

# **BAYESIAN FRAMEWORK FOR IMPROVED R&D DECISIONS**

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by

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# **BAYESIAN FRAMEWORK FOR IMPROVED R&D DECISIONS**

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*To my family*

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## SUMMARY

This thesis work describes the formulation of a Bayesian approach along with new tools to systematically reduce uncertainty in Research & Development (R&D) alternatives. During the initial stages of R&D many alternatives are considered and high uncertainty exists for all the alternatives. The ideal approach in addressing the many R&D alternatives is to find the one alternative which is stochastically dominant i.e. the alternative which is better in all possible scenarios of uncertainty. Often a stochastically dominant alternative does not exist. This leaves the R&D manager with two alternatives, either to make a selection based on user defined utility function or to gather more information in order to reduce uncertainty in the various alternatives. From the decision makers perspective the second alternative has more intrinsic value, since reduction of uncertainty will improve the confidence in the selection and further reduce the high downside risk involved with the decisions made under high uncertainty.

The motivation for this work is derived from our preliminary work on the evaluation of biorefinery alternatives, which brought into limelight the key challenges and opportunities in the evaluation of R&D alternatives. The primary challenge in the evaluation of many R&D alternatives was the presence of uncertainty in the many unit operations within each and every alternative. Additionally, limited or non-existent experimental data made it infeasible to quantify the uncertainty and lead to inability to develop an even simple systematic strategy to reduce it. Moreover, even if the uncertainty could be quantified, the traditional approaches (scenario analysis or stochastic analysis), lacked the ability to evaluate the key group of uncertainty contributors. Lastly, the

traditional design of experiment approaches focus towards reduction in uncertainty in the parameter estimates of the model, whereas what is required is a design of experiment approach which focuses on the decision (selection of the key alternative). In order to tackle all the above mentioned challenges a Bayesian framework along with two new tools is proposed. The Bayesian framework consists of three main steps:

- a. Quantification of uncertainty
- b. Evaluation of key uncertainty contributors
- c. Design of experiment strategies, focussed on decision making rather than the traditional parameter uncertainty reduction

To quantify technical uncertainty using expert knowledge, existing elicitation methods in the literature (outside chemical engineering domain) are used. To illustrate the importance of quantifying technical uncertainty, a bio-refinery case study is considered. The case study is an alternative for producing ethanol as a value added product in a Kraft mill producing pulp from softwood. To produce ethanol, a hot water pre-extraction of hemi-cellulose is considered, prior to the pulping stage. Using this case study, the methodology to quantify technical uncertainty using experts' knowledge is demonstrated.

To limit the cost of R&D investment for selection or rejection of an R&D alternative, it is essential to evaluate the key uncertainty contributors. Global sensitivity analysis (GSA) is a tool which can be used to evaluate the key uncertainties. But quite often global sensitivity analysis fails to differentiate between the uncertainties and assigns them equal global sensitivity index. To counter this failing of GSA, a new method conditional global sensitivity (c-GSA) is presented, which is able to differentiate between

the uncertainties even when GSA fails to do so. To demonstrate the value of c-GSA many small examples are presented.

The third and the last key method in the Bayesian framework is the decision oriented design of experiment. Traditional ‘Design of Experiment’ (DOE) approaches focus on minimization of parameter error variance. In this work, a new “decision-oriented” DOE approach is proposed that takes into account how the generated data, and subsequently, the model developed based on them will be used in decision making. By doing so, the parameter variances get distributed in a manner such that its adverse impact on the targeted decision making is minimal. Results show that the new decision-oriented DOE approach significantly outperforms the standard D-optimal design approach. The new design method should be a valuable tool when experiments are conducted for the purpose of making R&D decisions.

Finally, to demonstrate the importance of the overall Bayesian framework a bio-refinery case study is considered. The case study consists of the alternative to introduce a hemi-cellulose pre-extraction stage prior to pulping in a thermo-mechanical pulp mill. Application of the Bayesian framework to address this alternative, results in significant improvement in the prediction of the true potential value of the alternative.

# CHAPTER I

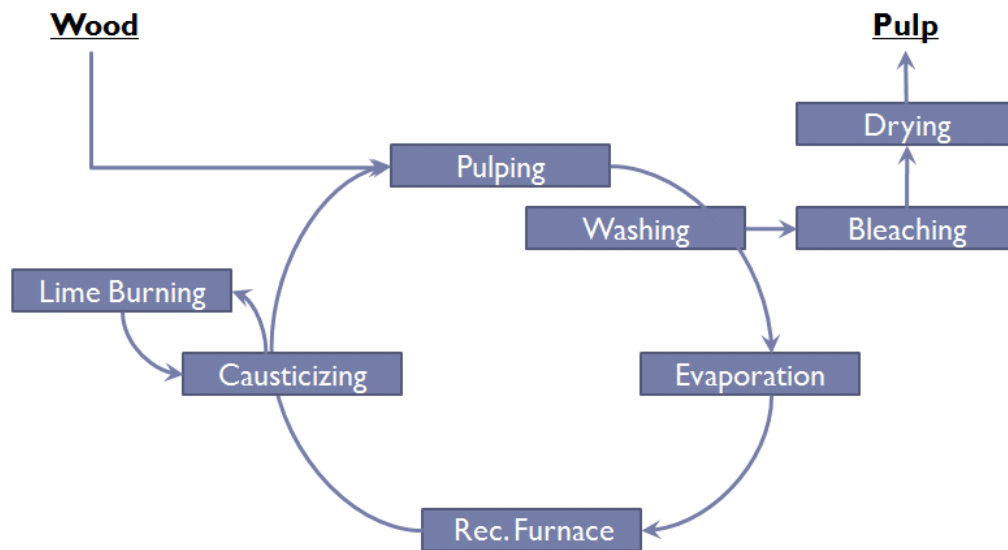
## INTRODUCTION

Development of new and improved processes and products through investment in research is a key driving force in the competitiveness of any industry. Investment in research and development (R&D) is considered high risk and high return. Hence, the systematic reduction of uncertainty in R&D options is undeniably an important problem. This has led to a significant body of research in the field of optimal R&D investment decision-making with the main focus on R&D portfolio optimization or the optimal timing of adoption or investment in R&D (Grenadier and Weiss 1997; Sampson 1998; Doraszelski 2004). This research is important and addresses the key issue when the objective is to select a portfolio of non-competing processes and products or select the optimal timing of the R&D investment.

Once the portfolio is selected, the second stage of the problem is to make R&D investment decisions within an individual R&D project. Alternatively, another class of problems is the selection of the best alternative among many R&D alternatives. A systematic method to optimally resolve the uncertainties is needed to address such problems.

Our motivation to address the problem of systematically reducing uncertainty in R&D alternatives comes from the issues, challenges, and opportunities we faced during our preliminary work on evaluation of various biorefinery alternatives. Among the various alternatives under consideration for biofuel production, the alternatives to produce biofuel within a pulp/paper mill (i.e. a biorefinery) are considered of significant

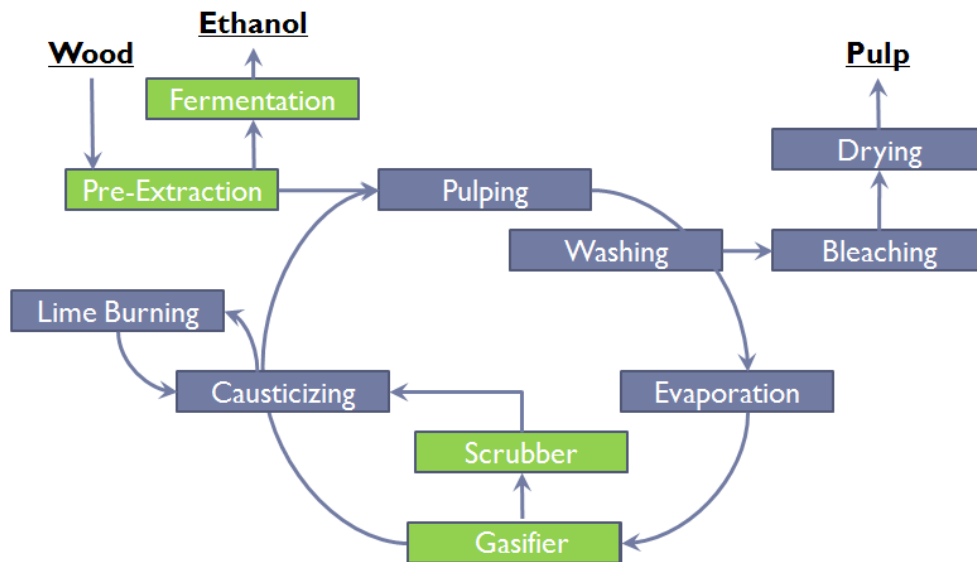
promise. The reason is that the pulp/paper mills already have significant infrastructure which can be exploited to convert them into a biorefinery(Larson, Consonni et al. 2003; Larson, Consonni et al. 2006).



**Figure 1.1:** Block diagram of the major unit operations in a kraft pulp mill

Figure 1.1 shows a block diagram of a traditional pulp/paper producing Kraft mill. In Kraft process, wood chips are fed to the digester along with the white liquor (mixture of sodium hydroxide and sodium sulfide), where pulping (process of converting wood or lignocellulosic non-wood material to separated pulp fibers for papermaking) takes place (Kocurek 1989). The highly basic conditions, high temperature and long process hours during pulping leads to degradation of lignin and some hemicelluloses giving fragments which are soluble in the strongly basic liquid. Pulping is followed by washing stage, where the solid pulp (called brown stock because of its color) is separated from the liquor (called black liquor because of its color). Black liquor (BL) contains lignin fragments, carbohydrates from the breakdown of hemicellulose, sodium sulphate, sodium

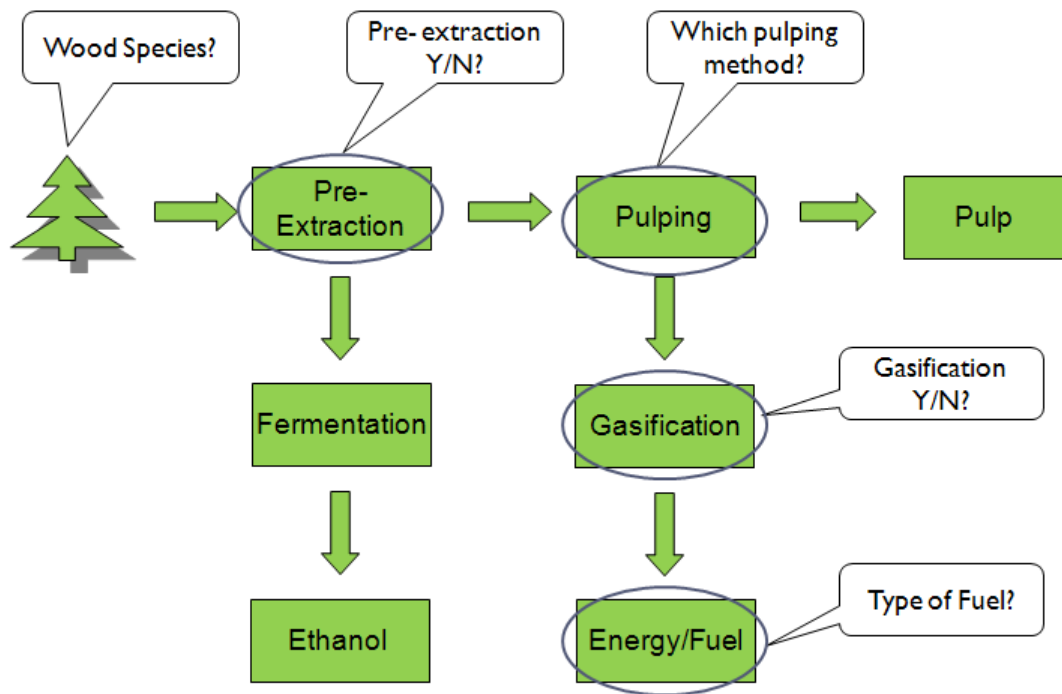
carbonate and other inorganic salts. Recovered pulp is bleached (to improve the brightness) and dried. The recovered black liquor is about 15% solid contents and is concentrated in a multiple effect evaporator to 60-80% solid content. This concentrated black liquor is then burned in the recovery furnace to recover the inorganic chemicals for reuse in the pulping process. The molten salts (“smelt”) recovered from the recovery boiler are sent to the causticizing section to regenerate the white liquor chemicals.



**Figure 1.2:** Block diagram of a modified pulp mill with the option to produce bio-fuels

Figure 1.2 shows the two main unit operations (hemicellulose pre-extraction and gasification) which can be introduced in a traditional paper mill leading to many R&D alternatives. The first unit operation is the pre-extraction stage prior to the ‘pulping’ step. Hemi-cellulose, one of the components of the wood, can be extracted during the pre-extraction stage and can be further fermented to produce ethanol as a value added product. Here ethanol is considered as the value added product because significant amount of hemicelluloses are lost during the pulping stage and end up being burnt in the recovery furnace as a part of the black liquor thus providing low value heat energy

compared to high value ethanol. The second alternative is to replace the recovery furnace by a gasification unit, which leads to the production of synthesis gas (syn-gas). Gasification unit provides the potential alternative to improved energy efficiency or production of various biofuels from the syngas (Consonni, Larson et al. 1998; Larson, Consonni et al. 2003).



**Figure 1.3:** Various questions to be answered for the selection of the best biorefinery alternative

Introduction of the two unit operations (pre-extraction and gasification unit) leads to many R&D alternatives and many questions which need to be answered before a best R&D alternative can be selected. Figure 1.3, lists some of the important questions:

- What wood species should be considered (Softwood or Hardwood)?
- Should pre-extraction be considered?

- Which pulping method should be used (MSSAQ, Kraft or Polysulphide)? (See appendix A and B for more information on MSSAQ, Kraft and polysulphide)
- Should gasification be considered? If yes, which type (low or high temperature)?
- How should the energy derived from the syngas be produced in the gasification (as energy or as liquid fuel)?

Moreover, within each of these bullets remain many other questions to be answered. For example, when considering a pre-extraction stage, should only hemicelluloses be pre-extracted or complete hydrolysis of wood should be considered. If considering hemicelluloses pre-extraction, which chemicals should be used, acidic, alkaline or neutral?

To answer some of these questions a preliminary analysis on various alternatives was undertaken. The description of various alternatives is listed in Table 1.1. The first four alternatives are based on high temperature gasification, producing mixed alcohol as a value added product. Alternative '1' and '2' are Kraft pulping based biorefineries with and without pre-extraction of hemicelluloses respectively. Similarly, alternative '3' and '4' are polysulphide based biorefineries with and without pre-extraction of hemicelluloses. Alternative '5' is a Kraft pulp mill based biorefinery, with the only value added product being the ethanol produced from the pre-extraction of hemicelluloses. Alternative '6' is a low temperature gasification process, based on MSSAQ pulping method, producing DME (dimethyl ether) as the value added product from the syngas from the gasifier. The details about the preliminary analysis of the alternatives '1'-'4' are presented in Appendix A, and of alternative '6' in Appendix B. Alternative '5' is presented as a case study in Chapter 3.

**Table 1.1:** Description of various R&D alternatives evaluated

Alternative No.		1	2	3	4	5	6
Pre Extraction		X		X		X	
Gasification	Low Temperature						X
	High Temperature	X	X	X	X		
Pulping Method	Kraft	X	X			X	
	Polysulphide + Gasification			X	X		
	MSSAQ						X
Product Mix	Ethanol	X		X		X	
	Mixed Alcohol	X	X	X	X		
	DME						X
	Paper	X	X	X	X	X	X

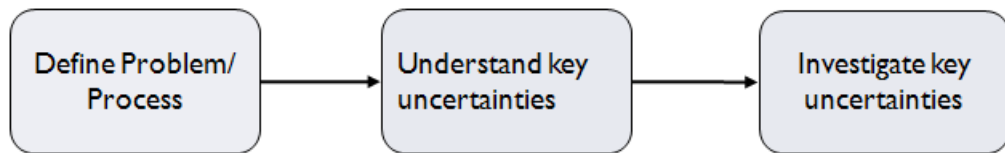
The efforts in the preliminary evaluation of the biorefinery alternatives suffered from the following challenges:

- a. Large number of biorefinery alternatives
- b. Limited or no experimental data (For example, for the kinetic of mixed alcohol synthesis (Gunturu, Kugler et al. 1998), effectively only two data points existed for a system of 18 ordinary differential equations with 19 parameters.)
- c. Inability to fully exploit the knowledge of the experts, i.e. inability to quantify the expert's qualitative knowledge and insights. At every step in the preliminary evaluation many assumptions were made, and values reported as point estimates, after discussion with the experts. However, this omits substantial components of

the experts' knowledge, and particularly their relative uncertainty in the values that they provide. Additionally, when considering similar alternatives, experts were able to provide qualitative knowledge, which was essentially the main source for the conception of the alternatives. But due to the lack of the quantitative estimates, this knowledge could not be used effectively to develop a systematic plan to reduce the uncertainty in the new alternatives.

