.37 it can be observed that the θ values are significantly larger for the average time to hotwash than for the other factors for all the designs, except for the d-optimal design. For the d-optimal design the largest θ is obtained for the minimum uptime for the main reactor.

Chapter 5

Results and Practical Application

5.1 Results

Two approximation models for the input-output relationship are compared, namely:

- Response Surface (Section 3.2).
- Kriging (Section 3.3).

For each of the designs in section 4.3 a Response Surface Model and Kriging model were fitted to the data. The Response Surface Model was fitted using Design Expert (Stat-Ease, 2006). The Kriging model was fitted using the DACE toolbox (Lophaven et al., 2002) in Matlab (Mathworks, 2007). A 20 run random Latin Hypercube design was created using the randomLHS function in the lhs (Carnell, 2006) package in R (R Development Core Team, 2008) for the validation grid in all 14 factors and ranges in Table 4.1. The Arena model was used to predict the plant availabilities for the validation grid. A validation grid is used to assess the accuracy of the models in predicting the plant availability at the new factor level combinations.

The philosophy behind generating the validation set over all 14 factors is to test if the factors that were screened out as “not significant” really

do not have an effect on the response. Therefore it is a validation of the effectiveness of the screening designs in determining the factors that do not have a significant effect on the response of interest. If the factors really do not have a significant effect on the response, the predictions of the approximation models should be accurate, regardless of the values of these factors.

For each approximation model in Figure 1.2 in Phase 3 the plant availabilities were predicted for the validation grid. The Mean Square Error (1.8) and Maximum Absolute Error (1.7) values for the predictions were calculated. The Arena model predictions were used as the “actual” values for these calculations.

The calculated mean square errors are summarized in Tables 5.1 and 5.2 for the response surface and kriging models respectively, and the calculated maximum absolute errors are summarized in Tables 5.3 and 5.4 for the response surface and kriging models respectively. The column names are the screening designs used to determine the significant factors, and the different rows are the second phase designs used to fit the response surface and kriging models. In interpreting these results care must be taken to keep in mind that the output from a simulation model is not deterministic. The results of each run is therefore a “sample” of the population. This is very similar to physical experiments. Therefore, the exact criteria values are not as important as the general trends between the different design and approximation model combinations. A small difference between two criteria values could be due to random variation.

The results in Tables 5.1 to 5.4 are also graphically depicted in Figures 5.1 to 5.4. The y axis depicts the criterion values, and the x axis depicts the Interaction Designs. The abbreviations used for the design names are summarized in Table 5.5. Each line in the graphs correspond to a different screening design.

5.2 Discussion

From Tables 5.1 to 5.4 and Figures 5.1 to 5.4 it can be observed that the lowest criterion values for both the Response Surface Models and the Kriging

Table 5.1: Mean Square Error Values for the Response Surface Model Predictions against the Arena model values.

Interaction Designs	Screening Designs				
	Fractional Factorial	Uniform Design	Latin Hypercube Design	Plackett-Burman	D-optimal
Fractional Factorial	2.50	1.43	1.07	0.85	2.67
Uniform Design	2.32	1.41	1.25	1.70	2.42
Latin Hypercube Design	2.37	1.42	1.42	1.56	2.35
D-optimal	2.53	1.47	1.05	0.86	2.62
Central Composite Design	2.28	1.35	1.08	1.05	2.53

Table 5.2: Mean Square Error Values for the Kriging Model Predictions against the Arena model values.

Interaction Designs	Screening Designs				
	Fractional Factorial	Uniform Design	Latin Hypercube Design	Plackett-Burman	D-optimal
Fractional Factorial	2.03	1.75	1.35	1.38	2.52
Uniform Design	2.02	1.81	1.24	2.39	2.43
Latin Hypercube Design	2.34	2.13	1.38	2.38	2.59
D-optimal	1.97	1.65	1.33	1.32	2.52
Central Composite Design	2.89	1.57	1.20	1.33	2.69

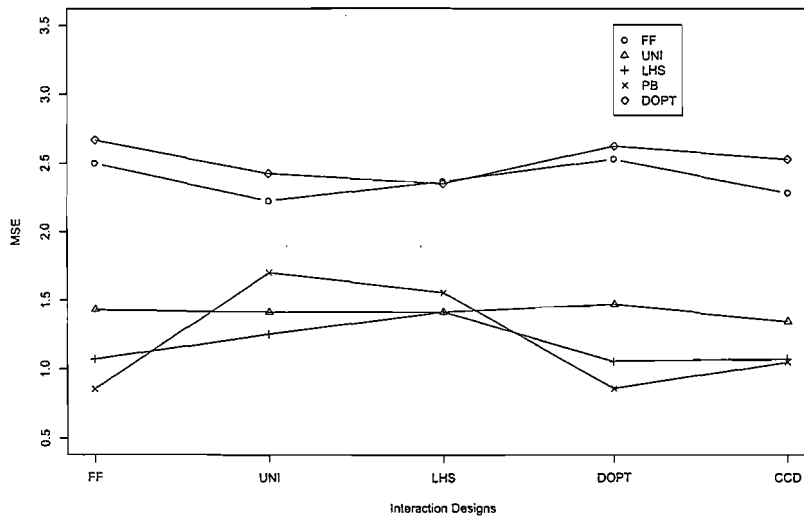


Figure 5.1: Plot of Mean Square Error Values for the Response Surface Model Predictions against the Arena model values.

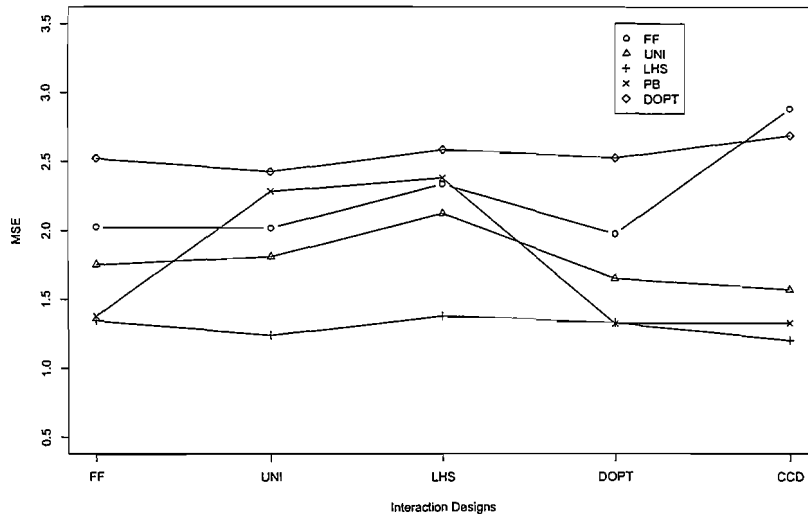


Figure 5.2: Plot of Mean Square Error Values for the Kriging Model Predictions against the Arena model values.

Table 5.3: Maximum Absolute Error Values for the Response Surface Model Predictions against the Arena model values.

Interaction Designs	Screening Designs				
	Fractional Factorial	Uniform Design	Latin Hypercube Design	Plackett-Burman	D-optimal
Fractional Factorial	4.79	3.13	2.08	1.60	5.65
Uniform Design	4.34	2.45	2.44	3.63	5.06
Latin Hypercube Design	4.17	2.88	2.99	2.99	4.63
D-optimal	4.98	3.43	1.89	1.68	5.56
Central Composite Design	4.61	2.83	2.21	2.36	4.86

Table 5.4: Maximum Absolute Error Values for the Kriging Model Predictions against the Arena model values.

Interaction Designs	Screening Designs				
	Fractional Factorial	Uniform Design	Latin Hypercube Design	Plackett-Burman	D-optimal
Fractional Factorial	4.00	3.82	2.80	2.55	6.24
Uniform Design	3.81	4.20	2.57	4.94	5.24
Latin Hypercube Design	4.10	5.84	2.41	5.45	5.62
D-optimal	3.35	3.85	2.84	2.51	6.24
Central Composite Design	6.08	3.88	3.14	2.58	5.85

Table 5.5: Design Abbreviations Used in Graph Legends.

Design Name	Design Abbreviation
Fractional Factorial Design	FF
Uniform Designs	UNI
Latin Hypercube Design	LHS
D-Optimal Design	DOP
Central Composite Design	CCD
Plackett-Burman Design	PB

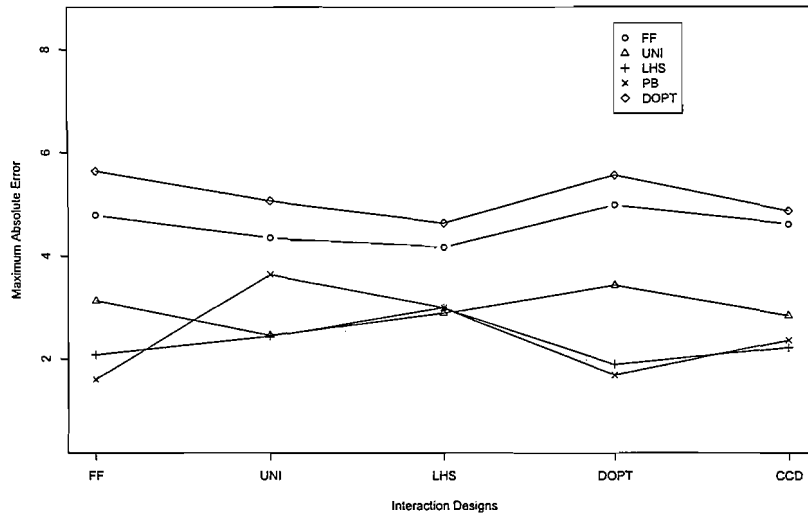


Figure 5.3: Plot of Maximum Absolute Error Values for the Response Surface Model Predictions against the Arena model values.

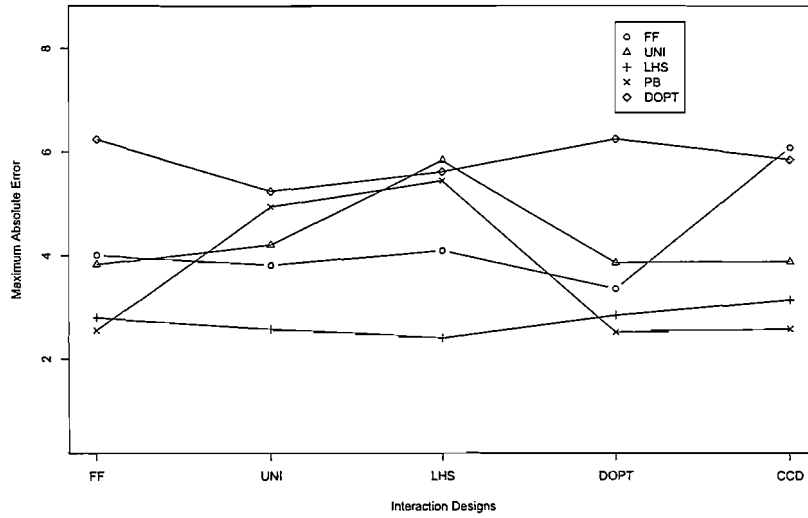


Figure 5.4: Plot of Maximum Absolute Error Values for the Kriging Model Predictions against the Arena model values.

models originate from the Plackett-Burman and Maximin Latin Hypercube screening designs. From these results it can be observed that the Plackett-Burman and Maximin Latin Hypercube designs are the most effective screening designs for this case study. Comparing the ANOVA tables in Table 7.2 (Plackett-Burman) and Table 7.4 (Maximin Latin Hypercube Design) in Appendix 7.1 the results for the two designs are very similar. The only difference between the significant factors indicated by these two screening designs are that the Plackett-Burman Design includes the hydroblasting days whereas the Maximin Latin Hypercube Design includes the minimum uptime for the post reactor.

Using effective and efficient screening designs are of great practical importance. In an industrial experimental design study, the screening results are the building blocks for the following experimental phases. If the incorrect factors are used in the following phases, it can lead to misleading and suboptimal findings.

From Tables 5.1 to 5.4 and Figures 5.1 to 5.4 it can be observed that the lowest criterion values for the Response Surface Models originate from

the Fractional Factorial and D-Optimal second phase designs for both the Plackett-Burman and Maximin Latin Hypercube screening legs. The Central Composite design also yields comparable results. For the Kriging Models it can be observed that the lowest criterion values are obtained from the Fractional Factorial and D-Optimal second phase designs for the Plackett-Burman screening legs, and all the second phase designs yields comparable results for the Maximin Latin Hypercube Design leg. Therefore it can be observed that the space filling designs (Uniform Design and Maximin Latin Hypercube Design) are more effective for fitting Kriging Models than for fitting Response Surface Models. This could be explained by the inherent differences between these two approximation models.

Kriging models and linear regression models share a common mathematical framework consisting of regressors and errors, but the emphasis is quite different. Linear regression focuses entirely on the regressors and their coefficient estimates, and makes simplistic assumptions about the errors (independence). In contrast, kriging makes simplistic assumptions about the regressors (just a constant term) and focuses entirely on the correlation structure of the errors. Thus, regression and kriging are probably best thought of as diametric opposites. Regression is about estimating regression coefficients that (together with the assumed functional form) completely describe what the function is. Kriging is about estimating correlation parameters that describe how the function typically behaves. As we have seen, kriging makes predictions by interpolating and extrapolating from the data in a way most consistent with the estimated typical behavior (Donald R. Jones, 1998).

Space filling designs would therefore be beneficial to the kriging models as they use interpolation to predict new values. Minimum distance between the design points would therefore ensure that any new value is as close as possible to a design point to minimize the distance that must be interpolated.

Overall the difference between using the Response Surface Models (Section 3.2) and the Kriging Models (Section 3.3) are not as pronounced. It would however seem that the Response Surface Models give slightly better results. This could possibly be due to the random nature of stochastic simulation models (Section 1.2.1). Each design point of the simulation model

is a sample from all possible replications. There is therefore uncertainty around the actual value of the response at the specific design point. As discussed above Kriging Models are interpolation models and are built on the assumption that the values of the design points are deterministic, i.e. two replications of the design point should yield the same response value.

- The overall best leg of the tree in Figure 1.2 is the Plackett-Burman Design for Phase 1, the Fractional Factorial Design for Phase 2, and the Response Surface Model for Phase 3, both in terms of the mean square error (1.8), and the maximum absolute error (1.7) criteria. This result might be specific to the case study. However, it is provided as a general recommendation for the design and analysis of simulation experiments in industry.

A plot of the predicted value from this approximation model versus the actual value from the Arena model is provided in Figure 5.5. The residual values (Actual - Predicted) are plotted in Figure 5.6. From these plots it can be observed that the response surface model is a good approximation of the arena model. This approximation model will be used to explore the design space for the case study.

5.3 Practical Application

5.3.1 Overall Plant Availability

Typical question in a study like the one presented here, centers around the risk of decisions. The engineers need to compare the risk of different scenarios. Risk is extremely difficult to quantify if you do not understand the design space well. In the current case study there are 14 factors involved, therefore, really understanding the design space and impacts are almost impossible without doing a simulation study combined with an experimental design strategy. Some of the results obtained from this approximation model will now be discussed.

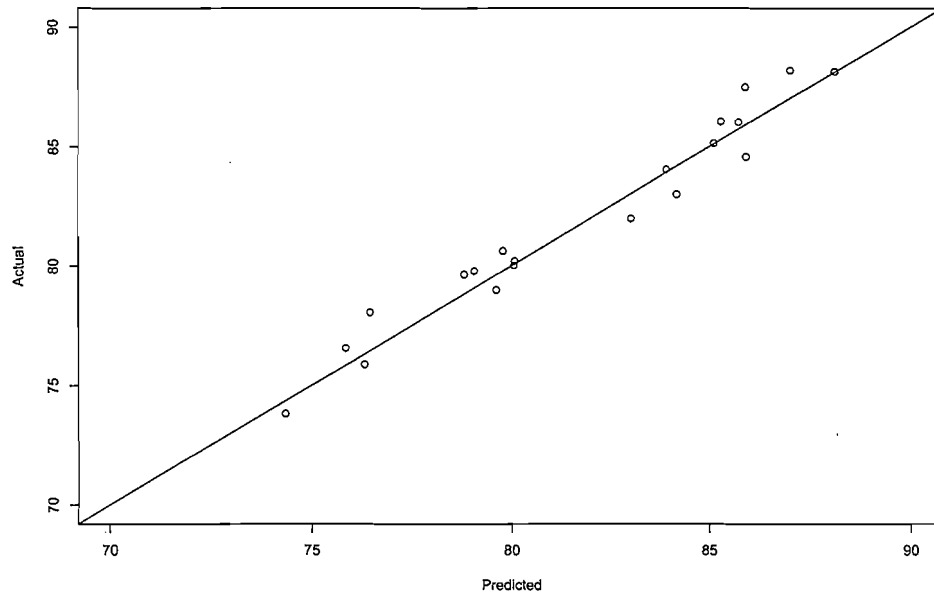


Figure 5.5: Plot of actual versus predicted values.

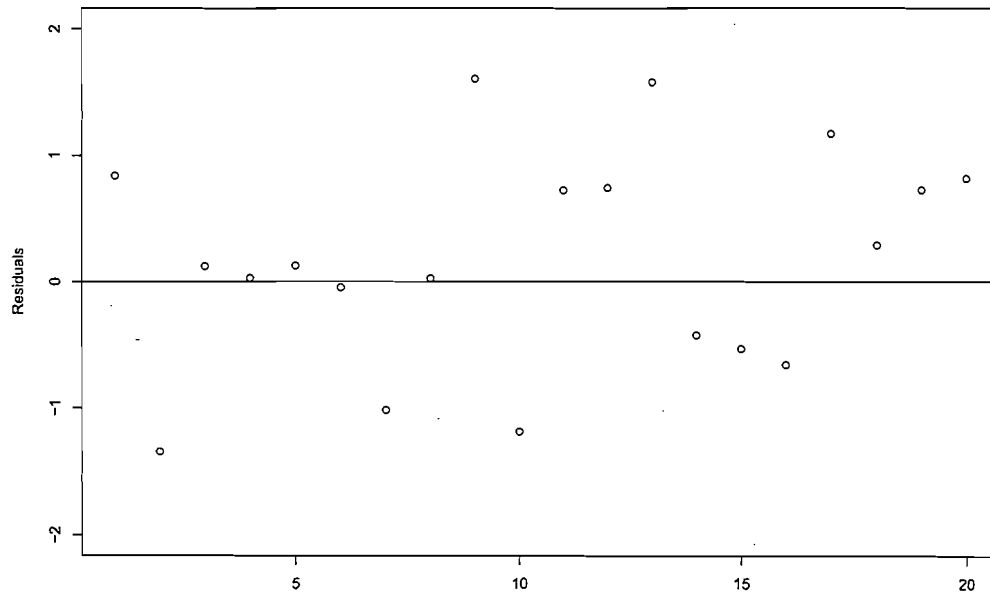


Figure 5.6: Residual plot.

As a first step, inspecting the ANOVA table (7.21) in Appendix 7.5 for the Fractional Factorial Design built on the significant factors observed from the Plackett-Burman design it can be observed that the sum of squares value for the average time to hotwash is much bigger than the sum of squares for the other factors. Therefore this factor has the largest effect on the plant availability. The minimum uptime for the main reactor has the second largest sum of squares value. The interaction between these two factors has the largest sum of squares value of all the interaction terms. From Figure 4.18 it is clear that the plant availability increases in the direction of an increase in minimum uptime for the main reactor, and decreasing average time to hotwash.

The design availability for the industrial plant has an impact on the sizing of the plant. A plant is designed for a certain throughput. The plant must be oversized to compensate for the downtime. This has a huge impact on cost. There is a trade-off between the risk that is involved and the cost. It is therefore very important to know the risk in designing for a certain availability, and to know which factors have the largest impact on the plant availability.