- d. Limited ability of the key uncertainty evaluation approaches (scenario analysis and stochastic analysis) to account for both the technical and economical uncertainty. When using scenario analysis for an alternative with a large number of uncertain parameters, it is not possible to comprehend the results. Further, both the methods have limited ability to ascertain the 'key group' of uncertainty contributors. For example, for alternatives '1' and '3', H<sub>2</sub>SO<sub>4</sub> based pre-extraction was considered as the key uncertainty based on the scenario analysis and some initial experimental data for pre-extraction yield was obtained but no experimental data was obtained for the effect of pre-extraction on the pulp yield. Even after incorporating the experimental data for the pre-extraction yield, significant uncertainty remained, mainly due to the uncertainty contributed by the affect of pre-extraction on the pulping yield, and no decision about the alternatives could be made.
- e. Failure to address decision-making needs
- f. How to reduce uncertainty around the decision? The traditional approaches focus on the reduction in the uncertainty in the parameter estimates, but what is needed

is an approach to assist in decision making, i.e. selection or rejection of the alternatives.



**Figure 1.4:** Three step intuitive approach to address the R&D problem

The existence of many R&D alternatives, along with the presence of uncertainty in the many unit operations within each alternative, makes the problem complex. The limited or non-existent experimental data makes it infeasible to quantify the uncertainty, and leads to the inability to develop a systematic strategy to reduce uncertainty. Even if the uncertainty can be quantified, using the traditional approaches (scenario analysis or stochastic analysis), the identification of key groups of contributors to uncertainty may be missed. Lastly, the traditional design of experiment approaches focus towards reduction in uncertainty in the parameter estimates of the model, whereas what is required is a design of experiment approach which focuses on the decision (selection of the key alternatives). In order to tackle all the above mentioned challenges a Bayesian framework based on the following three step intuitive approach (Figure 1.4) is proposed:

- a. Define the problem/process, gather all the information and define the scope of the problem
- b. Understand where the key uncertainties lie
- c. Investigate the key uncertainties by obtaining additional information, either through further modelling or experimentation

The fundamental key of the systematic approach is to bridge the gap between the decisions made by the scientists, whose decisions are based on the technical uncertainty, and the managers, whose decisions are based on the process modelling and economic uncertainty. Hence, the idea here is to develop a systematic approach, which can make use of the process models, experts' knowledge and the design of experiment strategies to improve the R&D decisions. Keeping the above in mind, a Bayesian framework composing the following three main steps is proposed:

- a. Quantification of uncertainty
- b. Evaluation of key uncertainty contributors under both technical and economic uncertainty
- c. Design of experiment (DOE) strategies which are focused on the decision making, not on the traditional parameter uncertainty reduction

The rest of the thesis is structured as follows: Chapter 2 provides background information about the various existing tools and methodologies which can be used in the developed framework. In Chapter 3, statistical methods to elicit expert's knowledge about uncertainty along with global sensitivity analysis (GSA) are applied to a real biofuel case study to quantify uncertainty and evaluate the key uncertainty contributors. Chapter 4 introduces a new methodology, conditional global sensitivity analysis (c-GSA) which is an improvement over the traditional approach (GSA), as it is able to differentiate between the various uncertainties when GSA fails to do so. A new decision based DOE approach is introduced in Chapter 5. The systematic approach to reduce uncertainty, the Bayesian framework along with the new tools, is introduced in the Chapter 6. To demonstrate the importance of the framework the systematic approach is applied to a

biofuel case-study. Chapter 7 concludes the thesis along with the suggestions for the future research directions.

## **CHAPTER II**

### **BACKGROUND**

This literature survey discusses the existing methodologies which are useful for the Bayesian framework. Section 2.1 discusses various existing methods which can be used to quantify the experts' knowledge and contrasts the benefits of using the predictive elicitation method. The advantages of the predictive elicitation method, discussed in this section, are the motivation for selecting it as the method for application for a real case study in Chapter 3. In Section 2.2 various methods to integrate the knowledge of experts are discussed. Finally recent literature is presented to support the selected methodology (simple average).

In quantification of uncertainty, it would be shown in Chapter 3 that it is important to account for all the correlations. Copula is a methodology which has significant advantages in accounting for correlations, hence more information about is presented in Section 2.3. To identify the key group of uncertainties one can use many methodologies and a discussion about the various methodologies is presented in Section 2.4.

#### **2.1 Expert opinion elicitation**

Traditionally elicited experts opinions have been used to deal with issues with significant uncertainty, issues that are controversial, issues that are complex and/or issues that have significant effect on the decisions and contribute significantly to the risk. Expert

opinion has been used extensively in a variety of sectors, such as nuclear applications, aerospace sector, military intelligence, occupational sector, the health sector and the banking sector. The earliest and the most common method is the Delphi method. The Delphi method was developed at the RAND Corporation in the early 1950's and is undoubtedly the best-known method for eliciting and aggregating expert opinions in order to achieve a high degree of consensus. The Delphi method has enjoyed considerable popularity among managers, policy analysts, and corporate planners.

In a broad sense, the elicitation methods can be classified as indirect methods, direct methods and parametric elicitation. **Indirect methods** (betting rates) methods were the popular methods among the theoreticians but they did not find many practical applications because of their artificial character (Cooke 1991). **Direct methods** measure an expert's degree of belief by directly inquiring about their degree of beliefs. They are the most common but not very useful when the experts are not familiar with the notion of probability. *Delphi* method falls into this category of direct methods. **Parametric elicitation** (Preyssl and Cooke 1989) is used to assess confidence intervals on a parameter of interest.

There are some pitfalls related to the above mentioned methods and some heuristics exists, which one should be aware of in elicitation. The pitfalls summarized by (Cooke 1991), (Kadane and Wolfson 1998) and (Wolfson 1995) are as follows:

- a. Availability: assessors link their probabilities to the frequency with which they remember the event.

- b. Anchoring: Experts anchor their judgments to some starting value and then adjust outward and usually insufficiently.
- c. Overconfidence: Experts are fairly coherent in the center of the distribution but there exists difficulty in assessing the tail of the distribution
- d. Conjunction fallacy: Many non-expert assessors will assign a greater probability to an event they deem to be “more common”, when in fact that event may be a subset of another event they assign lower probability to.
- e. Hindsight bias: When an assessor has seen the data about which the opinion is being solicited and their opinions already updated on the basis of the data.

In order to reduce and avoid the risk of above pitfalls, (Kadane and Wolfson 1998) recommends and found predictive questions to perform better than the structural questions. For example, they assumed regression likelihood and inquired about the expert's view of the dependent variables given various values of the predictor variables. In contrast the structural questions are the ones used in the parametric elicitation or *direct methods*.

According to the basic agreement in the statistical literature about the elicitation procedure, summarized in (Wolfson 1995), the elicitation procedure should account for the following:

- a. Experts should be asked to give opinions about observable quantities

- b. Quantiles should be elicited instead of the moments of the distribution (except the first moment possibly), especially when model parameters are not meaningful to the expert.
- c. Frequent feedback should be given to the expert during the elicitation process
- d. Experts should be asked to give assessments both conditionally and unconditionally on hypothetical observed data.

In light of the above the (Kadane and Wolfson 1998) recommends the normal linear model originally developed by (Kadane, Dickey et al. 1980) and further in (Wolfson 1995), as it evades the pitfalls and accommodates the acceptable principles. Moreover in (Kadane, Dickey et al. 1980) a t-distribution is considered for the dependent variable which provides greater flexibility in the type of distribution function. This important property is further vouched by D.V.Lindley in (1998) “*Reality includes outliers and sensible measurement would involve models, like those on a t-distribution, which naturally contain them*”.

## **2.2 Expert opinion aggregation**

Similar to expert opinion elicitation expert opinion aggregation techniques are used in various fields such as reliability engineering (Kumar and Hinds 2005), nuclear applications, aerospace sector, military intelligence and health sector.

Expert judgments can provide valuable information about important uncertainties, in the absence of experimental data. Eliciting expert opinions from more than one expert can be viewed as increasing the sample size of the experiment. Often experts differ in

their opinions, and then it becomes important to aggregate their opinions in a reasonable way. The importance and challenges in expert opinion aggregation can be understood by both the long history and the relative amount of literature on aggregation (Eisenberg and Gale 1959), (Winkler 1968), (Winkler 1981), (Bordley 1982), (Clemen 1987),(Clemen 1989), (Winkler and Clemen 1992), (Clemen and Winkler 1993), (Myung, Ramamorrti et al. 1996), (Rantilla and Budescu 1999), (Kumar and Hinds 2005) compared to elicitation (Kadane, Dickey et al. 1980) ,(O'Hagan 1998); (Craig, Goldstein et al. 1998); (E. 2002).

There are various mathematical and behavioral approaches to aggregate expert opinions and a good review is available in (Clemen and Winkler 1999). In this work we focus on the mathematical approaches. Mathematical approaches are subdivided into axiomatic and Bayesian approaches.

### 2.2.1 Axiomatic approaches

Earlier work on aggregation of expert opinions was focused towards axiomatic approaches. The two main approaches are the *linear opinion pool* (Stone 1961) and the *logarithmic opinion pool*. The linear opinion pool is just a weighted linear combination of the expert's probabilities:

$$p(\theta) = \sum_{i=1}^n w_i p_i(\theta) \quad (2.1)$$

where  $n$  is the number of experts and  $p_i(\theta)$  is the  $i^{\text{th}}$  expert's probability distribution about the parameter  $\theta$  and  $w_i$  are the fraction weights corresponding to each expert  $i$ . The logarithmic opinion pool which is the multiplicative averaging of the expert's opinions is of the form:

$$p(\theta) = \lambda \prod_{i=1}^n p_i(\theta)^{w_i} \quad (2.2)$$

where  $\lambda$  is the normalizing constant and  $w_i$  are the weights which satisfy some restrictions so that  $p(\theta)$  is a distribution. Typically the sum of the weights is restricted to equate one. Finding the appropriate weights for either of the approach has been problematic (Winkler and Clemen 1992) which lead to the focus towards considering individual expert opinions. Though recent findings (Soll and Larrick 2009) suggest averaging as in linear opinion pools is better than considering any individuals opinions.

### 2.2.2 Bayesian approaches

From mathematical/scientific viewpoint Bayesian approaches have more appeal. Morris (Morris 1974; Morris 1977) formally established the Bayesian paradigm for aggregation information from experts. Suppose  $n$  experts provide information  $g_1, g_2, \dots, g_n$  to a decision maker about a quantity of interest  $\theta$ , then the decision maker can use Bayes theorem to update the prior distribution  $p(\theta)$ :

$$p^* = \frac{p(\theta)L(g_1, g_2, \dots, g_n | \theta)}{p(g_1, g_2, \dots, g_n)} \quad (2.3)$$

where  $L$  represents the likelihood function associated with the experts opinions. The attention the Bayesian methods have received over the last few decades, is compelling but they are very challenging to apply, especially because of the difficulty to assess the likelihood function. The likelihood function should be able to capture the information given in  $g_1, g_2, \dots, g_n$  and as such it should also capture the interrelationship between  $\theta$  and  $g_1, g_2, \dots, g_n$ . In simple terms  $L$  should account for precision and bias of  $g_i$ 's and

should also account for the dependence between  $g_i$ 's. Dependence here signifies the extent the forecast errors of the experts are interrelated.

Winkler (R.L.Winkler 1981) presents a model for combining expert probability distributions; when expert probability distributions are normal and much work has been done on to refine the various aspects of this model. But the use of this method has been limited due to the restriction on the type of expert probability distribution. Another Bayesian model that has gained traction is by Mendel and Sheridan (Mendel and Sheridan 1989), which allow for aggregation of probability distributions that are not normal. Though Mendel and Sheridan's model conveniently combines the issues of both individual calibration and dependence, it assumes that the past data will be used for the estimation of the parameters of the likelihood function. However rarely is past data/information available, and in such cases it is important to look at the Bayesian aggregation methods that use subjective judgment in determining the likelihood function.

Jouini and Clemen (Jouini and Clemen 1996) develop a method in which likelihood function is expressed as a function (copula) of marginal distributions. This approach allows the Bayesian decision maker performing the aggregation to separate two difficult aspects of the model-construction procedure. Qualities of the individual sources, such as bias and precision, are incorporated into the marginal distributions. Dependence among the sources is encoded into the copula, which serves as a dependence function and joins the marginal distributions into a single multivariate distribution. Consider that expert  $i$  assess a continuous density for  $\theta$ ,  $f_i(\theta)$ , with the corresponding CDF  $F_i(\theta)$ . Now the decision makers posterior distribution is given by

$$P(\theta | f_1, f_2, \dots, f_n) \propto c[1 - F_1(\theta), \dots, 1 - F_n(\theta)] \prod_{i=1}^n f_i(\theta) \quad (2.4)$$

where  $c$  represents the copula density function. The conditional dependence among  $F_1, F_2, \dots, F_n$  given  $\theta$ , is measured by using the concept of *concordance*. In simple terms concordance measures the extent to which a set of random variables “move in the same direction”. Further, they evaluated Archimedean copulas for the expert opinion aggregation, and the following two constraints were noted:

- Archimedean copulas can be used to model only positive dependence.
- Archimedean copulas by their nature treat experts equivalently in terms of dependence.

The first constraint does not seem to be limiting, as (R.T.Clemen 1989) pointed out that there are very few cases when negative dependence have been observed. Moreover under the similar information sets and often similar methodology, positive dependence seems reasonable. The second constraint is limiting though as it does not let the decision maker differentiate between the experts.

In another development, Clemen and Reilly (Clemen and Reilly 1999) make use of a normal copula that underlies the multivariate normal distribution to construct a probabilistic model, which accounts for the correlation among various parameters. Insight into how one can assess dependence, among the various parameters by using three methods, specifically statistical approaches, probability of concordance and conditional fractile estimate, is also provided.

Literature on expert opinion aggregation shows that using aggregating opinions from multiple experts is useful. Moreover, simple average of forecasts seem to work well in comparison to more complex techniques (Clemen 1989) (Soll and Larrick 2009). (Winkler and Clemen 2004) evaluate the effect of considering multiple experts and multiple methods for combining assessments. The motivation behind using multiple experts or/and multiple methods is to obtain more accurate information, which would lead to better decisions. They concluded that considering more experts and more methods both are useful but considering more experts is better than considering more methods.

### **2.3 Copulas**

A copula is a general way of formulating a joint distribution from marginal distributions of the random variables. (Sklar 1959) coined the term copula in mathematical and statistical sense to describe the coupling of the marginal distributions to form the multivariate distribution. Copulas are applied in variety of fields, for example to model dependencies in economic costs (Herath and Kumar 2007), to aggregate expert opinions (Jouini and Clemen 1996) and extensively in finance to model dependencies (Rodriguez 2007), (Cherubini, Luciano et al. 2004), (Li 2000), (Frees, Carriere et al. 1996; Frees and Valdez 1998). The main advantage of using copulas is their ability to combine arbitrary marginal distributions to obtain a joint distribution. Moreover copulas offer greater flexibility in modeling correlation: they have the ability to use rank correlation (spearman's rho or kendall tau) instead of correlation (Pearson's product-moment coefficient). This is useful since correlation has several drawbacks (Herath and Kumar 2007):

- Correlation is the correct dependence if the marginal and joint distribution of the random variables is normal
- Correlation ignores any nonlinear dependencies
- Correlation is not invariant under strictly increasing transformation of the random variables

According to Sklar's theorem (Sklar 1959), Given a joint cumulative distribution function  $F(x_1, \dots, x_n)$  for random variables  $X_1, \dots, X_n$  with marginal cumulative distribution functions  $F_1(x_1), \dots, F_n(x_n)$ ,  $F$  can be written as a function of its marginal's:

$$F(x_1, \dots, x_n) = C[F_1(x_1), \dots, F_n(x_n)] \quad (2.5)$$

where  $C$  is a joint distribution function with uniform marginal's. Moreover, if each  $F_i$  is continuous then  $C$  is unique and if each  $F_i$  is discrete then  $C$  is uniquely determined on  $\text{Ran}(F_1) \times \dots \times \text{Ran}(F_n)$ .

## 2.4 Sensitivity analysis

Sensitivity analysis (SA) of a model output aims to quantify the relative importance of each input model parameter in determining the value of an assigned output variable. This discipline is being very much application driven and many different methods (differential analysis, global sensitivity analysis, etc.) have been developed for SA. SA can then help to identify key parameters whose uncertainty affects most the output. This in turn can be used to establish experimental (or field) research priorities, eventually leading to a better definition of the unknown parameter and hence to a

reduction of its uncertainty range. The process can be iterated until an acceptable uncertainty range of the output is achieved (Homma and Saltelli 1996).

### 2.4.1 Differential analysis

Differential analysis is based on the partial derivatives of model output 'y' with respect to the elements of  $x = [x_1, x_2, \dots, x_k]$ . In its simplest form differential analysis involves approximating the model output 'y' by the Taylor series:

$$y(x) \approx y(x_0) + \sum_{j=1}^k \left[ \frac{\partial f(x_0)}{\partial x_j} \right] [x_j - x_{j0}] \quad (2.6)$$

where  $x_0 = (x_{10}, x_{20}, \dots, x_{k0})$  is a vector of base case values for the  $x_j$  (i.e. the expected values for the  $x_j$ ). Based on (2.6) the mean and variance of the model can be calculated using (2.7) and (2.8) respectively.

$$E(y) = y(x_0) \quad (2.7)$$

$$V(y) \approx \sum_{j=1}^k \left[ \frac{\partial f(x_0)}{\partial x_j} \right]^2 V(x_j) + 2 \sum_{j=1}^k \sum_{i=j+1}^k \left[ \frac{\partial f(x_0)}{\partial x_j} \right] \times \left[ \frac{\partial f(x_0)}{\partial x_i} \right] Cov(x_j, x_i) \quad (2.8)$$

If  $x_j$  are uncorrelated then  $V(y)$  is given by (2.9). Sensitivity analysis is based on the use of the partial derivatives associated with a Taylor series to determine the effects of the individual elements of  $x$  on  $y$ . For example if the Taylor series in (2.6) is used and the elements of  $x$  are independent, then the fractional contribution of  $x_j$  to the variance of  $y$  can be approximated by (2.10).

$$V(y) \approx \sum_{j=1}^k \left[ \frac{\partial f(x_0)}{\partial x_j} \right]^2 V(x_j) \quad (2.9)$$

$$V(y | x_j) \approx \left[ \frac{\partial f(x_0)}{\partial x_j} \right]^2 V(x_j) / V(y) \quad (2.10)$$

An ordering of  $x_j$  on the basis of the size of fractional contribution  $V(y|x_j)$  provides a ranking of variable importance on the basis of how much of the variance of  $y$  can be accounted by each element of  $x$ .

The primary drawback of the differential analysis is that is inherently local sensitivity analysis. Moreover, the quality of the results is limited by the quality of the underlying Taylor series approximation (2.6). In particular, if  $y$  is a nonlinear function of the elements of  $x$ , then the first-order Taylor series approximation in (2.6) may be a provide a poor representation of the of the relationships between  $y$  and the elements of  $x$ .

#### 2.4.2. Global sensitivity analysis

The variance  $V(y)$  associate with the model  $y = f(x)$  is given by (2.11). The analysis for global sensitivity analysis is based on the decomposition of  $V(y)$  into components due to individual variables and interactions between individual variables. Specifically,  $V(y)$  can be decomposed into the form given by (2.12) under the assumption that the individual elements of  $x_j$  are independent.

$$V(y) = \int_x [f(x) - E(y)]^2 d(x) \quad (2.11)$$

$$V(y) = \sum_{1 \leq j \leq k} V_j + \sum_{1 \leq j < i \leq k} V_{ji} + \dots + V_{1,2,\dots,k} \quad (2.12)$$

In (2.12)  $V_j$  is the part of  $V(y)$  due solely to  $x_j$ ,  $V_{ji}$  is the part of  $V(y)$  due to the interaction of  $x_j$  and  $x_i$ , and so on upto  $V_{1,2,\dots,k}$ , which is part of  $V(y)$  due to interaction of  $x_1, x_2, \dots, x_k$ . The various sensitivity measures main effect ( $S_j$ ), second order effect ( $S_{ji}$ ) and total effect ( $S_{.j}$ ) are given by (2.13), (2.14) and (2.15) respectively.

$$S_j = V_j / V(y) \quad (2.13)$$

$$S_{ji} = V_{ji} / V(y) \quad (2.14)$$

$$S_{-j} = \left( V_j + \sum_{\substack{1 \leq i \leq k \\ i \neq j}} V_{ji} + \dots + V_{1,2,\dots,k} \right) / V(y) \quad (2.15)$$

Related to the methods for GSA is the concept of analysis of variance (ANOVA) in classical Design of Experiments (DOE) that identifies the factor effects through statistical analysis of computer experiments. Since ANOVA employs the statistical representation of model parameters, the same concept can be used to study the behavior of a model with probabilistic inputs. However, due to the computational complexity, the standard ANOVA often only provides linear effects and second-order interaction effects of variables, but seldom evaluates the nonlinear effect and the total effect (including linear, nonlinear main effects and interaction effects) of an input variable, information that is critical for understanding the true model behavior and ranking variable importance. To extend the traditional ANOVA to GSA, a number of variance-based methods have been developed, including the Fourier Amplitude Sensitivity Test (FAST) (Saltelli, Tarantola et al. 1999), correlation ratio (McKay, Morrison et al. 1999), various importance measures, Sobol's total effect indices, etc. Similar to the concept as used in ANOVA, many of these methods decompose the total variance of an output to items contributed by various sources of input variations, and then derive sensitivity indices as the ratios of a partial variance contributed by an effect of interest over the total variance of the output.

**Table 2.1** Comparison of various GSA techniques based on the computational load

Method	# of runs “Main Effects”	# of runs “Total Effects”	# of runs “Main + Total Effects”	# of runs “Main + Total + 2 & k-2 Effects”	# of runs “All Effects”
SOBOL	$n(k+1)$	$n(k+1)$	$n(2k+2)$	--	$n2^k$
Extended SOBOL	$n(k+1)$	$n(k+1)$	$n(k+2)$	Double* $n(2k+2)$	--
FAST	$n$	--	--	--	--
Extended Fast	$nk$	$nk$	$nk$	--	--

\*Here double means, that ‘Main Effects’ are measured twice.

k: # of model parameters

n: Sample size used to calculate individual effect

Global sensitivity indices for rather complex mathematical models can be efficiently computed by Monte Carlo (or quasi-Monte Carlo) methods. These indices are used for estimating the influence of individual variables or groups of variables on the model output. Among the various proposed methodologies, global sensitivity indices can be most efficiently and effectively calculated by using the methodology proposed by I. M. Sobol (Sobol 2001). It is important to understand here, that the Sobol technique performs better than the FAST techniques especially when uncertainty contribution is mainly due to the interaction among the parameters and not due to their individual effects. Table 2.1, gives a detailed comparison of the various FAST and SOBOL sensitivity methods. GSA has the following advantages:

- Extensive sampling from the ranges of the uncertain variables

- Uncertainty results that are obtained without the use of surrogate models (e.g. Taylor series in differential analysis)
- Extensive modifications of, or manipulations with the original models are not required.
- The extensive sampling from the individual variables facilitates the identification of non-linearity

For more detailed information about GSA along with applications one is referred to the following: (Sobol and Kucherenko), (Homma and Saltelli 1996), (Mara), (Tarantola, Gatelli et al. 2006), (Hofer, Kloos et al. 2002), (Helton, Johnson et al. 2006), (Helton and Davis 2003), (D. 1997), (Saltelli 2002), (Krzykacz-Hausmann 2006) and (Saltelli and Tarantola 2002). For comprehensive review about the various sensitivity analysis methods one is referred to (Christopher Frey and Patil 2002).

### **2.4.3 GSA with correlated factors**

All the approaches considered in the last section deal with the calculation of the GSA when the underlying factors are uncorrelated. But many times in real applications the underlying factors are correlated and it is important to understand how one can handle these situations when evaluating the uncertainty contributions of different factors. Global sensitivity analysis problem for correlated factor distributions has been addressed in literature (McKay 1995), (Saltelli and Tarantola 2002), (Jacques, Lavergne et al. 2006) and (Xu and Gertner 2007). The generic idea is to follow the same approach for unconditional GSA but introduce correlation between the parameters by re-ordering the samples from the factor distributions by following the ordering scheme introduced in

(Iman and Conover 1982). Moreover, the measure of uncertainty contribution for each factor is considered the same as for the traditional GSA approach, i.e.  $V(E(Y|X_j))$  (Saltelli and Tarantola 2002).

## 2.5. Expected value of information (EVOI)

Suppose one wishes to estimate the value of the parameter  $\theta \in \Theta$  where  $\Theta$  is the real line or a convex subset of it. Current information about the value of  $\theta$  is summarized by the prior density  $f(\theta)$ . An experiment is available that will estimate  $\theta$  subject to measurement error. The outcome of the experiment is represented by a random variable  $x \in X$ , with known distribution  $g(x|\theta)$ . Once the experimental outcome  $x'$  is observed, one can derive the posterior density function  $p(\theta|x')$  using Bayes' rule as shown in (2.16). The predictive density of  $x$  is given by (2.17).

$$p(\theta|x') = \frac{f(\theta)g(x'|\theta)}{\int_{\theta \in \Theta} f(\theta)g(x|\theta)d\theta} \quad (2.16)$$

$$h(x) = \int_{\theta \in \Theta} f(\theta)g(x|\theta)d\theta \quad (2.17)$$

The expected value of information depends on the set of alternative decisions that are available and on how the payoff depends on the decision and the uncertain parameters. Let  $u(d,u)$  denote the utility or payoff that results from choosing decision  $d$  when there is a single uncertain parameter  $\theta$ . Let  $d_{prior}^*$  and  $d_{post}^*$  denote the decision that maximizes the expected payoff when information about  $\theta$  is given by the distribution  $f(\theta)$  and  $p(\theta|x)$  respectively. The expected value of information provided by the experiment is given by (2.18).

$$EVOI = \int_{x \in X} \left[ \int_{\theta \in \Theta} u(d_{post}^*, \theta) p(\theta | x) d\theta \right] h(x) dx - \int_{\theta \in \Theta} u(d_{prior}^*, \theta) f(\theta) d\theta \quad (2.18)$$

In words, the expected value of information is the difference between the expected payoff if one observes  $x$  and then selects the optimal decision for the posterior distribution  $p(\theta | x)$ , and the expected payoff if the optimal decision given the prior information  $f(\theta)$  is selected.

## **CHAPTER III**

### **EXPERT OPINION ELICITATION**

The key challenge in the evaluation of R&D alternatives for new product/process development is technical uncertainty. Technical uncertainty exists because either there is a complete lack of experimental data or some limited experimental data exists but is not sufficient to resolve alternatives. A systematic reduction in uncertainty through the application of R&D resources requires that the initial state of knowledge be quantified. The qualitative knowledge of experts, which is often the main source of initial knowledge for the various R&D alternatives, is one source.

In this chapter we demonstrate how the experts' qualitative knowledge can be quantified and how the quantification of uncertainty can be used to improve R&D decisions. We apply the framework in the context of a real bio-refinery case study. To elicit and aggregate expert opinions existing techniques used in risk and decision analysis are used. A mathematical technique, global sensitivity analysis (GSA), is applied to translate uncertainty into its impact on the outcome of system designs. Hence, GSA provides the decision makers with the ability to estimate the relative importance of various uncertainties, so that the R&D resources can be optimally allocated.

#### **3.1. Introduction**

Given evolving business competitiveness, engineers and scientists involved in research and development have to solve increasingly complex problems more rapidly with limited resources. Significant challenges in the evaluation of R&D alternatives for a

new product/process are the underlying technical and economic uncertainties. Management is trained to quantify the economic uncertainties by using forecasting tools. On the contrary, with regard to the technical uncertainties, researchers may completely lack, or have limited, experimental data, which can make technical uncertainty hard to quantify. An efficient systematic R&D investment strategy depends on ensuring that the important sources of uncertainty are identified and reduced. The performance of the strategy essentially depends on the ability to reduce uncertainty, and without both estimates of the uncertainty and a quantitative framework to represent it, it will be hard to measure and improve performance.


In addition to the experimental data, there exists another source of information. This source is the knowledge of experts working on generating the ideas for the R&D alternatives or the experienced researchers in the field. Since the R&D alternatives or ideas are often based on intuitions or insights of experienced researchers there exists qualitative knowledge/information which can potentially be used. The knowledge of experts is often qualitative in nature, so what is needed is a methodology to translate the qualitative knowledge of these experts into quantitative knowledge that recognizes the inherent uncertainty in their understanding expressed in quantitative terms.

For example, consider an expert having 20 years of research experience in fibre morphology and chemical treatment of wood. If such an expert proposes a new chemical treatment method for wood as an R&D alternative, it would be reasonable to expect that s/he would have some qualitative sense of the effectiveness of the chemical treatment. But this qualitative knowledge is essentially of limited use in developing a systematic R&D investment strategy for evaluating this R&D alternative, unless this knowledge is

quantified. The importance of this qualitative knowledge is well recognized and is extensively used in other engineering fields and its importance has been recently recognized in the chemical engineering domain. For example, Coleman and Block (Coleman and Block 2006) demonstrates the importance of informative priors provided by the experts but does not show how they can be elicited. Even though the importance of experts' qualitative knowledge is recognized, its practical usage has been limited in chemical engineering domain. In this work, we demonstrate how qualitative knowledge of experts can be quantified for real problems by using the existing uncertainty quantification methodologies in the field of risk analysis.

To demonstrate the application of uncertainty quantification methodologies, we consider a bio-refinery case-study. Renewable energy system development is a formidable challenge and among the alternatives, fuels derived from biomass (bio-fuels) are one of the most advanced approaches. For the production of bio-fuels, the concept of bio-refinery (production of bio-fuel and paper at a paper mill) is a prominent one (Larson et.al.), (Anand, Realff et al. 2006), (Frederick Jr., Lien et al. 2008), (Frederick Jr., Lien et al. 2008) and it motivates the selection of the bio-refinery case study.

Product Type	Bio-chemical Route	Thermo-chemical Route	Chemical Treatment Process	Wood Species
<ul style="list-style-type: none"> <li>• Liquid Hydrocarbons</li> <li>• Mix. Alcohol</li> <li>• Ethanol</li> </ul>	<ul style="list-style-type: none"> <li>• Complete hydrolysis of wood</li> <li>• Pre-extraction of hemicellulose</li> </ul>	<ul style="list-style-type: none"> <li>• Low Temperature Gasification</li> <li>• High Temperature Gasification</li> </ul>	<ul style="list-style-type: none"> <li>• Kraft</li> <li>• MSSAQ</li> <li>• Polysulphide</li> </ul>	<ul style="list-style-type: none"> <li>• Hardwood</li> <li>• Softwood</li> </ul>



<ol style="list-style-type: none"> <li>1. Acid based</li> <li>2. Water based</li> <li>3. Others...</li> </ol>
---

**Figure 3.1:** Decision choices to consider when evaluating the concept of bio-refinery

The challenges and opportunities in the evaluation of bio-refinery alternatives are the same (many R&D alternatives, limited or no experimental data, availability of technical experts) as in traditional R&D. For example, Figure 3.1 illustrates many bio-refinery R&D alternatives/choices ranging from the selection of type of bio-fuel, type of wood pre-treatment, type of chemical treatment of pre-treated wood, to the type of wood species to consider. Even within a single pathway, for example pre-extraction of hemicelluloses, one has many process alternatives (acid based, water based or alkali based treatment). Evaluation of all these alternatives/choices/options and further reduction of uncertainty can be both very uneconomical and challenging. Further, the lack of quantification of technical uncertainty makes it difficult to evaluate the economics of the various R&D alternatives, making the selection of alternatives highly subjective.

Quantified technical uncertainty can be used as priors for further design of experiments, if the decision is made in favour of further experimental investigation. This advantage is important as the Bayesian design of experimental and parameter estimation approaches become computationally feasible. Both (Hsu, Stamatis et al. 2009) and (Matthew C. Coleman 2006) demonstrate the importance of such approaches. Though the advantages of quantifying expert knowledge are evident, to the authors knowledge there does not exist any literature in the chemical engineering domain focussed on this topic.

The task of quantifying expert knowledge is not straight forward as evidenced by the comments of Lawrence Phillips in *Discussion on the papers on 'Elicitation'* (1998) “*the process of assessing expert uncertainty deserves careful attention, in my view at least as much as is devoted to the design of experiments*”. In light of the above, we apply tools of ‘Expert Opinion Elicitation’ and ‘Expert Opinion Aggregation’ from the field of

Risk and Decision Analysis along with statistical tools like copula's, to quantify uncertainty. Finally, global sensitivity analysis (GSA) is applied to develop a systematic strategy to reduce uncertainty.