One way to quantify the risk involved in designing for an availability is to calculate the area of the design space where the availability is at least as large as the design availability over the total design space. This is indicated as a percentage of the design space. In a system as complex as this it is not possible to analytically calculate this area, but it can be approximated by random sampling techniques. Uniform random data can be generated for all the variables in their ranges, and the availabilities predicted with the model. The number of values above a certain availability divided by the total number of simulations is an approximation of the percentage of design area that have at least the chosen availability. This value is obviously dependent on the ranges of the factors used. The larger the number of simulations performed, the better the approximation will be. Using the Arena Simulation model the runtime will soon be prohibitively large. However, using the approximation model, this technique is practical and easy to apply.

For this study 1000000 uniform random values were generated for each

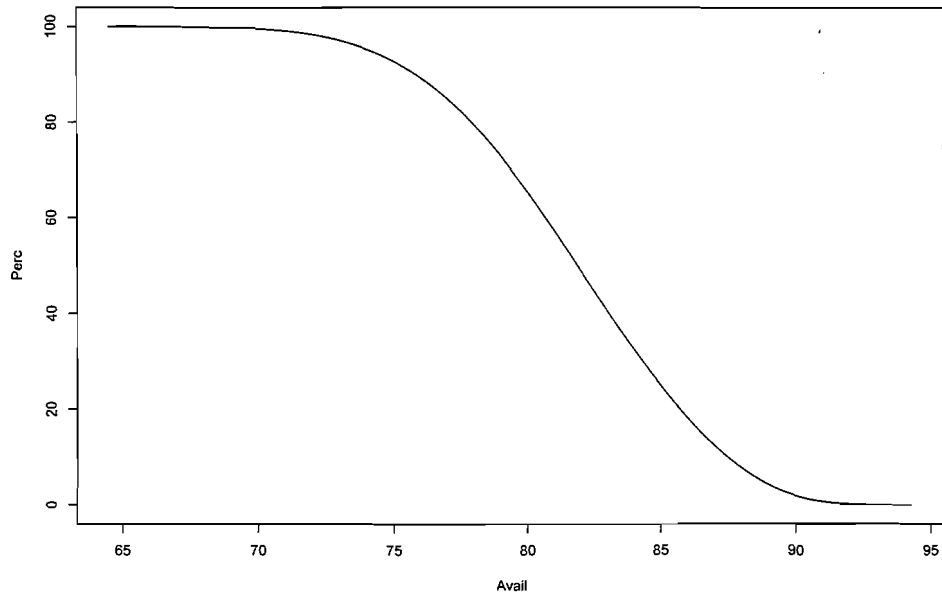


Figure 5.7: Plot of percentage design space above percent availability values.

factor using the `runif` function in R (R Development Core Team, 2008). The upper and lower ranges of the factors in Table 4.35 were used for generating random samples. For the “Hotwash Parallel or Series” factor the values below 0.5 were combined to create “Hotwash Series”, coded as 0, and values greater than 0.5 were combined to create “Hotwash Parallel” coded as 1. The model in Table 4.36 was coded in R and used to predict the plant availability for each of the factor combinations.

The plot in Figure 5.7 was generated by finding all the data points with an availability above the specified availability on the x axis, and calculating the percentage of values that satisfies this criterion divided by the total number of points (1000000). This gives an approximation of the percentage of the space that is covered by the data greater than the specified availability. This plot can be used to make an informed decision regarding the risk involved in designing the plant for a given availability.

The median of the variables which satisfies the criterion is summarized in Table 5.6 . For instance at an Availability Target = 92.5% the median of the factor values for the generated data which has availability greater

Table 5.6: Median Values of Factors for Different Availability Targets.

Availability Target	Hotwash Fail Factor	Hydroblasting Days	Hotwash Average	Main Reactor Fail Factor	Min Uptime Main Reactor	Main Reactor Beta	HotWash Parralel	Percentage Of Total Design Space
92.50	1.19	4.62	12.71	0.27	7.71	3.61	3.00	0.07
90.00	1.38	4.70	13.56	0.54	7.38	3.33	3.00	1.91
87.50	1.58	4.78	14.76	0.72	7.04	3.21	3.00	9.94
85.00	1.72	4.84	16.34	0.83	6.76	3.14	3.00	25.07
82.50	1.82	4.88	18.27	0.89	6.58	3.09	3.00	44.74
80.00	1.89	4.92	20.33	0.93	6.43	3.06	3.00	65.45
77.50	1.93	4.95	22.05	0.96	6.26	3.04	3.00	82.26
75.00	1.97	4.97	23.18	0.98	6.12	3.02	3.00	92.83
72.50	1.99	4.99	23.75	0.99	6.04	3.01	3.00	97.83
70.00	2.00	5.00	23.96	1.00	6.01	3.00	3.00	99.59
67.50	2.00	5.00	24.00	1.00	6.00	3.00	1.00	99.97
65.00	2.00	5.00	24.01	1.00	6.00	3.00	1.00	100.00
62.50	2.00	5.00	24.01	1.00	6.00	3.00	1.00	100.00

than 92.5% are depicted. The Percentage of Total Design Space column gives an approximation of the percentage of the space that is covered by the data greater than the availability target. This information can be used to approximate the sensitivity of the availability at the target value to the factors. The more constrained the region gets, the closer to their boundary values some of the factors become. This is an indication that the availabilities are more sensitive to these factors.

The histograms in Figure 5.8 are those of the factors which satisfies an availability greater than 90%. The histograms make it easy to visualize which factors are forced very close to one of their boundary values. For instance, the average time to hotwash has no values above the center point of 24, and is skewed to the lower boundary (12). The minimum uptime for the main reactor data is skewed to the upper limit (8). This confirms the findings from the ANOVA table.

These results were used to make practical decisions on additional laboratory experiments and plant sizing. The techniques discussed here makes it possible to really explore the design space, understand the system under investigation and optimization. Making decisions without this level of understanding has a real monetary risk. The “safe” practice would be to over-design the plant to make sure the production volumes can be reached. Quantifying the risk, and understanding on which factors to focus to decrease this risk saves money and time.

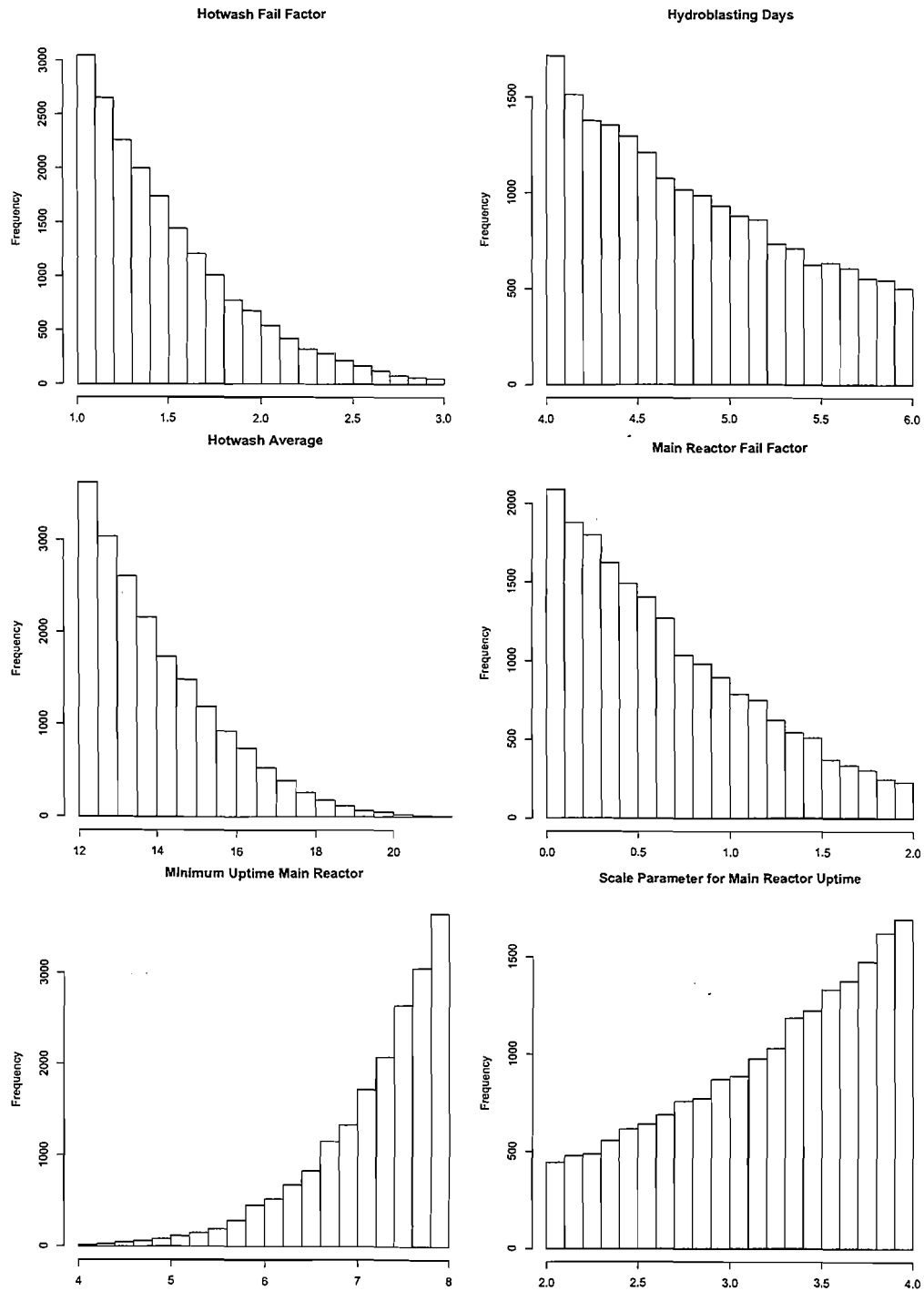


Figure 5.8: Histograms of factor values when plant availability is constrained to be larger than 90%.

5.3.2 Percentage Time Offline

In the case study some additional responses were tracked. Specifically, the percentage of the time that the plant are at 0% availability (offline). From the flowchart in Figure 1.2 and the discussion in Section 4.1, it can be observed that at any specific moment in time the overall plant availability can be either 100% (e.g. both trains are on line), 50% (one train is on line) or 0% (both trains are offline). The availability discussed above is calculated as the average availability over time. This is the most common way to report availability. However, the percentage time that the availability is at 0% has practical significance. During these periods, the plant can not receive any feed, and no output is produced. Considering that a plant in a refinery slots into the overall system, the feed will have to be diverted to another unit, or stored in a buffer. If the output is processed by another unit, the receiving unit will have to receive alternative feed, or source the feed from a buffer. If no such flexibility is available these units will have to shut down during this period. Buffers are expensive equipment, and the cost is related to the size of the buffer. The percentage time that the total plant is offline should therefore be minimized. The ANOVA table is provided in Table 5.8. The R-squared value for this model is 0.93. A square root transformation was performed on this data as suggested by the Box Cox transformation plot in Design Expert (Stat-Ease, 2006). The data are transformed to conform to the assumption of independent and identically distributed normal errors of the model.

The approximation model for the percentage time offline is provided in Table 5.9. This model was coded in the R software. 1000000 uniform random values for each factor was created using the `runif` function in R, using the upper and lower ranges of the factors in Table 4.35. For the “Hotwash Parallel or Series” factor the values below 2 were combined to create “Hotwash Series”, coded as 0, and values greater than 2 were combined to create “Hotwash Parallel” coded as 1. The percentage time offline was predicted with the model in R.

The plot in Figure 5.9 was generated by finding all the data points with a

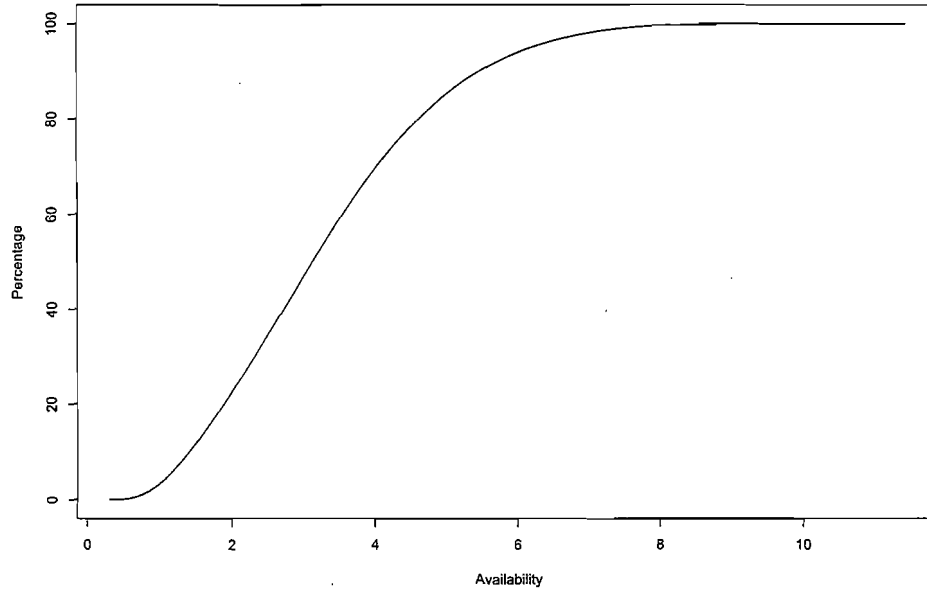


Figure 5.9: Plot of percentage design space above percentage time offline target value.

percentage time offline below the specified value on the x axis, and calculating the percentage of values that satisfies this criterion divided by the total number of points (1000000). This gives an approximation of the percentage of the space that is covered by the data with a percentage of time offline lower than the specified value. This plot can be used to make an informed decision regarding the risk involved in designing the plant for a given percentage time offline.

The median of the variables that satisfies the criterion is summarized in Table 5.7. For example, at an Offline Target = 1% the median of the factor values for the generated data that has percentage time offline lower than 1% are depicted. The Percentage of Total Design Space column gives an approximation of the percentage of the space that is covered by the data at the specified percentage time offline target value. This information can be used to approximate the sensitivity of the availability at the target value to the factors. The more constrained the region gets, the closer to their boundary values some of the factors become. This is an indication that the percentage time offline is more sensitive to these factors.

Table 5.7: Median Values of Factors for Different Percentage Time Offline Targets.

Offline Target	Hotwash Fail Factor	Hydroblasting Days	Hotwash Average	Main Reactor Fail Factor	Min Uptime Main Reactor	Main Reactor Beta	HotWash Parralel	Percentage Of Total Volume
11.00	2.00	5.00	24.01	1.00	6.00	3.00	1.00	100.00
10.00	2.00	5.00	24.01	1.00	6.00	3.00	1.00	99.99
9.00	2.00	5.00	24.00	1.00	6.00	3.00	3.00	99.92
8.00	1.99	4.99	23.95	1.00	6.01	3.00	3.00	99.52
7.00	1.98	4.98	23.83	0.99	6.04	3.01	3.00	98.02
6.00	1.96	4.96	23.59	0.98	6.11	3.02	3.00	94.03
5.00	1.93	4.92	23.17	0.96	6.24	3.03	3.00	85.31
4.00	1.87	4.86	22.39	0.93	6.42	3.05	3.00	69.49
3.00	1.82	4.82	20.65	0.89	6.60	3.08	3.00	46.98
2.00	1.75	4.82	17.46	0.87	6.73	3.12	3.00	22.36
1.00	1.43	4.66	14.19	0.82	7.23	3.27	3.00	3.16

The histograms in Figure 5.10 are those of the factors which satisfy the percentage time Offline lower than 1%. The histograms make it easy to visualize which factors are forced very close to one of their boundary values. For instance the average time to hotwash has no values above the center point of 24, and is skewed to the lower boundary (12). The minimum uptime for the main reactor data is skewed to the upper limit (8). These histograms are very similar to the histograms in Figure 5.8 for the total availability larger than 90%.

5.3.3 Multiple Response Optimization

In the case study it would obviously be beneficial to find the region where both the percentage time offline and overall availability are in an acceptable range. This can be achieved by using the numerical and graphical optimization techniques in Design Expert (Stat-Ease, 2006). For this case study the following criteria were specified:

- Percentage time offline between 0 and 1.
- Total availability between 90 and 100%

Design expert uses the Derringer and Suich (Coetzer et al., 2008b) desirability function approach to do the Multiple Response Optimization. The optimized results obtained by Design expert were then used to set the factor levels for the graphical optimization. An overlay plot (Figure 5.11) was cre-

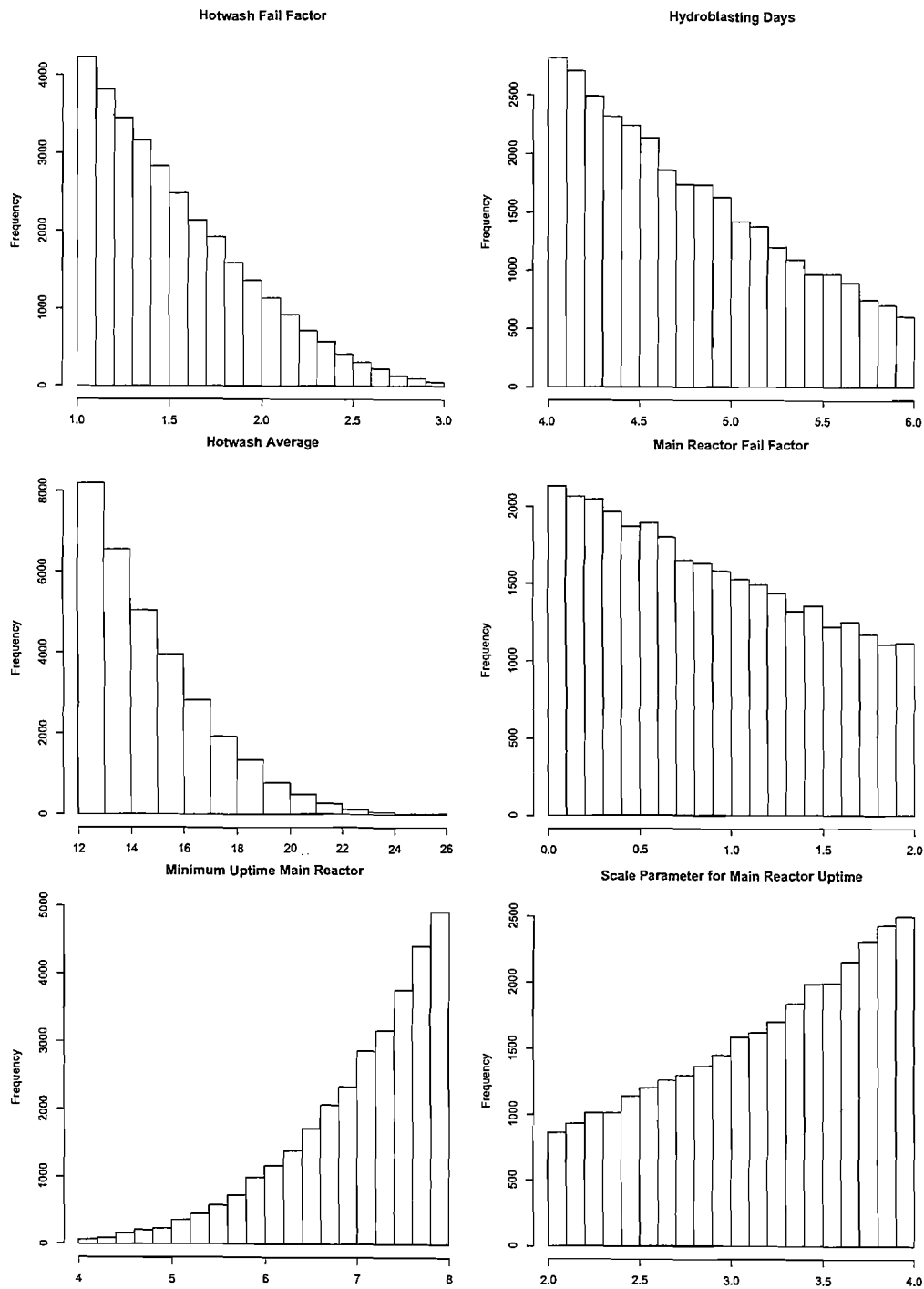


Figure 5.10: Histograms of factor values when percentage of time offline is constrained to be less than 1%.