The rest of the chapter is structured as follows: Section 3.2 provides background information about the expert opinion elicitation method. Section 3.3 introduces the biorefinery case study and Section 3.4 demonstrates the implementation of the various methods for the case study. Results of the implementation of the methods are given in Section 3.5 and Section 3.6 concludes the chapter.

### **3.2 Background (Expert opinion elicitation)**

Elicited experts opinions have been used in complex and controversial situations with significant uncertainty, requiring decision making under risk. Expert opinion has been used extensively in a variety of sectors, such as nuclear, aerospace, military intelligence, occupational health and banking. In a broad sense, the elicitation methods can be classified as indirect methods, direct methods and parametric elicitation. There are some pitfalls (See section 2.1 for more information) related to the above mentioned methods and some heuristics exists. In order to reduce and avoid the risk of above pitfalls (Kadane and Wolfson 1998), recommends a strategy based on predictive questions. Their strategy considers the conjugate prior structure for the model parameters:

$$y | X, \beta, \sigma^2 \sim N(X^T \beta, \sigma^2) \quad (3.1)$$

$$\beta | \sigma^2 \sim N(b, \sigma^2 R^{-1}) \quad (3.2)$$

$$1/\sigma^2 \sim \chi_\delta^2 / \omega\delta \quad (3.3)$$

where,  $y$  is the model output,  $X$  is the vector for the operating conditions,  $N$  symbolizes a normal distribution,  $\chi_\delta^2$  is a chi-square distribution with  $\delta$  degree of freedom,  $\beta$  is a vector of the mean estimates of the model parameters, and the rest  $(b, R, \omega, \delta)$  are the hyper-parameters. The main steps of the elicitation procedure are as follows:

**Step 0:** Define the range for the operating conditions

**Step 1:** Create or select a design matrix for operating conditions

**Step 2:** Given the operating conditions, the expert is inquired about the most probable value for the output values at each operating condition.

**Step 3:** Next, the expert is queried about his/her perception of the 75<sup>th</sup> and 90<sup>th</sup> percentiles (i.e. the value of the output below which 75% and 90% of the time the output is observed) for the same operating conditions.

**Step 4:** The least square estimate of the model parameters along with residuals are estimated and the expert is given the opportunity to review his/her opinions.

**Step 5:** Next, hypothetical experimental realizations are provided to the expert about his/her initial estimates of the output. And they are asked to revise their opinions in the light of the new hypothetical experimental data. This helps in capturing the confidence of the expert in their initial opinions and also quantifies their belief about external noise.

**Step 6:** Based on the experts revised opinions, the rest of the hyper-parameters are calculated

The overall procedure has two parts: First part (i.e. step 0 to step 4 of the above procedure) consists of calculating the mean and variance properties of the model output

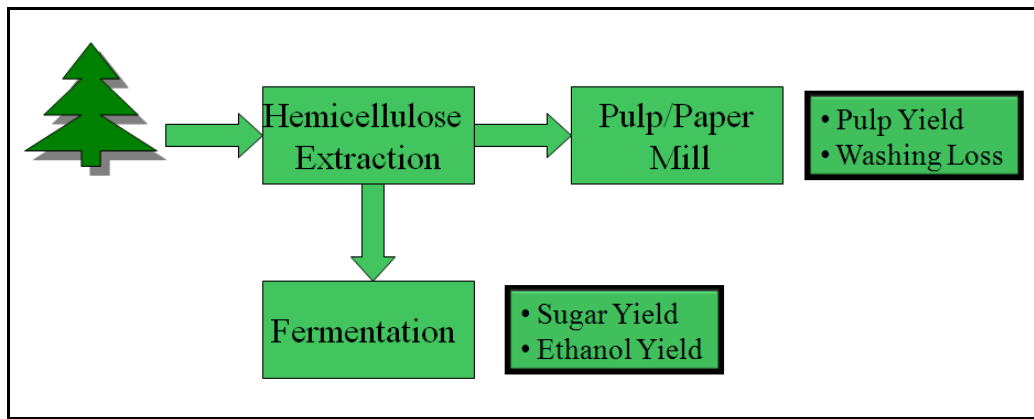
Y. The second part (i.e. step 5 and 6) consists of capturing the expert's beliefs and confidence about the elicited opinions and the external noise.

### **3.3. Case study (Hemicellulose pre-extraction in a Kraft mill)**

The idea we explore in this case study is that experts can provide useful predictions for process information that is related to their underlying domain of expertise. For example, consider an expert having experience/knowledge about the chemical treatment of wood and wood morphology. If this expert is provided with experimental results about a new chemical treatment for a wood species 'A' and queried about his beliefs about the wood species 'B', it is very likely that the expert would be able to provide some sensible qualitative information. Though this qualitative knowledge of the expert is useful in postulating the wood species 'B' as a potential R&D alternative, this knowledge is of limited use in systematically evaluating, or devising an efficient R&D investment strategy for this new R&D alternative, unless and until this knowledge of the expert is made quantitative.

We consider one of the R&D alternative case studies (presented in Figure 3.1 in section 1), where hemicelluloses pre-extraction (using hot water as a pre-extraction solvent) stage is introduced in a softwood based Kraft mill. The alternative is shown in Figure 3.2, where softwood wood is first pre-treated with hot water to extract hemicelluloses and extracted hemicelluloses are sent for fermentation to produce ethanol. The remaining wood material is sent to the Kraft mill for the production of paper following Kraft pulping method. There are several uncertainties such as pulp yield, washing loss, sugar yield in pre-extraction and fermentation (ethanol) yield, when

evaluating this alternative. Moreover, for these uncertainties no or very limited experimental data is available. To evaluate the hot water based hemicellulose pre-extraction for softwood, a modified version of the BioRefinOpt model is used, which has been previously employed in (Anand, Realff et al. 2006), (Frederick Jr., Lien et al. 2008) and (Frederick Jr., Lien et al. 2008).



**Figure 3.2:** Block diagram for hemicelluloses pre-extraction and pulp production along with key uncertainties

The motivation for the selection of the case study is based on the fact that considerable experimental data is available for sugar yield for a hot water based pre-extraction process for hardwood (a wood species). Based on this information the researchers/scientists have suggested investigating another wood species (Softwood) as a potential R&D alternative. If the expert is queried about predicting sugar yield (for softwood) at certain operating conditions, they can provide some information on what the yield values will be, given the literature information on the experimental data for hardwood and wood morphology information for the two wood species.

**Table 3.1** List of technical uncertainties and economical uncertainties along with their grouping structure

	<b>Factors</b>	<b>Units</b>	<b>Uncertainty</b>	<b>Groups</b>
Epistemic Uncertainty	Time for Pre-extraction	Hrs	U(1,3)	1
	Temperature for Pre-extraction	°C	U(120,170)	
	Arabinose Yield	%	U(50,80)	
	Galactose Yield	%	U(5,15)	
	Glucose Yield	%	U(2,10)	
	Xylose Yield	%	U(10,25)	
	Mannose Yield	%	U(10,20)	
	Effective Alkali	Wt-% OD Wood	U(14,18)	2
	Active Alkali	Wt-% OD Wood	U(16.8,20.8)	
	Unbleached Yield	%	± 2	3
	Washing Loss	lb Na <sub>2</sub> SO <sub>4</sub> /ODTUP	U(17,23)	
	Arabinose Yield	%	U(80,85)	4
	Galactose Yield	%	U(87,92)	
	Glucose Yield	%	U(87,92)	
	Xylose Yield	%	U(80,85)	
Mannose Yield	%	U(87,92)		
Aleatory Uncertainty	Wood Moisture	%	± 10	5
	Wood cost	%	± 5	
	Pulp Net Value	%	± 5	
	Pulping Chemical Cost	%	± 5	
	Bleaching Chemical Cost	%	± 5	
	Exportable Power value	%	± 5	
	Lime Kiln Fuel Cost	%	± 5	
	Fixed Cost	%	± 5	
	Annual capital cost for ethanol plant	%	± 5	
	Annual cost of 2 <sup>nd</sup> boiler & turbine	%	± 5	
	Annual cost of other pulp mill capital	%	± 5	
	Annual cost of chemicals for ethanol plant	%	± 5	
	Annual fixed operating cost for ethanol plant	%	± 5	
	Price of ethanol	\$/gal	N(2.04,0.06)	

### 3.4. Implementation description

As a first step, both the technical and economical uncertainties are elicited using the direct method and the results are presented in Table 3.1. In table 3.1 U[*a*,*b*] represents a uniform distribution between *a* and *b* and the representation ± *c* means the range of

uncertainty around the parameter is of  $c$  units. Many of these factors have some underlying formula, which is not accurate and  $\pm c$  signifies that the value of the parameter can equally lie  $c$  units below/above the value given by the formula.

### 3.4.1. Elicitation procedure

In order to perform the expert opinion elicitation, two experts with combined thirty year of research experience in the field of wood morphology, chemical treatment of wood and pre-extraction of wood were selected, to provide information on the pre-extraction of hemicellulose.

Based on the initial discussion with the experts and in light of the existing information about the wood composition and the pre-extraction experimental data for the hardwood species (which also a similar linear model for the different sugars) the following linear model for the pre-extraction yield of different sugars was considered:

$$Y_i = \theta_0^i + \theta_1^i \times \log(t) + \theta_2^i \times T \quad (3.4)$$

where, ' $t$ ' is the pre-extraction time (min), ' $T$ ' is temperature ( $^{\circ}\text{C}$ ) and  $\theta_0$ ,  $\theta_1$  and  $\theta_2$  are the uncertain parameters. The vector ' $X$ ' for the operating conditions, as used in equation (3.1) is  $[1 \quad \log(t) \quad T]^T$ . Here index ' $i$ ' represents different sugar units ( $i = 1,2,3,4$  and  $5$  represent arabinose, galactose, glucose, xylose and mannose respectively).

To quantify the uncertainty in the model parameters of (3.4), the methodology presented by (Wolfson 1995) is considered (See Section 3.2). To elicit the experts opinions a deployable VBA (visual basic for applications) macro based excel model was developed, which experts can use with limited supervision (See Appendix C, for further details about the elicitation procedure).

Based on the above methodology one can elicit the parameter uncertainty in the yield models for the five sugar units. But it is also important to account for the correlation between the different distributions for the pre-extraction yield of the individual sugars. To account for this correlation we use normal copulas to form the joint distribution, combining individual t-distributions corresponding to each sugar unit. To perform this elicitation we employ the predictive elicitation method in (Clemen and Reilly 1999). See appendix D, for further details about the elicitation procedure for the correlation structure.

Once the expert's opinions are elicited, one needs to aggregate their opinions. Given the complexity of the problem and the recent literature (Clemen 1989; Soll and Larrick 2009) we use the approach of linear opinion pool with equal weight, i.e. we average the yield values based on the elicited models/parameter uncertainty from the two experts, to aggregate their opinions.

### **3.4.2. Global sensitivity analysis**

It is also important to note that the R&D alternative consists of many technical uncertainties as shown in Table 3.1. Calculation of GSI for each and every uncertainty factor would be both computationally expensive and would not provide much information. Hence the technical uncertainties are grouped together to make sense out of them. Table 3.1 shows assignment of the various technical uncertainties into different groups. Groups 1,2,3,4 and 5 represent pre-extraction yield, digester yield, washing loss, fermentation yield and economic uncertainties respectively.

### 3.5. Results

#### 3.5.1. Elicited marginal distributions

The quantification of the technical uncertainty in terms of the mean and hyper-parameters, as illustrated in (3.1) - (3.4), is evaluated and the result for the two experts are given in the Table 3.2 and Table 3.3. It is clearly observed that the two experts have different opinions about the yields of the various sugar units. Figure 3.3 and Figure 3.4 further compare the opinions of the two experts at two different sets of operating conditions. As observed from Figure 3.3 and Figure 3.4, the prediction of the experts overlaps significantly for the glucose yield but differ significantly for the arabinose and xylose yield.

**Table 3.2:** Elicited model parameter estimates for the Expert 1

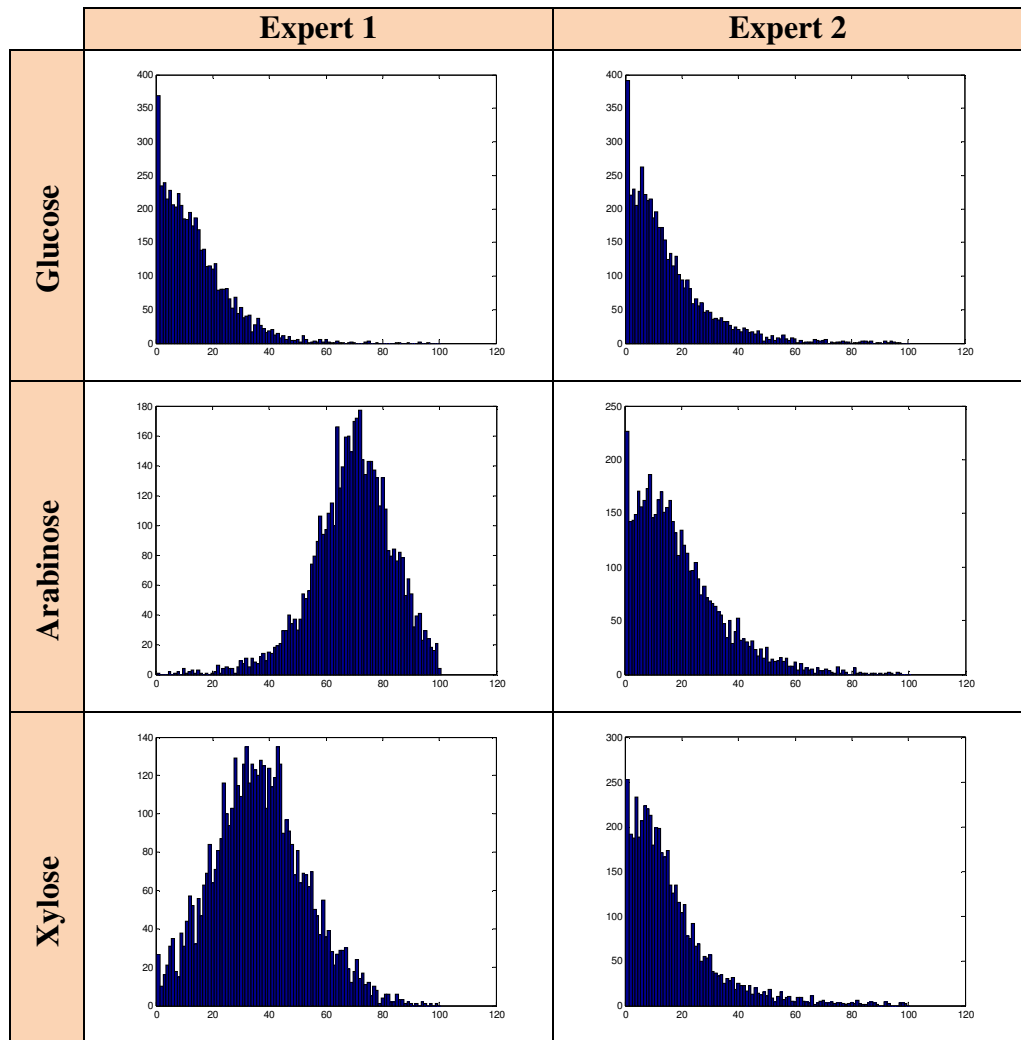
Sugar Units	$\delta$	$\omega$	$\beta$	$R^{-1}$
Arabinose	4	0.051	$\begin{bmatrix} -84 \\ 24 \\ 31 \end{bmatrix}$	$10^3 * \begin{bmatrix} 97.0 & -14.8 & -6.4 \\ -14.8 & 2.6 & -0.2 \\ -6.4 & -0.2 & 4.6 \end{bmatrix}$
Galactose	5	0.051	$\begin{bmatrix} -67 \\ 20 \\ 21 \end{bmatrix}$	$10^3 * \begin{bmatrix} 97.0 & -14.8 & -6.4 \\ -14.8 & 2.6 & -0.2 \\ -6.4 & -0.2 & 4.6 \end{bmatrix}$
Glucose	7	0.009	$\begin{bmatrix} -6 \\ 1 \\ 2 \end{bmatrix}$	$10^4 * \begin{bmatrix} 83.4 & -12.7 & -5.5 \\ -12.7 & 2.2 & -0.2 \\ -5.5 & -0.2 & 3.9 \end{bmatrix}$
Xylose	8	0.0001	$\begin{bmatrix} -65 \\ 16 \\ 18 \end{bmatrix}$	$10^5 * \begin{bmatrix} 825.7 & -125.4 & -53.9 \\ -125.4 & 21.9 & -1.8 \\ -53.9 & -1.8 & 38.9 \end{bmatrix}$
Mannose	4	0.0001	$\begin{bmatrix} -40 \\ 10 \\ 13 \end{bmatrix}$	$10^5 * \begin{bmatrix} 825.7 & -125.4 & -53.9 \\ -125.4 & 21.9 & -1.8 \\ -53.9 & -1.8 & 38.9 \end{bmatrix}$

### 3.5.2. Elicited correlation structures

The correlation structure between the various sugar yields is captured using a Gaussian copula. Since five sugars units are extracted on the pre-extraction process, the dimension of the correlation matrix is (5 x 5), where the indexes represent arabinose, galactose, glucose, xylose and mannose respectively. The elicited correlation matrices for the two experts are shown in Table 3.4. Expert 1 does not perceive any systematic relation between the yields of arabinose to yield of galactose, glucose and mannose, which is signified by the zero correlation. But expert 1 percieves a strong relationship between yields of galactose and mannose, which can be attributed to the presence of glucomannan (composed of galactose and mannose) in the wood.