Table 5.8: ANOVA table for percentage time offline

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	26.68	15	1.78	50.84	< 0.0001
A-HotwashFailFactor	2.61	1	2.61	74.68	< 0.0001
B-HydroblastingDays	2.37	1	2.37	67.64	< 0.0001
C-HotwashAverage	7.14	1	7.14	203.89	< 0.0001
D-MainReactorSmallFailFact	0.67	1	0.67	19.20	< 0.0001
E-MainReactorMin	6.47	1	6.47	184.78	< 0.0001
F-MainReactorBeta	0.49	1	0.49	14.13	0.0004
G-HotWashParralel	4.24	1	4.24	121.21	< 0.0001
AC	0.14	1	0.14	3.86	0.0546
AG	0.17	1	0.17	4.95	0.0303
BG	0.59	1	0.59	16.74	0.0001
CD	0.38	1	0.38	10.80	0.0018
CE	0.27	1	0.27	7.61	0.0079
CG	1.12	1	1.12	31.93	< 0.0001
EF	0.12	1	0.12	3.33	0.0733
EG	0.18	1	0.18	5.26	0.0256
Curvature	0.02	2	0.01	0.35	0.7090
Residual	1.92	55	0.03		

Table 5.9: Response Surface Model for the percentage time offline.

HotWashParralel	0
Sqrt(Availability0)	=
0.908140074	
0.349530928	* HotwashFailFactor
0.290971096	* HydroblastingDays
0.034543447	* HotwashAverage
-0.05175327	* MainReactorSmallFailFact
-0.18722762	* MainReactorMin
-0.218224505	* MainReactorBeta
-0.003867316	* HotwashFailFactor * HotwashAverage
0.006469389	* HotwashAverage * MainReactorSmallFailFact
-0.002715083	* HotwashAverage * MainReactorMin
0.021568344	* MainReactorMin * MainReactorBeta
HotWashParralel	1
Sqrt(Availability0)	=
0.705405077	
0.244450462	* HotwashFailFactor
0.097652379	* HydroblastingDays
0.056794269	* HotwashAverage
-0.05175327	* MainReactorSmallFailFact
-0.133018532	* MainReactorMin
-0.218224505	* MainReactorBeta
-0.003867316	* HotwashFailFactor * HotwashAverage
0.006469389	* HotwashAverage * MainReactorSmallFailFact
-0.002715083	* HotwashAverage * MainReactorMin
0.021568344	* MainReactorMin * MainReactorBeta

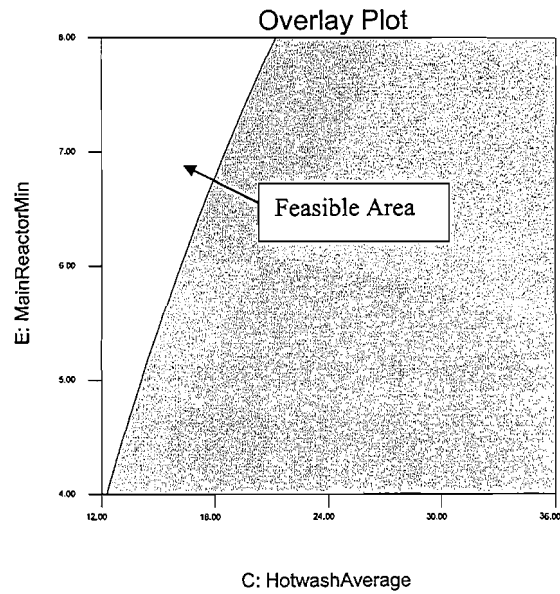


Figure 5.11: Overlay Plot.

ated for the average time to hotwash and the minimum uptime for the main reactor satisfying the criteria.

This plot can be used to aid design decisions regarding the average time to hotwash, given a minimum uptime for the main reactor. It is always beneficial to have a range of options available, as this allows for flexibility in choosing the most practical and cost effective factor levels for the design.

Chapter 6

Conclusions and Future Research

6.1 Conclusions

In this study different design and approximation models were compared, and the results were used to provide valuable answers concerning the configuration of the plant.

The Plackett-Burman (Section 2.2.3) and Maximin Latin Hypercube (Section 2.3.1) designs were found to be the best screening designs for the case study discussed. Both the Plackett-Burman (Section 2.2.3) and Maximin Latin Hypercube (Section 2.3.1) designs are easy and convenient designs to create and to use. Most modern statistical design packages should include these designs. Choosing between these two designs would mostly be a matter of personal preference and modeling considerations. A possible benefit of the Latin Hypercube family of designs is that it can be created for any number of runs and factor levels. The Plackett-Burman design would however be beneficial if setting the factor levels in a simulation model is not trivial. Using the Latin Hypercube designs each design point is at a different factor level, whereas for the Plackett-Burman designs the factor levels are only varied between their upper and lower levels. In some simulation studies setting the factor levels is not easy. A lot of modeling work is involved in

setting the factors at each level of the design. For these kinds of models the Plackett-Burman design could be advantageous.

For the second phase the Fractional Factorial design, D-Optimal design and Central Composite design gave comparable results when fitting response surface models. If curvature is observed in the design space the Central Composite Design or second order D-Optimal design should be used. For the kriging model all the designs gave comparable results. An interesting observation is that the two space filling designs (Maximin Latin Hypercube and Uniform design) performed much better with the kriging model than with the response surface model.

Response Surface Models and Kriging models differs in ease of use. Kriging models are much more difficult to fit and to interpret. In this study the only software found to be able to reliably and efficiently fit the kriging models was the DACE toolbox (Lophaven et al., 2002) in Matlab (Mathworks, 2007). Interpreting the optimal θ values for the model is also very difficult. It would also be problematic to release the model to a client, or use the model as 'n black box in a current simulation model. Response surface models are however easy to fit with most statistical packages. The coefficients are easy to interpret, and it is trivial to built the approximation model into a simulation model, or any other software to release to a client.

- The overall best leg of the tree in Figure 1.2 were found to be the Plackett-Burman Design for Phase 1, the Fractional Factorial Design for Phase 2, and the Response Surface Model for Phase 3, both in term of the mean square error (1.8), and the maximum absolute error (1.7) criteria. This result might be specific to the case study. However, it is provided as a general recommendation for the design and analysis of simulation experiments in industry.

This approximation model was used to analyze the case study, and make recommendations to the engineers. The case study consists of 14 factors, and it would have been extremely difficult to get a good understanding of such a complex system without making use of simulation and design of experiments. The resulting approximation model can be used to effectively and efficiently

explore the design space, and gain valuable insight about the system under investigation. These results were used to decide on what factors to focus on in further experimental work in the pilot plant, and to make informed decisions about the sizing of the reactors.

The work in this study clearly indicated that the average time to hotwash the system and the minimum uptime for the main reactor are the two variables that have the biggest effect on the plant availability. Additional information regarding the risk of designing for a specified plant availability was also generated. This allows for informed decision making regarding the over sizing of the plant to compensate for the required plant availability.

Additional to the results for the overall availability the percentage time offline was also analyzed. This gave additional insight into the plant performance. The average time to hotwash the system and the minimum uptime for the main reactor were again identified as the factors with the largest effect on the percentage of time that the plant is offline.

These two criteria were combined in a multiple response optimization study (Coetzee et al., 2008b; Kim and Lin, 1998, 2000) to find a feasible operating region of the average time to hotwash and the minimum uptime for the main reactor which satisfies the dual criterion. This is a powerful technique that can be used to find the optimal compromise between multiple response criteria.

Building a simulation model is a difficult and time consuming process. It is therefore only natural to expect the maximum amount of value to be gained from the model. Experimental Design techniques can be used to greatly enhance the quality and quantity of information and understanding that can be extracted from the simulation model. This ensures that the returns on the time and money put into building the model are maximized. As was demonstrated in the industrial case study discussed, once the approximation models are obtained countless possibilities are opened for further investigation and optimization. An experimental design strategy should therefore form a critical part of any simulation study, if possible.

6.2 Future Research

Experimental Design and Analysis for Simulation Experiments (DASE) is a powerful tool. This study only considered a small subset of the designs that currently exist. It would be specifically worthwhile to investigate alternative screening designs and techniques, for instance:

- Supersaturated Designs (Li and Lin, 2002; Lin, 1993, 1995, 2003; Yamada and Lin, 1997)
- Sequential Bifurcation (Bert Bettonvil, 1996; Kleijnen, 2008a,b; Kleijnen et al., 2005; Sanchez, 2007)

Kriging models in simulation studies are currently receiving a lot of attention (Jack, 2007; Kleijnen and van Beers, 2004; Kleijnen, 2008a; Law, 2007; van Beers and Kleijnen, 2003, 2004). Investigating the use of these models in simulation, and the designs to use in conjunction with kriging models, would be a worthwhile exercise.

Most simulation models in the petrochemical industry contains inputs and outputs that consists of mixtures. Experimental Design approaches for simulation models containing mixtures as inputs and outputs is in need of future research (Kleijnen et al., 2005).

Simulation studies normally have more than one conflicting output. The use of multiple response optimization approaches (Coetzer et al., 2008b; Kim and Lin, 1998, 2000) can help the analyst to find a good compromise between these responses. Future research in multiple response optimization would definitely be beneficial for application in simulation models.

The model used in this paper turned out to be very linear. It is possible that the results will differ for more nonlinear simulation models. Examples of models that might behave very differently are supply chain models, consisting of tankers, trucks etc, process models which have a lot of interaction between different units, and an overall mass balance over the system etc. It would be worthwhile to investigate the behaviour of the different model “families” and find an experimental design framework specific to each type of model.