**Table 3.3:** Elicited model parameter estimates for the Expert 2

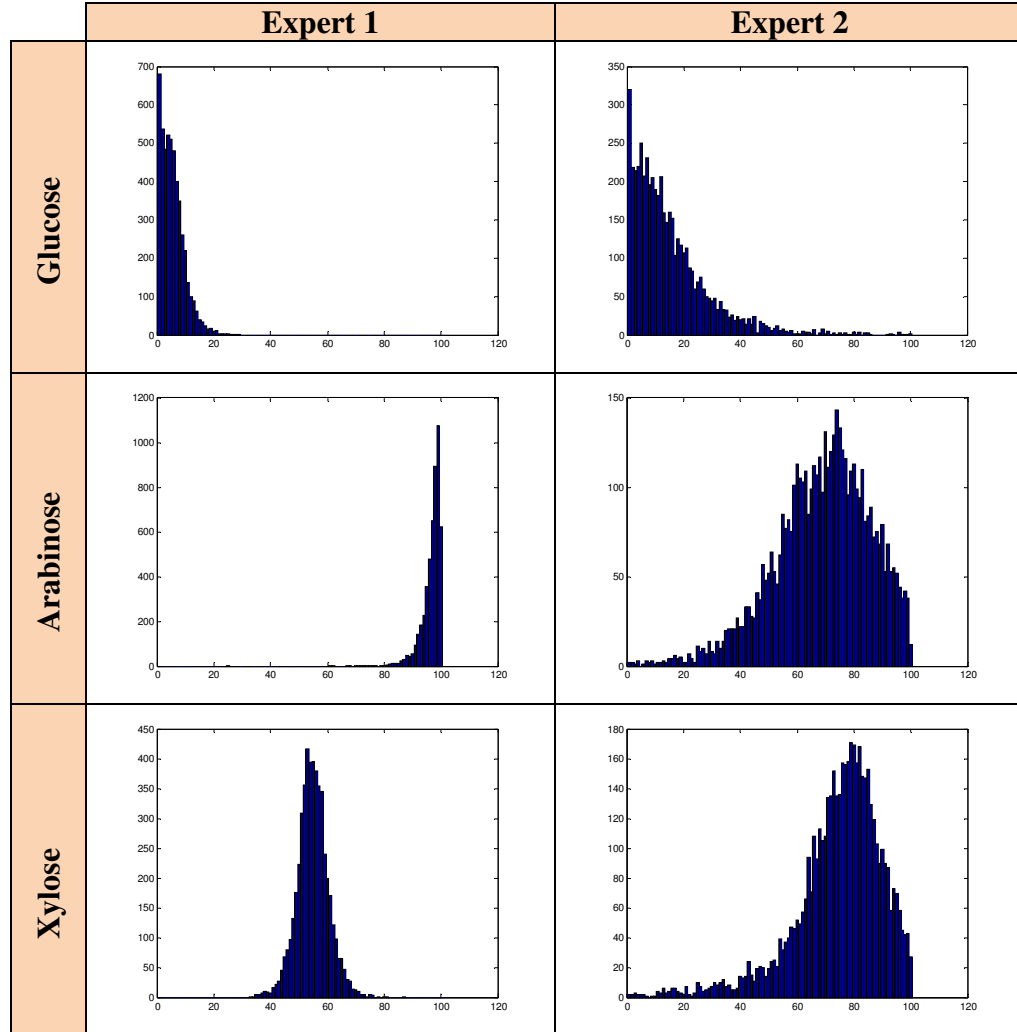
Sugar Units	$\delta$	$\omega$	$\beta$	$R^{-1}$
Arabinose	6	0.0006	$\begin{bmatrix} -192 \\ 14 \\ 109 \end{bmatrix}$	$10^5 * \begin{bmatrix} 10.8 & -15.8 & -13.9 \\ -15.8 & 2.5 & 1.8 \\ -13.9 & 1.8 & 2.5 \end{bmatrix}$
Galactose	5	0.0006	$\begin{bmatrix} -201 \\ 14 \\ 113 \end{bmatrix}$	$10^5 * \begin{bmatrix} 10.8 & -15.8 & -13.9 \\ -15.8 & 2.5 & 1.8 \\ -13.9 & 1.8 & 2.5 \end{bmatrix}$
Glucose	3	0.0001	$\begin{bmatrix} -9 \\ 1 \\ 4 \end{bmatrix}$	$10^5 * \begin{bmatrix} 394.8 & -57.5 & -5.1 \\ -57.5 & 9.2 & 6.6 \\ -5.1 & 6.6 & 8.9 \end{bmatrix}$
Xylose	2	0.49	$\begin{bmatrix} -216 \\ 15 \\ 122 \end{bmatrix}$	$10^2 * \begin{bmatrix} 64.7 & -9.4 & -8.4 \\ -9.4 & 1.5 & 1.1 \\ -8.4 & 1.1 & 1.2 \end{bmatrix}$
Mannose	2	0.49	$\begin{bmatrix} -112 \\ 8 \\ 65 \end{bmatrix}$	$10^2 * \begin{bmatrix} 64.7 & -9.4 & -8.4 \\ -9.4 & 1.5 & 1.1 \\ -8.4 & 1.1 & 1.2 \end{bmatrix}$



**Figure 3.3:** Predictive distribution of yields of various sugar units at 150 min and 120°C for Loblolly Pine

**Table 3.4:** Correlation matrices elicited from the two experts

Correlation matrix for Expert 1					Correlation matrix for Expert 2				
1	0	0	0.823	0	1	0.9326	0.0402	0.6234	0.4253
0	1	0.3439	0	0.9451	0.9326	1	0.1488	0.5743	0.3720
0	0.3439	1	0	0.8326	0.0402	0.1488	1	0.8685	0.7363
0.823	0	0	1	0	0.6234	0.5743	0.8685	1	0.7944
0	0.9451	0.8326	0	1	0.4253	0.3720	0.7363	0.7944	1



**Figure 3.4:** Predictive distribution of yields of various sugar units at 300 min and 170°C for Loblolly Pine

### 3.5.3. Global sensitivity analysis

The ideal approach to quantify technical uncertainty for the evaluation of the key uncertainty contributor, in the scenarios of complete lack of experimental data, is to elicit expert knowledge in terms of uncertainty in model parameter value (as done in Section 3.5.2). For the evaluation of the key uncertainty contributor, it's important to consider

both the technical and economic uncertainty. In order to demonstrate the impact of using an improper method to quantify the uncertainty we consider three cases. Case 1 considers uncertainty defined as range of values (i.e. a min and max value defined for the uncertain variable) and does not consider the economic uncertainty. Case 2, considers uncertainty defined as range of values but additionally considers the economic uncertainty. Case 3 considers the technical uncertainty in terms of model parameter uncertainty along with the economic uncertainty. Case 3 is the correct approach for the quantification of uncertainty, as predictive elicitation is considered as the better approach as discussed in Chapter 2. As demonstrated in (Herath and Kumar 2007) it's important to account for the correlation between various uncertainties, hence we consider an additional case (case 4) which is similar to case 3 but we also account for the correlation between the sugar yields.

#### 3.5.3.1. Case 1 (Technical uncertainties as range)

Quantification of uncertainty as a range of values, i.e. a uniform distribution with lower and upper limit, is easier than the elicitation of the detailed distribution (as discussed in section 3.2). The results of quantification of uncertainty as range of values are listed in Table 3.1. The results for the GSI for the technical uncertainties (quantified as range of values) are shown in Table 3.5. These results based on only the technical uncertainties show that pre-extraction yield and the digester yield are the main uncertainty contributing factors. Moreover, the pre-extraction yield is the main uncertainty contributor.

**Table 3.5:** GSA results based on technical uncertainties defined as a range of values

	Pre-extraction Yield	Digester Yield	Washing	Ethanol Yield
Main Effect	0.54	0.38	0.02	0.02
Total Effect	0.58	0.40	0.01	0.00

3.5.3.2. Case 2 (Technical uncertainties as range, along with economical uncertainties)

In case 1, we only considered the technical uncertainties (i.e. epistemic uncertainties, which can be resolved by further experimentation) but there also exist economic uncertainties (i.e. aleatory uncertainties, which cannot be reduced by further experimentation). It is important to account for both epistemic and aleatory uncertainties when we evaluate the GSI, since it is possible that some factors which might not be very significant when only accounting for epistemic uncertainty may become very important when accounting for both the epistemic and aleatory uncertainties. Table 3.6 shows the GSA results when one accounts for both the epistemic and aleatory uncertainty and clearly indicate that the economic uncertainty have larger effect on the digester yield.

**Table 3.6:** GSA results based on both technical and economical uncertainties

	Pre-extraction Yield	Digester Yield	Washing	Ethanol Yield
Main Effect	0.46	0.55	0.00	0.00

3.5.3.3. Case 3 (Quantified technical uncertainty by experts along with economical uncertainty)

Experts demonstrated limited confidence on the knowledge about the affect of pre-extraction on the digester yield. Moreover the limited pool of experts we had aces to, expressed some confidence on their knowledge about the pre-extraction yield. So, using elicited expert’s opinions about the pre-extraction yield are used and GSA (still accounting for the economic uncertainty) is performed. In this case Pre-extraction yield turns out to be the most uncertainty contributing factor followed by Digester yield (see Table 3.7).

**Table 3.7:** GSA results based on expert opinions and economic uncertainty

	Pre-extraction Yield	Digester Yield	Washing	Ethanol Yield
Main Effect	0.56	0.38	0.00	0.00

3.5.3.4. Case 4 (Quantified technical uncertainty and sugar yield correlations by experts along with economical uncertainty)

**Table 3.8:** GSA results based on expert opinions, correlation structure and economic uncertainty

	Pre-extraction Yield	Digester Yield	Washing	Ethanol Yield
Main Effect	0.58	0.35	0.00	0.00

The GSA results based on the expert opinion and the correlation structure between the sugar yields further highlights the uncertainty contribution of the pre-

extraction yield (see Table 3.8). Further, the overall impact of the digester yield uncertainty is reduced, reflecting that pre-extraction yield is the most important factor.

### **3.6. Conclusions**

In this chapter, to demonstrate the importance of quantifying uncertainty in the expert's knowledge, a real bio-fuel case study is considered. Since experts' qualitative knowledge is used to generate ideas for the R&D alternatives, it is important to quantify this knowledge for developing a systematic R&D investment approach. To demonstrate the importance of quantification of expert knowledge, global sensitivity analysis (GSA) is used to evaluate the key uncertainty contributors.

The Case 1 considers quantification of experts' knowledge by direct elicitation method but ignores the economic uncertainty knowledge R&D managers can provide. Case 2, uses both the quantified experts knowledge (based on the direct elicitation method) and the economic uncertainty knowledge of the R&D managers. The results based on Case 1 and Case 2 indicate the importance of accounting for both technical and economic uncertainty in developing R&D investment strategy. Case 1 signifies that pre-extraction yield is the main uncertainty (i.e. key factor) while case 2 signifies digester yield is the main uncertainty. Though the global sensitivity index for the two key factors is the same magnitude order, in a situation of limited R&D resources this differentiation of key factor would make a difference. Moreover, the comparison of the case study 1 and 2 clearly indicates that use of both the technical knowledge of the experts and the economic uncertainty knowledge of the R&D managers is essential.

As discussed in Section 2.1, there are certain pitfalls related to the direct elicitation method (used for case 1 and 2) and it fails to accurately quantify the experts'

knowledge. The predictive elicitation methodology by (Wolfson 1995), which is regarded to counter all the pitfalls is used to elicit experts knowledge for case study 3. Case 2 suggests that digester yield is the main uncertainty contributor, whereas case 3 indicates that pre-extraction yield is the major uncertainty contributor. This differentiation is mainly because of the methodology used for quantification of experts' knowledge, thus methodological choices can influence the outcome.

As suggested in (Herath and Kumar 2007), the importance of accounting correlations between various uncertainties is important. Hence the correlation between the various sugar yields is also elicited using predictive elicitation method. The GSA results when accounting for the technical uncertainties and the correlation between the sugar yields, i.e. case 4, further highlights for the biorefinery case study that pre-extraction yield in the key uncertainty contrary to digester yield.

The case study considered in this chapter has only four groups of technical uncertainties, and use of inappropriate method to quantify expert knowledge or missing on the using both the experts knowledge and R&D managers knowledge does make a difference in the identification of key uncertainties. The method used for the quantification of uncertainty makes difference in identification of the pre-extraction yield or digester yield as the main uncertainty, but in every case both of them are the top two uncertainties. This result is specific to the case study under consideration but for other case studies with large groups of uncertainties the use of inappropriate method for quantification of experts knowledge, missing on the R&D managers knowledge on economic uncertainty and failing to account for correlation can make a significant difference.

Once the key group uncertainties are identified the next step is to reduce those uncertainties. Chapter 5 discusses how decision oriented design of experiments are better for decision making compared to the traditional design of experiment approaches which focus on reduction in uncertainty in the model parameters.

## CHAPTER IV

### CONDITIONAL GLOBAL SENSITIVITY ANALYSIS

Decisions during the early stages of R&D are made under substantial uncertainty. Evaluation of R&D alternatives under uncertainty generally does not provide a clear choice that is best under all possible scenarios. In such cases, the decision maker may either make the selection based on a user defined utility function, or conduct more experiments to further reduce the key uncertainty in the most promising alternatives, so that a better decision can be reached. The latter option has more intrinsic appeal, but conducting experiments to reduce uncertainty can be both time consuming and expensive. Hence, it is important to focus on the key uncertainty contributors from a decision maker's perspective. Global sensitivity analysis (*GSA*) is a tool that can be used to determine key uncertainties that contribute the most to the variance of the bottom-line objective. It is often the case, however, that *GSA* is not able to distinguish between the uncertainties. To supplement *GSA*, in this chapter we propose a new tool called conditional – global sensitivity analysis ( $cGSA^{up} / cGSA^{down}$ ), that further considers the decision-makers risk preference. The conditional sensitivity measures quantify the contributions of different individual uncertainty factors to the upper and lower half of the objective function. The lower or upper half of the objective function is defined as the part of the distribution below or above the mean of the objective function respectively. It is argued that the use of  $cGSA^{up}$  may appeal to a risk-averse decision maker as it leads to more rejection decisions (and also a lower rate of false acceptance decisions at the

expense of a higher rate of false rejection decisions), whereas the use of  $cGSA^{down}$  leads to more acceptance decisions (and also a lower rate of false rejection decisions at the expense of a higher rate of false acceptance decisions and).

#### 4.1 Introduction

Evaluation of the key uncertainty contributors in the R&D process is an essential step to reduce the cost of the whole process. Global sensitivity analysis ( $GSA$ ) and expected value of information ( $EVOI$ ) are two tools that can be used to estimate the key uncertainty contributors. Global sensitivity analysis considers variance as a measure of risk and the importance of various uncertainties is measured as the fraction of the overall variance contributed by each uncertain factor. On the other hand,  $EVOI$  directly measures the value reduction in uncertainty in each factor brings.

The evaluation of  $GSA$  is significantly simpler than that of  $EVOI$  since the calculation of  $EVOI$  requires more detailed information about the effect of experimentation on the uncertainty. Though, from a decision makers perspective  $EVOI$  provides more useful information compared to  $GSA$ , the practical limitations with the calculation of the  $EVOI$  limits its usefulness. In this work we supplement the traditional  $GSA$  approach with a new tool called *conditional global sensitivity analysis* ( $cGSA$ ), which provides insight into the selection of the key uncertainty when  $GSI$  (global sensitivity index) is unable to do so.

For a R&D investment decision, there are two sides of the problem. First is the R&D investment cost, e.g., the experimentation cost. Second is the return or profits when the R&D project becomes successful. In order to make the overall process more

profitable one can either focus on the reduction in the R&D cost or on maximizing the probability of success of the project. To address the two different strategies we consider two different risk behaviours of the decision maker:

(a). **Decision Delayer / Just A Few Alternatives:** One who wants to maximize the probability of success and is ready to accept a relatively higher R&D investment. If there are few alternatives, one is more focused on maximizing the probability of success. In such cases, one is more concerned with not removing a potentially successful alternative at the cost of higher R&D investment. Hence such a decision maker would prefer an approach that will lead to lower FALSE REJECTION rate, even if it requires that the decision maker has to bear higher FALSE ACCEPTANCE rates.

(b). **Decision Maker / Many Alternatives:** One who wants to minimize the R&D investment and is ready to accept a relative lower probability of success. If there are large numbers of alternatives, one wants to minimize the R&D cost to find a successful alternative. This is a more aggressive approach in terms of selection and the objective is to quickly trim down the options to just a few alternatives. Hence such a decision maker would prefer an approach that will lead to lower FALSE ACCEPTANCE rate, even if it entails that the decision maker has to bear a higher FALSE REJECTION rate.

When *GSA* is not able to distinguish between the uncertainties, *cGSA* (either  $cGSA^{down}$  or  $cGSA^{up}$ ) can be used for selection of the key uncertainty to reduce, depending on the situation and the decision maker's attitude.

The rest of the chapter is structured as follows: Section 4.2 presents the background about *GSA*. Section 4.3 presents the new approach, *cGSA*, along with the

algorithm to calculate  $cGSA$  and discusses the risk behaviours  $cGSA^{up}$  and  $cGSA^{down}$  support Various examples to illustrate the utility of  $cGSA$  are presented in Section 4.4 and Section 4.5 concludes the chapter.

## 4.2 Global sensitivity analysis (GSA)

$GSA$  calculates the relative importance of input variables or factors  $(x_1, x_2, \dots, x_k)$  in determining the value of the output variable  $y$ . Assume a model  $y = f(x_1, x_2, \dots, x_k)$  is composed of independent random variables  $x_1, x_2, \dots, x_k$ . Moreover assume that the probability density functions of  $x_1, x_2, \dots, x_k$  are  $p_1(x_1), p_2(x_2), \dots, p_k(x_k)$ . Then,

$$P(x_1, x_2, \dots, x_k) = \prod_{i=1}^k p_i(x_i) \quad (4.1)$$

The mean and variance of  $y$  can be calculates as:

$$E(y) = \int \dots \int f(x_1, x_2, \dots, x_k) \prod_{i=1}^k p_i(x_i) dx_i \quad (4.2)$$

$$\begin{aligned} V(y) &= \int \dots \int \left( f(x_1, x_2, \dots, x_k) - E(y) \right)^2 \prod_{i=1}^k p_i(x_i) dx_i \\ &= \int \dots \int f^2(x_1, x_2, \dots, x_k) \prod_{i=1}^k p_i(x_i) dx_i - E^2(y) \end{aligned} \quad (4.3)$$

If one of the input factors is  $x_j$  is fixed to a generic value  $\tilde{x}_j$ , the resulting variance of  $y$  will be equal to:

$$\begin{aligned} V(y | x_j = \tilde{x}_j) &= \int \dots \int \left( f(x_1, x_2, \dots, \tilde{x}_j, \dots, x_k) - E(y | x_j = \tilde{x}_j) \right)^2 \prod_{\substack{i=1 \\ j \neq i}}^k p_i(x_i) dx_i \\ &= \int \dots \int \left( f^2(x_1, x_2, \dots, \tilde{x}_j, \dots, x_k) \right) \prod_{\substack{i=1 \\ j \neq i}}^k p_i(x_i) dx_i - E^2(y | x_j = \tilde{x}_j) \end{aligned} \quad (4.4)$$

For sensitivity analysis, the dependence on value  $\tilde{x}_j$  is eliminated by integrating the above equation over the probability density function of value  $\tilde{x}_j$ . This leads to,

$$E\left(V\left(y \mid x_j\right)\right)=\iint \dots \int f^2\left(x_1, x_2, \dots, x_j, \dots, x_k\right) \prod_{\substack{i=1 \\ i \neq j}}^k p_i\left(x_i\right) d x_i - \int E^2\left(y \mid x_j = \tilde{x}_j\right) p_j\left(\tilde{x}_j\right) d \tilde{x}_j \quad (4.5)$$

From above we get,

$$V(y)-E\left(V\left(y \mid x_j\right)\right)=\int E^2\left(y \mid x_j = \tilde{x}_j\right) p_j\left(\tilde{x}_j\right) d \tilde{x}_j - E^2(y) \quad (4.6)$$

The left hand side of (4.6) is equal to  $V\left(E\left(y \mid x_j\right)\right)$ , which is considered as a good measure of the sensitivity of  $y$  with respect to factor  $x_j$ . The first order sensitivity index is defined as:

$$GSI_j = V\left(E\left(y \mid x_j\right)\right) / V(y) \quad (4.7)$$

In a Monte Carlo framework, the exact computation of the above equation is impractical due the need to evaluate the double integral in calculating  $V\left(E\left(y \mid x_j\right)\right)$ . To ease the calculation of the double integral, Ishigami and Homma (1990) suggested the following simplification:

$$\begin{aligned} & \int E^2\left(y \mid x_j = \tilde{x}_j\right) p_j\left(\tilde{x}_j\right) d \tilde{x}_j \\ &= \int \left\{ \iint \dots \int f\left(x_1, x_2, \dots, \tilde{x}_j, \dots, x_k\right) \prod_{\substack{i=1 \\ i \neq j}}^k p_i\left(x_i\right) d x_i \right\}^2 p_j\left(\tilde{x}_j\right) d \tilde{x}_j \\ &= \iint \dots \int f\left(x_1, x_2, \dots, \tilde{x}_j, \dots, x_k\right) f\left(x'_1, x'_2, \dots, \tilde{x}_j, \dots, x'_k\right) \prod_{\substack{i=1 \\ i \neq j}}^k\left(p_i\left(x_i\right) d x_i\right) \prod_{\substack{i=1 \\ i \neq j}}^k\left(p_i\left(x'_i\right) d x'_i\right) p_j\left(\tilde{x}_j\right) d \tilde{x}_j \\ &= \iint \dots \int f\left(x_1, x_2, \dots, x_j, \dots, x_k\right) f\left(x'_1, x'_2, \dots, x_j, \dots, x'_k\right) \prod_{i=1}^k\left(p_i\left(x_i\right) d x_i\right) \end{aligned} \quad (4.8)$$

The creation of artificial primed variables in the above equation makes us realize that the above is the expectation of the function  $F$  of a set of  $(2k-1)$  factors:

$$\begin{aligned} F(x_1, x_2, \dots, x_j, \dots, x_k, x'_1, x'_2, \dots, x'_{j-1}, x'_{j+1}, \dots, x'_k) \\ = f(x_1, x_2, \dots, x_k) f(x'_1, x'_2, \dots, x'_{j-1}, x'_j, x'_{j+1}, \dots, x'_k) \end{aligned} \quad (4.9)$$

The above simplification suggested in (Ishigami and Homma 1990) makes the calculation of the above using a single Monte Carlo loop. (Saltelli, Andres et al. 1993) suggested the following Monte Carlo based procedure for calculation of global sensitivity indices.

Consider the two input sample matrices  $M_1$  and  $M_2$  as follows:

$$M_1 = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \dots & & & \\ x_{n1} & x_{n2} & \dots & x_{nk} \end{pmatrix}, M_2 = \begin{pmatrix} x'_{11} & x'_{12} & \dots & x'_{1k} \\ x'_{21} & x'_{22} & \dots & x'_{2k} \\ \dots & & & \\ x'_{n1} & x'_{n2} & \dots & x'_{nk} \end{pmatrix}$$

where  $n$  is the sample size used for the Monte Carlo estimation. To estimate the sensitivity measure for a generic factor  $x_j$ , using the following equations we need to estimate both  $E(y)$  and  $U_j$ .

$$GSI_j = \frac{V(E(y|x_j))}{V(y)} = \frac{(U_j - E^2(y))}{V(y)} \quad (4.10)$$

$$U_j = \int E^2(y|x_j = \tilde{x}_j) p_j(\tilde{x}_j) d\tilde{x}_j \quad (4.11)$$

$E(y)$  can be calculated based on the values of  $y$  computed on matrices samples either from  $M_1$  or  $M_2$ , whereas  $U_j$  can be calculated from values of  $y$  computed from sample from matrices  $M_1$  and  $N_j$ .

$$N_j = \begin{pmatrix} x'_{11} & x'_{12} & \dots & x_{1j} & \dots & x'_{1k} \\ x'_{21} & x'_{22} & \dots & x_{2j} & \dots & x'_{2k} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ x'_{n1} & x'_{n2} & \dots & x_{nj} & \dots & x'_{nk} \end{pmatrix} \quad (4.12)$$

The approximation for  $U_j$  is as follows:

$$\hat{U}_j = \frac{1}{n-1} \sum_{r=1}^n f(x_{r1}, x_{r2}, \dots, x_{rk}) f(x'_{r1}, x'_{r2}, \dots, x'_{r(j-1)}, x_{rj}, x'_{r(j+1)}, \dots, x'_{rk}) \quad (4.13)$$

The computational cost associated with the calculation of the all first order sensitivity indices is  $n.(k+1)$ , where  $n$  evaluations of  $f$  are needed to calculate  $E(y)$  and  $n$  sets of  $f$  for each first order sensitivity index.

### 4.3 Conditional global sensitivity analysis (*cGSA*)

As explained in Section 4.2, *GSA* provides information about the contribution by individual factors to the overall uncertainty, where uncertainty is measured in terms of variance. But there are problems where *GSA* is unable to distinguish among several uncertain factors in terms of their importance, i.e. two or more factors have equal or nearly equal global sensitivity index (*GSI*). From a decision makers perspective then it is not possible to differentiate between the factors and decide in which factor to reduce uncertainty through experimentation. In order to accommodate such a situation, a new tool called *cGSA* is presented, which may be able to differentiate between the factors having equal *GSI* based on the situation at hand and the decision makers risk preference.

### 4.3.1 Definition

Conditional global sensitivity analysis is the measure of the contribution of variance by individual factors to the conditional objective function. Here conditional distribution refers to the part of the distribution of model output  $y$  above or below its mean  $E(y)$ , for  $cGSA^{up}$  or  $cGSA^{down}$ , respectively. The conditional (upside or downside) global sensitivity index ( $cGSI^{up}$  or  $cGSI^{down}$ ) can be calculated using (4.14) or (4.15) compared to  $GSI$  which is calculated using (4.10).

$$cGSI_j^{up} = \frac{V(E(y|x_j, y > E(y)))}{V(y|y > E(y))} \quad (4.14)$$

$$cGSI_j^{down} = \frac{V(E(y|x_j, y < E(y)))}{V(y|y < E(y))} \quad (4.15)$$

### 4.3.2 Algorithm

Calculation of  $cGSI^{up}/cGSI^{down}$  follows the same approach as  $GSI$  with the difference being that the random samples for the various factors conform to the conditionality constraint, i.e. the factors transformed by the model to the objective function value should lie above/below the mean of the model output  $E(y)$ . So, in essence the problem is how to sample from the distribution of the factors so that the objective function values belong to the respective side of the distribution. This problem can be addressed by developing classification functions, which make sure that the model output will lie on the desired side of the mean of the model output distribution.

It is important to note, that the sampling from the factor distributions introduces correlation between the factors. Global sensitivity analysis problem for correlated factor

distributions has been addressed in the literature (McKay 1995), (Saltelli 2002),(Jacques, Lavergne et al. 2006), (Xu and Gertner 2008). The generic idea is to follow the same approach for unconditional *GSA* but introduce correlation between the parameters by re-ordering the samples from the factor distributions by following the ordering scheme introduced in (Iman and Conover 1982). Moreover, the measure of uncertainty contribution for each factor is considered the same as for the traditional *GSA* approach, i.e.,  $V(E(Y|X_j))$  (Saltelli 2002).

The correlation introduced in *cGSA* cannot be calculated by using the re-ordering scheme of (Iman and Conover 1982), since the conditionality induces a relationship between the input factors that cannot be easily represented by either correlation or rank correlation. Hence in order to maintain the original distribution properties of the factors and account for the natural relationship introduced by the ‘conditionality’, we first sample the factors from their original distribution functions and then accept or reject the sample based on the result of the classification function separating the objective function values below and above the cut-off. (Note: this is very similar to the Acceptance-Rejection algorithm). The importance of using the classification function instead of the model is that the model can be computationally intensive and a high rejection rate can significantly increase the computational load.

Moreover, since the classification function would be an approximation, we would consider an enveloping classification function i.e. a classification function with high priority for acceptance of all possible valid combinations of factor values at the cost of relatively low priority for rejection of invalid combination of factor values. Though this would require additionally checking the validity of the sample point it would make the

*cGSI* calculation more accurate. The complete procedure to calculate the *cGSI* given below assumes that *GSI* has been performed already and the user wants to perform *cGSI* for follow-up analysis:

**Step 1:** Use the generated sample matrices for the main effect calculation to generate the classification function, which segregates the model output to values above or below the mean value of the model output.

**Step 2:** Generate sampling matrix  $M_1$  ( $N \times k$ ), where  $N$  is the number of rows signifying the number of Monte Carlo runs required for convergence and  $k$  is the number of uncertain factors. To generate the matrix  $M_1$ , first generate a  $k$  dimensional vector from the  $k$  factor distributions. Based on the classification function select or reject the sample.

$$M_1 = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \dots & & & \\ x_{n1} & x_{n2} & \dots & x_{nk} \end{pmatrix} \quad (4.16)$$

**Step 3:** Similarly sample the  $N^j$  matrices corresponding to each factor. A different notation  $N^j$  is used here compared to the earlier notation of  $N_j$  in (4.12) as there is difference between the two matrices.  $N_j$  can be generated from  $M_1$  and  $M_2$  as shown in Section 4.2. However, for  $N^j$ , elements of each row would have to be independently generated, since for a given value of  $x_{ij}$  the other elements of the row are not sampled independently. The elements other than  $x_{ij}$  are dependent on the model output to be less than or greater than the mean  $E(y)$  for the calculation of  $cGSI_j^{down}$  or  $cGSI_j^{up}$  respectively.

$$N^j = \begin{pmatrix} x_{11}^j & x_{12}^j & \dots & x_{1j} & \dots & x_{1k}^j \\ x_{21}^j & x_{22}^j & \dots & x_{2j} & \dots & x_{2k}^j \\ \dots & \dots & \dots & \dots & \dots & \dots \\ x_{n1}^j & x_{n2}^j & \dots & x_{nj} & \dots & x_{nk}^j \end{pmatrix} \quad (4.17)$$

**Step 4:** Calculate the model output values with respect to the corresponding input factor values corresponding to each row of the matrices  $M_I$  and  $N_j^j$ 's.

**Step 5:** Calculate the  $cGSI$  based on the following two equations:

$$U_j = \frac{1}{n-1} \sum_{r=1}^n f(x_{r1}, x_{r2}, \dots, x_{rk}) f(x_{r1}^j, x_{r2}^j, \dots, x_{r(j-1)}^j, x_{rj}, x_{r(j+1)}^j, \dots, x_{rk}^j) \quad (4.18)$$

$$cGSI_j = \frac{(U_j - E^2(y))}{V(y)} \quad (4.19)$$

### 4.3.3 Theoretical Interpretation

To understand the theoretical interpretation of the results of reducing uncertainty in the key  $cGSA^{up}$  and  $cGSA^{down}$  uncertainty and its application consider the following model output  $y$  given by (4.20).

$$y = x_1 + x_2 \quad (4.20)$$

$$x_1 = \text{beta}(2,10) \quad (4.21)$$

$$x_2 = \text{beta}(10,2) \quad (4.22)$$

The input uncertainties ( $x_1$  and  $x_2$ ) are given by (4.21) and (4.22). The distributions of  $x_1$  and  $x_2$  are positively and negatively skewed respectively as shown in

figure 4.1. The distribution of model output  $y$  is shown in figure 4.2. Properties of the input uncertainties along with the model output are shown in Table 4.1.