Chapter 7

Appendix

7.1 ANOVA Tables for Screening Design

Table 7.1: ANOVA table for Fractional Factorial Design for Screening Phase

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	815.72	8	101.96	87.18	< 0.0001
A-HotwashFailFactor	74.81	1	74.81	63.96	< 0.0001
B-HydroblastingDays	28.32	1	28.32	24.21	0.0017
C-HotwashAverage	467.76	1	467.76	399.93	< 0.0001
E-ActivationReactorMin	18.16	1	18.16	15.52	0.0056
F-ActivationReactorAlpha	23.36	1	23.36	19.97	0.0029
H-MainReactorSmallFailFact	16.79	1	16.79	14.36	0.0068
J-MainReactorMin	148.87	1	148.87	127.28	< 0.0001
L-MainReactorBeta	37.66	1	37.66	32.20	0.0008
Residual	8.19	7	1.17		
Cor Total	823.90	15			

Table 7.2: ANOVA table for the Plackett-Burman Design for Screening Phase

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1129.41	7	161.34	54.06	< 0.0001
A-HotwashFailFactor	157.07	1	157.07	52.63	< 0.0001
B-HydroblastingDays	41.37	1	41.37	13.86	0.0029
C-HotwashAverage	556.73	1	556.73	186.55	< 0.0001
H-MainReactorSmallFailFact	73.17	1	73.17	24.52	0.0003
J-MainReactorMin	192.06	1	192.06	64.35	< 0.0001
L-MainReactorBeta	34.77	1	34.77	11.65	0.0051
O-HotWashParralel	74.25	1	74.25	24.88	0.0003
Residual	35.81	12	2.98		
Cor Total	1165.23	19			

Table 7.3: ANOVA table for the Uniform Design for Screening Phase

ANOVA for Response Surface Reduced Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	612.06	5	122.41	42.07	< 0.0001
A-HotwashFailFactor	39.50	1	39.50	13.57	0.0025
B-HydroblastingDays	28.01	1	28.01	9.63	0.0078
C-HotwashAverage	304.01	1	304.01	104.48	< 0.0001
J-MainReactorMin	131.65	1	131.65	45.24	< 0.0001
O-HotWashParralel	39.22	1	39.22	13.48	0.0025
Residual	40.74	14	2.91		
Cor Total	652.80	19			

Table 7.4: ANOVA table for the Latin Hypercube Design for Screening Phase

ANOVA for Response Surface Reduced Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	355.98	7	50.85	86.71	< 0.0001
A-HotwashFailFactor	13.85	1	13.85	23.61	0.0004
C-HotwashAverage	156.21	1	156.21	266.35	< 0.0001
H-MainReactorSmallFailFact	7.88	1	7.88	13.44	0.0032
J-MainReactorMin	53.92	1	53.92	91.95	< 0.0001
L-MainReactorBeta	2.88	1	2.88	4.92	0.0466
M-PostReactorMin	8.42	1	8.42	14.35	0.0026
O-HotWashParralel	13.30	1	13.30	22.68	0.0005
Residual	7.04	12	0.59		
Cor Total	363.02	19			

Table 7.5: ANOVA table for the D-Optimal Design for Screening Phase

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	810.80	4	202.70	83.01	< 0.0001
C-HotwashAverage	389.78	1	389.78	159.62	< 0.0001
G-ActivationReactorBeta	39.50	1	39.50	16.17	0.0024
H-MainReactorSmallFailFact	37.66	1	37.66	15.42	0.0028
J-MainReactorMin	153.59	1	153.59	62.89	< 0.0001
Residual	24.42	10	2.44		
Cor Total	835.22	14			

7.2 ANOVA Tables for Second Order Designs From Fractional Factorial Design

Table 7.6: ANOVA table for Fractional Factorial Design for Second Order Model

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	3740.87	18	207.83	275.36	< 0.0001
A-HotwashFailFactor	458.99	1	458.99	608.13	< 0.0001
B-HydroblastingDays	204.65	1	204.65	271.15	< 0.0001
C-HotwashAverage	1890.78	1	1890.78	2505.18	< 0.0001
D-ActivationReactorMin	98.49	1	98.49	130.50	< 0.0001
F-MainReactorSmallFailFact	104.37	1	104.37	138.28	< 0.0001
G-MainReactorMin	741.42	1	741.42	982.34	< 0.0001
H-MainReactorBeta	80.63	1	80.63	106.83	< 0.0001
AB	30.53	1	30.53	40.45	< 0.0001
AC	23.96	1	23.96	31.75	< 0.0001
AD	8.65	1	8.65	11.46	0.0014
AG	7.16	1	7.16	9.48	0.0034
AH	3.18	1	3.18	4.21	0.0454
BC	8.13	1	8.13	10.78	0.0019
CD	4.73	1	4.73	6.27	0.0157
CF	10.39	1	10.39	13.77	0.0005
CG	47.84	1	47.84	63.38	< 0.0001
FG	4.84	1	4.84	6.42	0.0146
GH	12.13	1	12.13	16.07	0.0002
Curvature	2.07	1	2.07	2.74	0.1040
Residual	36.98	49	0.75		
Lack of Fit	30.82	45	0.68	0.44	0.9215
Pure Error	6.16	4	1.54		
Cor Total	3779.92	68			

Table 7.7: ANOVA table for the Uniform Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1653.17	8	206.65	198.84	< 0.0001
A-HotwashFailFactor	182.00	1	182.00	175.12	< 0.0001
B-HydroblastingDays	99.89	1	99.89	96.12	< 0.0001
C-HotwashAverage	844.69	1	844.69	812.79	< 0.0001
D-ActivationReactorMin	31.21	1	31.21	30.03	< 0.0001
F-MainReactorSmallFailFact	39.45	1	39.45	37.96	< 0.0001
G-MainReactorMin	326.67	1	326.67	314.34	< 0.0001
H-MainReactorBeta	37.98	1	37.98	36.55	< 0.0001
CF	12.35	1	12.35	11.89	0.0013
Residual	45.73	44	1.04		
Lack of Fit	39.56	40	0.99	0.64	0.7958
Pure Error	6.16	4	1.54		
Cor Total	1698.90	52			

Table 7.8: ANOVA table for the Latin Hypercube Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	633.90	15	42.26	96.89	< 0.0001
A-HotwashFailFactor	79.64	1	79.64	182.60	< 0.0001
B-HydroblastingDays	24.29	1	24.29	55.69	< 0.0001
C-HotwashAverage	255.84	1	255.84	586.55	< 0.0001
D-ActivationReactorMin	3.64	1	3.64	8.35	0.0064
E-ActivationReactorAlpha	0.05	1	0.05	0.12	0.7283
F-MainReactorSmallFailFact	17.96	1	17.96	41.17	< 0.0001
G-MainReactorMin	86.96	1	86.96	199.37	< 0.0001
H-MainReactorBeta	24.65	1	24.65	56.52	< 0.0001
BE	2.07	1	2.07	4.74	0.0359
BG	7.60	1	7.60	17.42	0.0002
BH	3.07	1	3.07	7.04	0.0117
CG	6.63	1	6.63	15.21	0.0004
CH	1.87	1	1.87	4.29	0.0454
EH	2.69	1	2.69	6.18	0.0176
FH	5.26	1	5.26	12.07	0.0013
Residual	16.14	37	0.44		
Lack of Fit	9.97	33	0.30	0.20	0.9974
Pure Error	6.16	4	1.54		
Cor Total	650.04	52			

Table 7.9: ANOVA table for the D-Optimal Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	2317.77	17	136.34	166.50	< 0.0001
A-HotwashFailFactor	303.32	1	303.32	370.43	< 0.0001
B-HydroblastingDays	133.03	1	133.03	162.46	< 0.0001
C-HotwashAverage	1129.23	1	1129.23	1379.06	< 0.0001
D-ActivationReactorMin	67.07	1	67.07	81.90	< 0.0001
F-MainReactorSmallFailFact	86.27	1	86.27	105.36	< 0.0001
G-MainReactorMin	388.78	1	388.78	474.80	< 0.0001
H-MainReactorBeta	42.96	1	42.96	52.47	< 0.0001
AB	29.09	1	29.09	35.52	< 0.0001
AC	22.59	1	22.59	27.58	< 0.0001
AD	9.31	1	9.31	11.37	0.0021
AG	7.39	1	7.39	9.03	0.0054
BC	4.56	1	4.56	5.57	0.0252
BD	4.00	1	4.00	4.89	0.0351
BF	3.49	1	3.49	4.26	0.0480
CF	4.60	1	4.60	5.62	0.0246
CG	32.20	1	32.20	39.33	< 0.0001
GH	3.82	1	3.82	4.66	0.0393
Residual	23.75	29	0.82		
Lack of Fit	17.58	25	0.70	0.46	0.9008
Pure Error	6.16	4	1.54		
Cor Total	2341.51	46			

Table 7.10: ANOVA table for the Central Composite Design for Second Order Model

ANOVA for Response Surface Reduced Quadratic Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	2191.37	18	121.74	221.28	< 0.0001
A-HotwashFailFactor	269.00	1	269.00	488.93	< 0.0001
B-HydroblastingDays	112.27	1	112.27	204.06	< 0.0001
C-HotwashAverage	1082.40	1	1082.40	1967.37	< 0.0001
D-ActivationReactorMin	68.29	1	68.29	124.13	< 0.0001
E-ActivationReactorAlpha	0.15	1	0.15	0.26	0.6103
F-MainReactorSmallFailFact	74.18	1	74.18	134.83	< 0.0001
G-MainReactorMin	447.32	1	447.32	813.05	< 0.0001
H-MainReactorBeta	44.48	1	44.48	80.85	< 0.0001
AB	20.63	1	20.63	37.50	< 0.0001
AC	9.80	1	9.80	17.82	0.0001
AD	7.33	1	7.33	13.32	0.0008
AG	4.22	1	4.22	7.67	0.0085
BC	4.09	1	4.09	7.43	0.0095
CF	5.85	1	5.85	10.64	0.0023
CG	21.82	1	21.82	39.67	< 0.0001
EG	1.68	1	1.68	3.06	0.0881
GH	11.68	1	11.68	21.23	< 0.0001
E^2	15.38	1	15.38	27.96	< 0.0001
Residual	22.01	40	0.55		
Lack of Fit	15.84	36	0.44	0.29	0.9837
Pure Error	6.16	4	1.54		
Cor Total	2213.38	58			