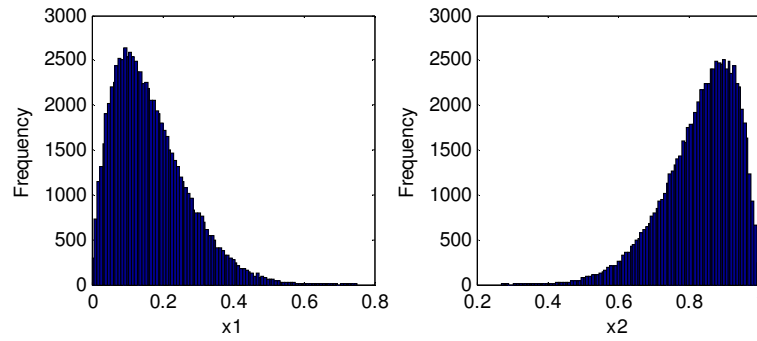
**Table 4.1:** Statistical properties of the input uncertainty and the model output

	<b>Mean</b>	<b>Standard Deviation</b>	<b>Skewness</b>
$x_1$	0.167	0.104	0.92
$x_2$	0.833	0.104	-0.92
$y$	1.0	0.147	0

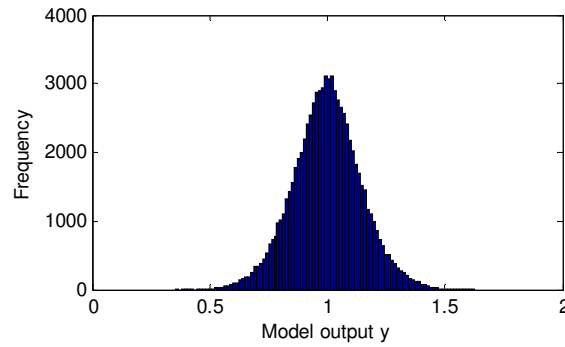
Consider that the true decision criterion (4.23) is based on a *cutoff*, i.e. if the correct value of the model output lie above the *cutoff* the decision maker would keep the R&D alternative and if the model output lie below the *cutoff* the decision maker would reject the R&D alternative. For simplicity, assume the *cutoff* to be at the mean of the model output  $y$  ( $= 1$ ). This means that the correct decision is to accept the technology 50% of the sampled cases and reject it in the other 50% of the cases. Consider the decision criterion under uncertainty (4.24) is driven by just the mean value, i.e. if the posterior mean ( $\mu_{y,posterior}^i$ , for realization  $i$ ), after uncertainty reduction, is below the *cutoff* the alternative is rejected and if the posterior mean ( $\mu_{y,posterior}^i$ ) is above the *cutoff* then the alternative is accepted. Further, assume that if the decision maker tries to reduce uncertainty in any input factor then the correct value of that uncertainty would be known exactly, i.e. the posterior value of that input factor would be a point estimate, though the actual point estimate that results would be a sample from the prior distribution.

$$\text{True Decision} = \begin{cases} \text{Accept,} & \text{if } y > \text{cutoff} \\ \text{Reject,} & \text{if } y < \text{cutoff} \\ \text{No Decision,} & \text{otherwise} \end{cases} \quad (4.23)$$

$$\text{Decision Criterion} = \begin{cases} \text{Accept,} & \text{if } \mu_{y,\text{posterior}}^i > \text{cutoff} \\ \text{Reject,} & \text{if } \mu_{y,\text{posterior}}^i < \text{cutoff} \\ \text{No Decision,} & \text{otherwise} \end{cases} \quad (4.24)$$



**Figure 4.1:** (a) Frequency distribution of random variable  $x_1$ , (b) Frequency distribution of random variable  $x_2$ .



**Figure 4.2:** Frequency distribution of model output  $y$ .

$$y_{\text{posterior}}^i = \hat{x}_1^i + x_2 \quad (4.25)$$

$$\mu_{y,posterior}^i = \hat{x}_1^i + \mu_2 \quad (4.26)$$

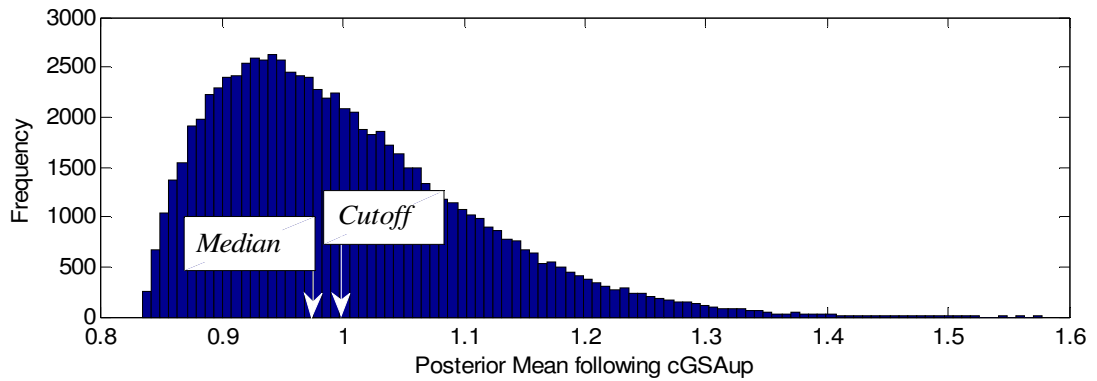
$$\mu_{y,posterior} = x_1 + \mu_2 \quad (4.27)$$

$$E(\mu_{y,posterior}) = \mu_1 + \mu_2 \quad (4.28)$$

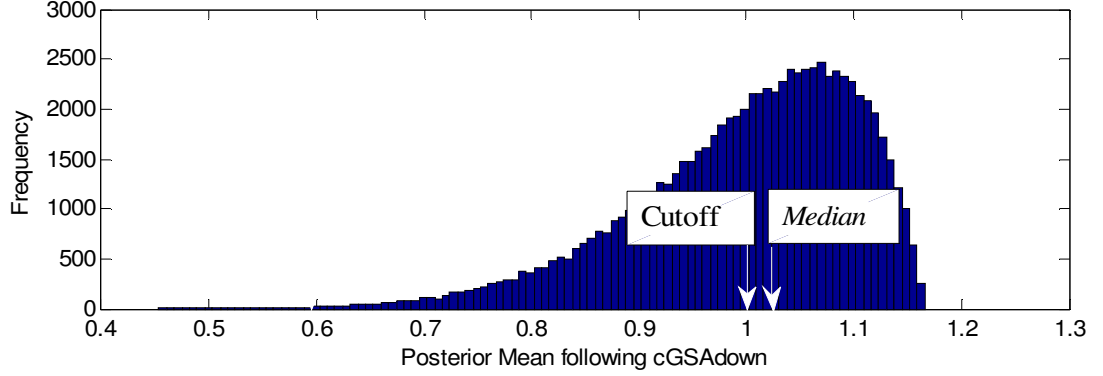
Since, the two input uncertainties have similar distributions and the model structure is simply the addition of the two uncertainties, it is obvious that both the uncertainties will equally contribute to the uncertainty in the model output, which means they would have equal *GSI* value. Additionally  $x_1$  is the key  $cGSA^{up}$  uncertainty and  $x_2$  is the key  $cGSA^{down}$  uncertainty. If the key  $cGSA^{up}$  uncertainty is reduced, we will obtain a negatively skewed posterior distribution ( $y_{posterior}^i$ ) for model output  $y$  for any realization  $i$ , but the mean of these posterior distributions ( $\mu_{y,posterior}$ ) would be positively distributed. To clarify, if uncertainty  $x_1$  is reduced then a posterior point estimate ( $\hat{x}_1$ ) of  $x_1$  is obtained, which is sampled from the prior positively skewed distribution of  $x_1$  (4.21). This point estimate only contributes in changing the location of the mean ( $\mu_{y,posterior}^i$ ) of the posterior model output  $y_{posterior}^i$  (4.25), when considered along with the other input uncertainty (i.e.  $x_2$  in this example). The shape of the posterior distribution is mainly driven by the input uncertainty  $x_2$ , hence  $y_{posterior}^i$  is a negatively skewed distribution. The mean of the posterior distribution ( $\mu_{y,posterior}^i$ ) for any realization  $i$  is given by (4.26), where  $\mu_2$  is the mean of the prior distribution of  $x_2$ . The contribution of the uncertainty  $x_2$  to the distribution of the posterior mean of  $y$  (i.e.  $\mu_{y,posterior}$ ) is constant, while the

realization of  $x_1$  contributes uncertainty to  $\mu_{y,posterior}$ , making it positively skewed (4.27).

The expected value of the posterior mean of  $y$  (i.e.  $\mu_{y,posterior}$ ) is constant (4.28), where  $\mu_1$  and  $\mu_2$  are the mean of the prior distributions of  $x_1$  and  $x_2$ , respectively. Similarly, if uncertainty in key  $cGSA^{down}$  uncertainty is reduced, we will obtain a positively skewed posterior distribution for model output  $y$ . The frequency distribution of the mean of the posterior model output for scenarios reducing uncertainty in key  $cGSA^{up}$  and key  $cGSA^{down}$  uncertainty are shown in figure 4.3 and figure 4.4.



**Figure 4.3:** Frequency distribution of mean of model output  $y$  when key  $cGSA^{up}$  uncertainty (i.e.  $x_1$ ) is reduced



**Figure 4.4:** Frequency distribution of mean of model output  $y$  when key  $cGSA^{down}$  uncertainty (i.e.  $x_2$ ) is reduced.

In order to evaluate the pros and cons of the  $cGSA^{up}$  and  $cGSA^{down}$ , false acceptance and false rejection is defined by (4.29) and (4.30) respectively, where  $N$  symbolizes the frequency. False acceptance is defined as the percentage of reject decisions which are falsely concluded to be acceptance decision. Similarly false rejection is defined as the percentage of the correct acceptance decisions which are falsely rejected.

$$\text{False Acceptance} = \frac{N(\text{Correct Decision} = \text{Reject}, \text{Predicted Decision} = \text{Accept})}{N(\text{Correct Decision} = \text{Reject})} * 100 \quad (4.29)$$

$$\text{False Rejection} = \frac{N(\text{Correct Decision} = \text{Accept}, \text{Predicted Decision} = \text{Reject})}{N(\text{Correct Decision} = \text{Accept})} * 100 \quad (4.30)$$

Consider the scenario, when the key  $cGSA^{up}$  uncertainty is reduced, this would lead to the positively skewed posterior mean distribution shown in Figure 4.3. For a positively skewed distribution the median lie below the mean, as also shown in figure 4.3. And hence for the mean based decision criterion shown in (4.23), higher percentage of the times the R&D alternative is rejected and lower percentage of the times the R&D

alternative is accepted (as also shown by the results in Table 4.2). Similarly reducing the uncertainty in the key  $cGSA^{down}$  uncertainty would lead to the negatively skewed posterior mean distribution shown in Figure 4.4. For a negatively skewed distribution the median lie above the mean, as also shown in Figure 4.4. And hence for the mean based decision criterion shown in (4.23), higher percentage of the times the R&D alternative is accepted and lower percentage of the times the R&D alternative is rejected (as also shown by the results in table 4.2).

From the above discussion it is obvious how the positive (negative) skewness of the distribution of the posterior mean of  $y$  (i.e.  $\mu_{y,posterior}$ ) leads to higher rejection (acceptance) decisions. In addition, the results presented in table 4.2, also indicate that the reduction in uncertainty in the key  $cGSA^{up}$  factor not only leads to higher rejection decisions but also higher false rejection decisions. Similarly, reduction in uncertainty in the key  $cGSA^{down}$  factor not only leads to higher acceptance decisions but also higher false acceptance decisions. This behaviour of the false acceptance and false rejection decision can be explained in either of the following ways:

- (a) Heuristically, in general an increase in prediction of absolute number of acceptance decisions always leads to an increased or equal, absolute number of both correct and false acceptance decisions. Similarly, an increase in prediction of number of rejection decisions always leads to an increased or equal, absolute number of both correct and false rejection decisions. Hence for  $cGSA^{up}$ , an increment in the number of rejection decisions would lead to increment in false rejections. Similarly, an increment in the number of acceptance decisions, leads to increment in the false acceptance.

(b) For the specific example considered, the R&D alternative can be equally accepted or rejected, i.e. 50% of the times the alternative is rejected and 50% of the times the alternative is accepted. Since both the correct acceptance and rejections is a fixed value equal to 50% in the example considered,  $cGSA^{up}$  with higher rejection decisions would lead to higher false rejections. Similarly,  $cGSA^{down}$  leads to higher false acceptance, which would lead to higher false acceptance decisions.

**Table 4.2:** Comparing prediction performance based on  $cGSA^{up}$  and  $cGSA^{down}$  approach

<b>Reducing Uncertainty in:</b>	$cGSA^{up}$ , i.e. $x_1$	$cGSA^{down}$ , i.e. $x_2$
Acceptance Decision	43%	57%
Rejection Decision	57%	43%
False Acceptance	18%	32%
False Rejection	32%	18%

Overall in general, reduction in uncertainty in key  $cGSA^{up}$  would lead to reduction in skewness of the posterior distribution but would lead to positively skewed distribution of the posterior mean of  $y$  (i.e.  $\mu_{y,posterior}$ ) (for factors having same or nearly equal  $GSA$ ). Moreover, compared to the prior distribution of  $y$ , the mean of the posterior distribution of  $y$  (i.e.  $\mu_{y,posterior}$ ) would be relatively positively skewed. Additionally, the mean of the prior distribution and the expected value of the distribution of the posterior mean is the

same. So, effectively, we are comparing two distributions with the same mean but different skewness and the one with higher skewness would lead to higher rejection rate. In this case  $\mu_{y,posterior}$  has higher skewness and hence higher rejection rate. Following the heuristic argument this would always lead to higher false rejection decisions.

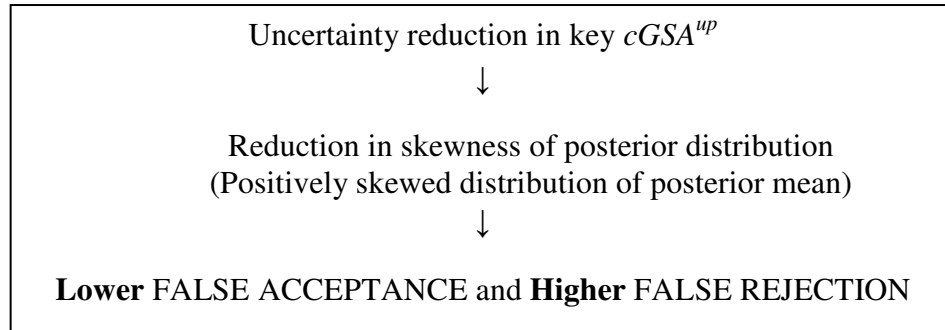
Similarly in general, reduction in uncertainty in key  $cGSA^{down}$  would lead to increase in skewness of the posterior distribution but would lead to a negatively skewed distribution of the posterior mean of  $y$  (i.e.  $\mu_{y,posterior}$ ) (for factors having same or nearly equal  $GSA$ ). Moreover, compared to the prior distribution of  $y$ , the mean of the posterior distribution of  $y$  (i.e.  $\mu_{y,posterior}$ ) would be relatively negatively skewed. Additionally the, the mean of the prior distribution and the expected value of the distribution of the posterior mean is the same. So, effectively, we are comparing two distributions with the same mean but different skewness and the one with lower skewness would lead to higher acceptance rate. In this case  $\mu_{y,posterior}$  has lower skewness and hence higher acceptance rate. Following the heuristic argument this would always lead to higher false acceptance decisions.

Since, we are considering the case with same or nearly equal  $GSA$ , if one factor has higher  $cGSI^{up}$  (conditional global sensitivity up index), the other variable would have higher  $cGSI^{down}$  (conditional global sensitivity down index). This means on a relative basis, the key  $cGSA^{up}$  factor would lead to higher false rejection decisions and lower acceptance decision, which in effect would lead to higher false rejection and lower false acceptance decisions (following the heuristic argument). Similarly, the key  $cGSA^{down}$  factor would lead to higher false acceptance decisions and lower rejection decisions,

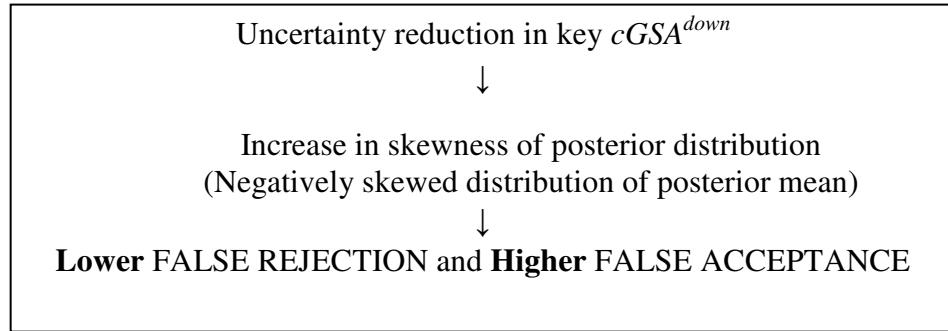
which in effect would lead to higher false acceptance and lower false rejection decisions (following the heuristic argument).