7.3 ANOVA Tables for Second Order Designs From Uniform Design

Table 7.11: ANOVA table for Fractional Factorial Design for Second Order Model

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	782.50	8	97.81	130.04	< 0.0001
A-HotwashFailFactor	71.47	1	71.47	95.02	< 0.0001
B-HydroblastingDays	26.28	1	26.28	34.94	< 0.0001
C-HotwashAverage	428.10	1	428.10	569.16	< 0.0001
D-MainReactorMin	180.70	1	180.70	240.24	< 0.0001
E-HotWashParralel	37.24	1	37.24	49.51	< 0.0001
AB	8.28	1	8.28	11.01	0.0047
AC	4.19	1	4.19	5.57	0.0323
CD	10.15	1	10.15	13.49	0.0023
Curvature	0.48	2	0.24	0.32	0.7305
Residual	11.28	15	0.75		
Lack of Fit	3.91	7	0.56	0.61	0.7380
Pure Error	7.37	8	0.92		
Cor Total	794.27	25			

Table 7.12: ANOVA table for the Uniform Design for Second Order Model

ANOVA for Response Surface Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	554.80	5	110.96	86.55	< 0.0001
A-HotwashFailFactor	50.29	1	50.29	39.23	< 0.0001
B-HydroblastingDays	28.77	1	28.77	22.45	< 0.0001
C-HotwashAverage	326.37	1	326.37	254.58	< 0.0001
D-MainReactorMin	85.70	1	85.70	66.85	< 0.0001
E-HotWashParralel	58.22	1	58.22	45.41	< 0.0001
Residual	30.77	24	1.28		
Lack of Fit	23.40	16	1.46	1.59	0.2584
Pure Error	7.37	8	0.92		
Cor Total	585.57	29			

Table 7.13: ANOVA table for the Latin Hypercube Design for Second Order Model

ANOVA for Response Surface Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	295.38	5	59.08	74.82	< 0.0001
A-HotwashFailFactor	26.70	1	26.70	33.82	< 0.0001
B-HydroblastingDays	5.59	1	5.59	7.09	0.0136
C-HotwashAverage	162.51	1	162.51	205.82	< 0.0001
D-MainReactorMin	74.23	1	74.23	94.01	< 0.0001
E-HotWashParralel	46.68	1	46.68	59.12	< 0.0001
Residual	18.95	24	0.79		
Lack of Fit	11.58	16	0.72	0.79	0.6770
Pure Error	7.37	8	0.92		
Cor Total	314.33	29			

Table 7.14: ANOVA table for the D-Optimal Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	805.04	8	100.63	144.27	< 0.0001
A-HotwashFailFactor	77.55	1	77.55	111.18	< 0.0001
B-HydroblastingDays	28.72	1	28.72	41.17	< 0.0001
C-HotwashAverage	457.71	1	457.71	656.19	< 0.0001
D-MainReactorMin	185.08	1	185.08	265.34	< 0.0001
E-HotWashParralel	56.42	1	56.42	80.89	< 0.0001
AB	8.17	1	8.17	11.72	0.0024
AC	4.45	1	4.45	6.38	0.0192
CD	11.87	1	11.87	17.02	0.0004
Residual	15.35	22	0.70		
Lack of Fit	6.33	13	0.49	0.49	0.8851
Pure Error	9.02	9	1.00		
Cor Total	820.39	30			

Table 7.15: ANOVA table for the Central Composite Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1124.34	10	112.43	201.50	< 0.0001
A-HotwashFailFactor	95.85	1	95.85	171.78	< 0.0001
B-HydroblastingDays	42.66	1	42.66	76.45	< 0.0001
C-HotwashAverage	599.67	1	599.67	1074.69	< 0.0001
D-MainReactorMin	36.07	1	36.07	64.63	< 0.0001
E-HotWashParralel	61.75	1	61.75	110.67	< 0.0001
AB	3.93	1	3.93	7.05	0.0124
AC	6.33	1	6.33	11.34	0.0020
AE	3.42	1	3.42	6.14	0.0189
BE	3.17	1	3.17	5.69	0.0234
CD	4.95	1	4.95	8.87	0.0056
Residual	17.30	31	0.56		
Lack of Fit	9.93	23	0.43	0.47	0.9259
Pure Error	7.37	8	0.92		
Cor Total	1141.64	41			

7.4 ANOVA Tables for Second Order Designs From Latin Hypercube Design

Table 7.16: ANOVA table for Fractional Factorial Design for Second Order Model

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	3147.79	15	209.85	343.53	< 0.0001
A-HotwashFailFactor	257.50	1	257.50	421.54	< 0.0001
B-HotwashAverage	1880.74	1	1880.74	3078.79	< 0.0001
C-MainReactorSmallFailFact	96.08	1	96.08	157.28	< 0.0001
D-MainReactorMin	614.05	1	614.05	1005.21	< 0.0001
E-MainReactorBeta	63.94	1	63.94	104.67	< 0.0001
G-HotWashParralel	114.59	1	114.59	187.59	< 0.0001
AB	11.75	1	11.75	19.23	< 0.0001
AD	5.42	1	5.42	8.87	0.0043
AE	3.56	1	3.56	5.83	0.0191
AG	12.98	1	12.98	21.25	< 0.0001
BC	7.05	1	7.05	11.55	0.0013
BD	42.33	1	42.33	69.29	< 0.0001
BE	4.35	1	4.35	7.12	0.0100
DE	9.19	1	9.19	15.05	0.0003
DG	7.82	1	7.82	12.81	0.0007
Curvature	1.21	2	0.61	0.99	0.3778
Residual	34.21	56	0.61		
Lack of Fit	26.84	48	0.56	0.61	0.8637
Pure Error	7.37	8	0.92		
Cor Total	3183.21	73			

Table 7.17: ANOVA table for the Uniform Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1441.72	12	120.14	204.88	< 0.0001
A-HotwashFailFactor	104.32	1	104.32	177.89	< 0.0001
B-HotwashAverage	814.71	1	814.71	1389.33	< 0.0001
C-MainReactorSmallFailFact	22.30	1	22.30	38.02	< 0.0001
D-MainReactorMin	264.61	1	264.61	451.25	< 0.0001
E-MainReactorBeta	25.06	1	25.06	42.73	< 0.0001
F-PostReactorMin	0.85	1	0.85	1.44	0.2360
G-HotWashParralel	82.24	1	82.24	140.24	< 0.0001
AE	4.81	1	4.81	8.21	0.0063
AF	3.69	1	3.69	6.29	0.0158
AG	5.43	1	5.43	9.26	0.0039
BD	14.87	1	14.87	25.36	< 0.0001
DE	2.33	1	2.33	3.97	0.0524
Residual	26.39	45	0.59		
Lack of Fit	19.02	37	0.51	0.56	0.8900
Pure Error	7.37	8	0.92		
Cor Total	1468.11	57			

Table 7.18: ANOVA table for the Latin Hypercube Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	831.80	8	103.97	153.37	< 0.0001
A-HotwashFailFactor	75.91	1	75.91	111.97	< 0.0001
B-HotwashAverage	327.86	1	327.86	483.61	< 0.0001
C-MainReactorSmallFailFact	14.76	1	14.76	21.77	< 0.0001
D-MainReactorMin	164.49	1	164.49	242.63	< 0.0001
E-MainReactorBeta	8.54	1	8.54	12.60	0.0009
F-PostReactorMin	3.34	1	3.34	4.92	0.0312
G-HotWashParralel	69.74	1	69.74	102.87	< 0.0001
AD	6.82	1	6.82	10.07	0.0026
Residual	33.22	49	0.68		
Lack of Fit	25.85	41	0.63	0.68	0.7988
Pure Error	7.37	8	0.92		
Cor Total	865.02	57			

Table 7.19: ANOVA table for the D-Optimal Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1588.75	12	132.40	151.54	< 0.0001
A-HotwashFailFactor	152.46	1	152.46	174.50	< 0.0001
B-HotwashAverage	961.04	1	961.04	1099.97	< 0.0001
C-MainReactorSmallFailFact	40.39	1	40.39	46.23	< 0.0001
D-MainReactorMin	245.91	1	245.91	281.46	< 0.0001
E-MainReactorBeta	25.15	1	25.15	28.79	< 0.0001
F-PostReactorMin	0.04	1	0.04	0.04	0.8351
G-HotWashParrallel	48.09	1	48.09	55.04	< 0.0001
AD	7.86	1	7.86	9.00	0.0053
AG	15.42	1	15.42	17.65	0.0002
BC	4.89	1	4.89	5.59	0.0245
BD	12.40	1	12.40	14.19	0.0007
CF	4.25	1	4.25	4.87	0.0349
Residual	27.08	31	0.87		
Lack of Fit	18.07	22	0.82	0.82	0.6674
Pure Error	9.02	9	1.00		
Cor Total	1615.84	43			

Table 7.20: ANOVA table for the Central Composite Design for Second Order Model

ANOVA for Response Surface Reduced Quadratic Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	3225.53	14	230.40	540.24	< 0.0001
A-HotwashFailFactor	168.03	1	168.03	394.01	< 0.0001
B-HotwashAverage	1419.51	1	1419.51	3328.54	< 0.0001
C-MainReactorSmallFailFact	84.54	1	84.54	198.22	< 0.0001
D-MainReactorMin	477.78	1	477.78	1120.32	< 0.0001
E-MainReactorBeta	64.73	1	64.73	151.79	< 0.0001
F-PostReactorMin	2.17	1	2.17	5.09	0.0276
G-HotWashParralel	151.28	1	151.28	354.73	< 0.0001
AB	7.21	1	7.21	16.92	0.0001
AG	8.37	1	8.37	19.64	< 0.0001
BC	2.25	1	2.25	5.27	0.0250
BD	16.12	1	16.12	37.81	< 0.0001
DE	7.46	1	7.46	17.50	< 0.0001
DG	6.11	1	6.11	14.33	0.0003
F^2	7.45	1	7.45	17.48	< 0.0001
Residual	26.87	63	0.43		
Lack of Fit	20.70	55	0.38	0.49	0.9425
Pure Error	6.16	8	0.77		
Cor Total	3252.40	77			

7.5 ANOVA Tables for Second Order Designs From Plackett-Burman Design

Table 7.21: ANOVA table for Fractional Factorial Design for Second Order Model

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	3498.23	14	249.87	236.53	< 0.0001
A-HotwashFailFactor	252.20	1	252.20	238.73	< 0.0001
B-HydroblastingDays	106.86	1	106.86	101.16	< 0.0001
C-HotwashAverage	1993.82	1	1993.82	1887.33	< 0.0001
D-MainReactorSmallFailFact	92.37	1	92.37	87.44	< 0.0001
E-MainReactorMin	681.57	1	681.57	645.17	< 0.0001
F-MainReactorBeta	71.82	1	71.82	67.98	< 0.0001
G-HotWashParralel	163.39	1	163.39	154.67	< 0.0001
AB	15.41	1	15.41	14.59	0.0003
AC	11.43	1	11.43	10.82	0.0017
AG	13.66	1	13.66	12.93	0.0007
BG	18.94	1	18.94	17.93	< 0.0001
CE	35.26	1	35.26	33.38	< 0.0001
EF	17.08	1	17.08	16.16	0.0002
EG	8.82	1	8.82	8.35	0.0055
Curvature	2.57	2	1.28	1.22	0.3041
Residual	60.22	57	1.06		
Lack of Fit	52.85	49	1.08	1.17	0.4393
Pure Error	7.37	8	0.92		
Cor Total	3561.02	73			

Table 7.22: ANOVA table for the Uniform Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1113.01	11	101.18	20.44	< 0.0001
A-HotwashFailFactor	80.25	1	80.25	16.21	0.0002
B-HydroblastingDays	20.94	1	20.94	4.23	0.0455
C-HotwashAverage	503.18	1	503.18	101.63	< 0.0001
D-MainReactorSmallFailFact	15.18	1	15.18	3.07	0.0866
E-MainReactorMin	183.46	1	183.46	37.05	< 0.0001
F-MainReactorBeta	18.29	1	18.29	3.69	0.0608
G-HotWashParralel	150.75	1	150.75	30.45	< 0.0001
AB	24.98	1	24.98	5.04	0.0296
CE	70.20	1	70.20	14.18	0.0005
CF	31.89	1	31.89	6.44	0.0146
FG	21.00	1	21.00	4.24	0.0451
Residual	227.76	46	4.95		
Lack of Fit	220.39	38	5.80	6.30	0.0050
Pure Error	7.37	8	0.92		
Cor Total	1340.77	57			

Table 7.23: ANOVA table for the Latin Hypercube Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	936.95	6	156.16	50.44	< 0.0001
A-HotwashFailFactor	92.60	1	92.60	29.91	< 0.0001
B-HydroblastingDays	12.76	1	12.76	4.12	0.0476
C-HotwashAverage	425.11	1	425.11	137.32	< 0.0001
E-MainReactorMin	89.55	1	89.55	28.93	< 0.0001
G-HotWashParralel	47.93	1	47.93	15.48	0.0003
BG	25.02	1	25.02	8.08	0.0064
Residual	157.88	51	3.10		
Lack of Fit	150.51	43	3.50	3.80	0.0256
Pure Error	7.37	8	0.92		
Cor Total	1094.83	57			

Table 7.24: ANOVA table for the D-Optimal Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	1684.79	13	129.60	134.57	< 0.0001
A-HotwashFailFactor	119.09	1	119.09	123.66	< 0.0001
B-HydroblastingDays	40.33	1	40.33	41.87	< 0.0001
C-HotwashAverage	927.95	1	927.95	963.57	< 0.0001
D-MainReactorSmallFailFact	34.51	1	34.51	35.84	< 0.0001
E-MainReactorMin	277.10	1	277.10	287.73	< 0.0001
F-MainReactorBeta	34.72	1	34.72	36.05	< 0.0001
G-HotWashParralel	66.22	1	66.22	68.76	< 0.0001
AC	5.08	1	5.08	5.27	0.0288
AE	8.01	1	8.01	8.32	0.0072
BG	7.35	1	7.35	7.63	0.0097
CE	17.74	1	17.74	18.42	0.0002
EF	5.62	1	5.62	5.84	0.0220
EG	6.18	1	6.18	6.41	0.0168
Residual	28.89	30	0.96		
Lack of Fit	19.87	21	0.95	0.94	0.5697
Pure Error	9.02	9	1.00		
Cor Total	1713.68	43			

Table 7.25: ANOVA table for the Central Composite Design for Second Order Model

ANOVA for Response Surface Reduced Quadratic Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	2977.07	17	175.12	213.47	< 0.0001
A-HotwashFailFactor	141.33	1	141.33	172.28	< 0.0001
B-HydroblastingDays	42.82	1	42.82	52.20	< 0.0001
C-HotwashAverage	1311.08	1	1311.08	1598.20	< 0.0001
D-MainReactorSmallFailFact	53.89	1	53.89	65.70	< 0.0001
E-MainReactorMin	351.12	1	351.12	428.02	< 0.0001
F-MainReactorBeta	56.80	1	56.80	69.24	< 0.0001
G-HotWashParralel	140.64	1	140.64	171.44	< 0.0001
AB	12.71	1	12.71	15.50	0.0002
AC	6.31	1	6.31	7.69	0.0074
AG	9.67	1	9.67	11.78	0.0011
BG	13.21	1	13.21	16.11	0.0002
CD	4.98	1	4.98	6.07	0.0166
CE	27.65	1	27.65	33.71	< 0.0001
CF	6.10	1	6.10	7.44	0.0084
DF	4.10	1	4.10	4.99	0.0292
EF	4.12	1	4.12	5.02	0.0288
F^2	3.38	1	3.38	4.12	0.0469
Residual	49.22	60	0.82		
Lack of Fit	41.85	52	0.80	0.87	0.6499
Pure Error	7.37	8	0.92		
Cor Total	3026.29	77			

7.6 ANOVA Tables for Second Order Designs From D-Optimal Design

Table 7.26: ANOVA table for Fractional Factorial Design for Second Order Model

ANOVA for selected factorial model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	764.98	5	153.00	225.04	< 0.0001
A-HotwashAverage	536.10	1	536.10	788.56	< 0.0001
B-ActivationReactorBeta	8.38	1	8.38	12.32	0.0035
C-MainReactorSmallFailFact	16.86	1	16.86	24.80	0.0002
D-MainReactorMin	195.24	1	195.24	287.19	< 0.0001
AD	8.40	1	8.40	12.36	0.0034
Curvature	0.54	1	0.54	0.80	0.3859
Residual	9.52	14	0.68		
Lack of Fit	3.35	10	0.34	0.22	0.9770
Pure Error	6.16	4	1.54		
Cor Total	775.04	20			

Table 7.27: ANOVA table for the Uniform Design for Second Order Model

ANOVA for Response Surface Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	559.97	4	139.99	170.43	< 0.0001
A-HotwashAverage	355.50	1	355.50	432.79	< 0.0001
B-ActivationReactorBeta	3.96	1	3.96	4.83	0.0400
C-MainReactorSmallFailFact	18.80	1	18.80	22.89	0.0001
D-MainReactorMin	161.67	1	161.67	196.82	< 0.0001
Residual	16.43	20	0.82		
Lack of Fit	10.26	16	0.64	0.42	0.9071
Pure Error	6.16	4	1.54		
Cor Total	576.40	24			

Table 7.28: ANOVA table for the Latin Hypercube Design for Second Order Model

ANOVA for Response Surface Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	345.03	4	86.26	134.25	< 0.0001
A-HotwashAverage	184.99	1	184.99	287.92	< 0.0001
B-ActivationReactorBeta	3.28	1	3.28	5.11	0.0351
C-MainReactorSmallFailFact	8.03	1	8.03	12.50	0.0021
D-MainReactorMin	64.20	1	64.20	99.92	< 0.0001
Residual	12.85	20	0.64		
Lack of Fit	6.69	16	0.42	0.27	0.9740
Pure Error	6.16	4	1.54		
Cor Total	357.88	24			

Table 7.29: ANOVA table for the D-Optimal Design for Second Order Model

ANOVA for Response Surface Reduced 2FI Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	764.98	5	153.00	228.07	< 0.0001
A-HotwashAverage	536.10	1	536.10	799.15	< 0.0001
B-ActivationReactorBeta	8.38	1	8.38	12.49	0.0030
C-MainReactorSmallFailFact	16.86	1	16.86	25.13	0.0002
D-MainReactorMin	195.24	1	195.24	291.04	< 0.0001
AD	8.40	1	8.40	12.52	0.0030
Residual	10.06	15	0.67		
Lack of Fit	3.90	11	0.35	0.23	0.9763
Pure Error	6.16	4	1.54		
Cor Total	775.04	20			

Table 7.30: ANOVA table for the Central Composite Design for Second Order Model

ANOVA for Response Surface Reduced Linear Model					
Analysis of variance table [Partial sum of squares - Type III]					
	Sum of		Mean	F	p-value
Source	Squares	df	Square	Value	Prob > F
Model	454.24	3	151.41	191.86	< 0.0001
A-HotwashAverage	336.58	1	336.58	426.49	< 0.0001
C-MainReactorSmallFailFact	14.72	1	14.72	18.65	0.0005
D-MainReactorMin	102.94	1	102.94	130.44	< 0.0001
Residual	13.42	17	0.79		
Lack of Fit	7.25	13	0.56	0.36	0.9269
Pure Error	6.16	4	1.54		
Cor Total	467.66	20			

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