Mean based decision criterion shown in (4.23) is a simplistic approach, which does not account for the risk involved in the decision. To consider for the risk in the decision, decision criterion based on both the mean and the variance of the distribution are prominent. One such decision criterion is shown in (4.31), where  $\mu_{y,posterior}^i$  is the mean of the posterior model output  $y$  and  $\sigma_{y,posterior}^i$  is the standard deviation of the posterior model output  $y$ , for the realization  $i$ .

$$\text{Decision Criterion} = \left\{ \begin{array}{ll} \text{Accept,} & \text{if } \mu_{y,posterior}^i - k\sigma_{y,posterior}^i > \text{cutoff} \\ \text{Reject,} & \text{if } \mu_{y,posterior}^i + k\sigma_{y,posterior}^i < \text{cutoff} \\ \text{No Decision,} & \text{otherwise} \end{array} \right\} \quad (4.31)$$



**Figure 4.5:** Interpretation of  $cGSA^{up}$  results, when the decision criterion involves both the mean and variance of the posterior distribution



**Figure 4.6:** Interpretation of  $cGSA^{down}$  results, when the decision criterion involves both the mean and variance of the posterior distribution

For the decision criterion (4.31),  $k$  and  $cutoff$  are constant and  $\sigma_{y,posterior}^i$  is the same immaterial of which uncertainty is reduced. So effectively, the decision criterion mainly depends on the distribution of  $\mu_{y,posterior}$ . Again the positive (negative) skewness of  $\mu_{y,posterior}$  leads to higher rejection (acceptance) decisions for  $cGSA^{up}$  ( $cGSA^{down}$ ). This based on the heuristic argument discussed earlier leads to higher (lower) false rejection and lower (higher) false acceptance when the key  $cGSA^{up}$  ( $cGSA^{down}$ ) uncertainty is reduced. Figure 4.5 and 4.6 diagrammatically illustrate the interpretation for the  $cGSA^{up}$  and  $cGSA^{down}$  respectively.

Another risk based decision criterion can be based on the conditional value at risk (CVaR). CVaR is a risk assessment method used to reduce the probability that a portfolio will incur large losses. Mathematically CVaR is the mean of the part of the distribution between the VaR (Value at Risk) and the values exceeding VaR losses. For example a VaR of 5% gives the maximum return in the worst 5% of the scenarios and CVaR measures the mean return for these worst 5% of the scenarios. If we look at profit

distribution, then the CVaR would always lie below the mean of the distribution. Additionally the distance between the CVaR and mean would be smaller for a positively skewed distribution compared to a negatively skewed distribution.

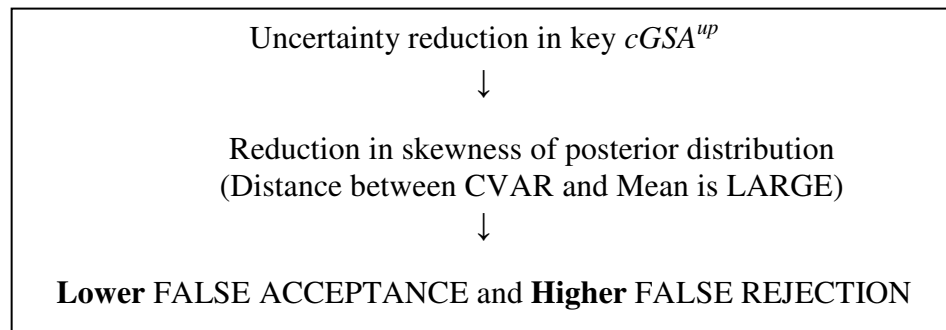
$$\text{Decision Criterion} = \left\{ \begin{array}{ll} \text{Accept,} & \text{if } CVaR_{y,posterior}^i > cutoff \\ \text{Reject,} & \text{if } CVaR_{y,posterior}^i < cutoff \\ \text{No Decision,} & \text{otherwise} \end{array} \right\} \quad (4.32)$$

Consider the scenario, where the uncertainty in the key  $cGSA^{up}$  uncertainty factor is reduced, this would lead to a negatively skewed posterior distribution of  $y$ , with large distance between the CVaR and the mean of the distribution. This clearly indicates a higher number of rejection decisions. Moreover, the positive skewed distribution of the posterior mean would also mean that the posterior mean would lie below the *cutoff* with higher frequency. These two effects, both drive towards higher reject decisions. Similarly, for the scenario where the uncertainty in the key  $cGSA^{down}$  uncertainty factor is reduced, this would lead to a positively skewed posterior distribution of  $y$ , with shorter distance between the CVaR and the mean of the distribution. Moreover, the mean of the posterior distributions is negatively skewed, signifying that with higher frequency the posterior mean would lie above the *cutoff*. Both these factors (shorter distance between CVaR and mean, posterior mean above the *cutoff* with higher frequency) would lead to higher acceptance decisions. Considering the heuristic argument (higher acceptance (rejection) decisions leads to non decrement in correct and false acceptance (rejections)), leads to argue that the  $cGSA^{down}$  ( $cGSA^{up}$ ) would lead to higher (lower) false acceptance and lower (higher) false rejections. Further, figure 4.7 and 4.8 diagrammatically illustrate

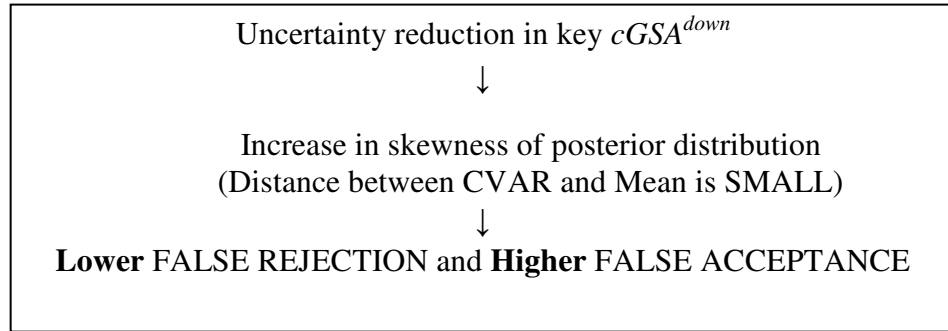
the interpretation for the  $cGSA^{up}$  and  $cGSA^{down}$  respectively. The result for the above example presented in table 4.3 supports the above argument.

**Table 4.3:** Comparing prediction performance based on  $cGSA^{up}$  and  $cGSA^{down}$  approach, for CVaR based decision criterion

Reducing Uncertainty in:	$cGSA^{up}$ , i.e. $x_1$	$cGSA^{down}$ , i.e. $x_2$
Acceptance Decision	2	2.3
Rejection Decision	98	97.7
False Acceptance	0.05	0.1
False Rejection	96.9	96.3



**Figure 4.7:** Interpretation of the  $cGSA^{up}$  results, with CVaR based decision criterion



**Figure 4.8:** Interpretation of the  $cGSA^{down}$  results, with CVaR based decision criterion

#### 4.3.4 Application

Two input uncertain factors ( $x_1$  and  $x_2$ ) which have similar  $GSI$ 's, means that both of them contribute equally to the variance of the model output. Then, the selection between the input factors,  $x_1$  or  $x_2$ , for uncertainty reduction could depend on the risk profile of the decision maker. If the decision maker has a conservative risk profile, i.e., is more worried about possible rejection of a potential good opportunity, then  $cGSA^{down}$  is the right approach as it leads to lower false rejection and higher false acceptance. On the other hand, if the decision maker wants to trim down a large number of alternatives to a few ones, then the  $cGSA^{up}$  is the right approach as it leads to lower false acceptance and higher false rejection.

If the decision maker is considering only a few highly promising R&D options, he or she would be more cautious in rejecting them and would prefer to reduce the uncertainty in a fashion that minimizes the probability of false rejection. For such a situation,  $cGSA^{down}$  would be the right tool to use for the variable selection for further uncertainty reduction. This is because the uncertainty reduction based on  $cGSA^{down}$  would

generally lead to more acceptance decisions with a higher false acceptance probability, which in turn would lead to higher R&D resource consumption, but it is unlikely that a potentially good alternative is rejected.

On the contrary, if many of the R&D options under consideration are likely not very promising and the decision makers does not want to spend too much resource to make a decision in terms of accepting or rejecting them, then  $cGSA^{up}$  would be the right tool as reducing uncertainty in the key  $cGSA^{up}$  uncertainty leads to a lower rate of false acceptance at the expense of a higher rate of false rejection. So  $cGSA^{up}$  compared to  $cGSA^{down}$  is a more aggressive strategy in terms of screening the candidates and hence is beneficial when working with a large number of R&D options with lower success probabilities.

#### 4.4. Test case studies

To obtain more insight and demonstrate the importance of  $cGSA$  we consider a generic model  $y$  given by (4.33), composed of two skewed model inputs ( $x_1$  and  $x_2$ ) and two symmetric distributed model inputs ( $h_1$  and  $h_2$ ). Parameters ( $y_0, a, b, c, d, e, f$ ) are assigned different value for different examples, but the general structure of the model remains the same for all the examples. Model inputs,  $x_1$  and  $x_2$  are derived from (4.34) and (4.35) respectively, while model inputs  $h_1$  and  $h_2$  are derived from (4.36) and (4.37) respectively. The values and prior distributions of the various underlying parameters ( $T_1, T_2, \theta_1, \theta_2$ ) of  $x_1, x_2, h_1$  and  $h_2$  are given by (4.41) – (4.45). The frequency distributions of the two model input factors  $x_1$  and  $x_2$  is shown in the figure 4.9 and for model inputs  $h_1$  and  $h_2$  is shown in figure 4.10. For reducing uncertainty of parameters  $\theta_1$  and  $\theta_2$

experiments are conducted for the models  $g_1$  and  $g_2$  given by (4.38) and (4.39) respectively. The gaussian noise in models  $g_1$  and  $g_2$  is given by (4.46) and (4.47) respectively and the variance of the noise is given by (4.48).

$$y = y_0 + a.x_1 + b.x_2 + c.x_1.x_2 + d.h_1 + e.h_2 + f.h_1.h_2 \quad (4.33)$$

$$x_1 = (z_1^T \theta_1 - T_1)^2 \quad (4.34)$$

$$x_2 = (z_2^T \theta_2 - T_2)^2 \quad (4.35)$$

$$h_1 = z_1^T \theta_1 \quad (4.36)$$

$$h_2 = z_2^T \theta_2 \quad (4.37)$$

$$g_1 = z_1^T \theta_1 + \varepsilon_1 \quad (4.38)$$

$$g_2 = z_2^T \theta_2 + \varepsilon_2 \quad (4.39)$$

$$z_1 = z_2 = [1 \quad 1 \quad 1]^T \quad (4.40)$$

$$\theta_1 \sim N(\mu_{\theta_1}, \Sigma_{\theta_1}) \quad (4.41)$$

$$\theta_2 \sim N(\mu_{\theta_2}, \Sigma_{\theta_2}) \quad (4.42)$$

$$\mu_{\theta_1} = \mu_{\theta_2} = [-5 \quad 10 \quad 5]^T \quad (4.43)$$

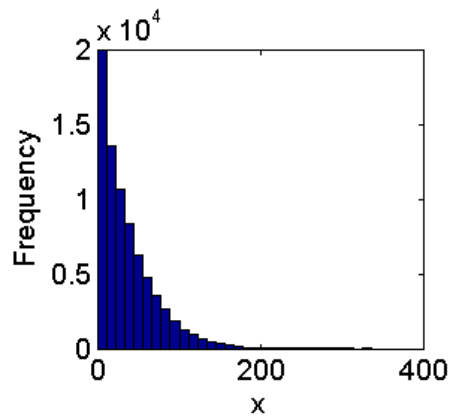
$$\Sigma_{\theta_1} = \Sigma_{\theta_2} = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.25 \end{bmatrix} \quad (4.44)$$

$$T_1 = T_2 = 5 \quad (4.45)$$

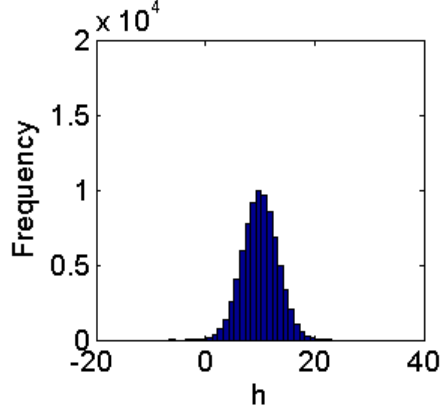
$$\varepsilon_1 \sim N(0, \sigma_1^2) \quad (4.46)$$

$$\varepsilon_2 \sim N(0, \sigma_2^2) \quad (4.47)$$

$$\sigma_1^2 = \sigma_2^2 = 0.05 \quad (4.48)$$



**Figure 4.9:** Frequency distribution of input uncertainties ( $x_1$  and  $x_2$ )



**Figure 4.10:** Frequency distribution of input uncertainties ( $h_1$  and  $h_2$ )

To evaluate the performance of the  $cGSA$ , both  $cGSI^{up}$  (4.14) and  $cGSI^{down}$  (4.15) are calculated, along with it the probability of false acceptance (4.29) and false rejection (4.30). Procedure to calculate the probabilities are explained as follows:

Consider the scenario when  $cGSA$  (either  $cGSA^{up}$  or  $cGSA^{down}$ ) identifies  $x_l$  as the key uncertainty. Hence more information should be obtained to reduce uncertainty on  $x_l$ . In order to acquire more information, one D-optimal design ( $\eta_l^{exp}$ ) based experiment is conducted on the model  $g_l$  (see (4.38)) and thereupon after obtaining the experimental realization ( $g_{1,exp}^i$ ) of  $g_l$ , the posterior distribution,  $\theta_{1,p}^i \sim N\left(\mu_{\theta_{1,p}^i}, \Sigma_{\theta_{1,p}^i}\right)$ , of  $\theta_1$  is obtained.

In order to systematically compare the  $cGSA^{up}$  and  $cGSA^{down}$ ,  $N$  ( $N = 5000 \times 8$ ) realizations of  $\theta_1, \theta_2, \varepsilon_1$  and  $\varepsilon_2$  are generated and stored in  $\theta_1^i, \theta_2^i, \varepsilon_1^i$  and  $\varepsilon_2^i$  (where  $i = 1, 2, \dots, N$ ). To generate the experimental realization  $g_{1,exp}^i$ , a sample  $\theta_1^i$  from the prior

distribution of  $\theta_1$  and a sample noise,  $\varepsilon_1^i$  from the noise distribution  $\varepsilon_1$  is considered. The posterior distribution for  $\theta_1$  can be calculated using (4.49) and (4.50).

$$\mu_{\theta_1^{posterior}} = \left( (\eta_1^{exp})^T (\eta_1^{exp}) + (\Sigma_{\theta_1} / \sigma_1^2)^{-1} \right) \left( (\eta_1^{exp})^T (g_1^{exp}) + (\Sigma_{\theta_1} / \sigma_1^2)^{-1} \mu_{\theta_1} \right) \quad (4.49)$$

$$\Sigma_{\theta_1^{posterior}} = \sigma_1^2 \left( (\eta_1^{exp})^T (\eta_1^{exp}) + (\Sigma_{\theta_1} / \sigma_1^2)^{-1} \right) \quad (4.50)$$

Now given this posterior distribution ( $\theta_{1,posterior}$ ) of  $\theta_1$ , the posterior distribution of  $x_1$  is easily obtained using (4.34). Next using the posterior distribution of  $x_1$  and prior distribution of  $x_2$  the updated distribution of  $y$  is obtained. Depending upon which decision criterion ((4.24), (4.31) or (4.32)) is used, the required properties of the posterior distribution are calculated and the decision is predicted.

In the above, one sample of experimental realization  $g_{1,exp}^i$  is considered and it leads to one updated distribution of  $y$  and then one decision of either selection, rejection or no decision, is made based on the decision criterion selected; this constitutes of one scenario. Similarly  $N$  ( $N = 8000$ ) scenarios are generated and using the definition of false acceptance (4.29) and false rejection (4.30) the values are reported.

To demonstrate the importance of *cGSA*, we consider two set of examples. Section 4.4.1 presents examples where decision criterion is based on both the posterior mean and the variance of the distribution (4.31) and Section 4.4.2 presents examples, where decision criterion is based on the CVaR (4.32).

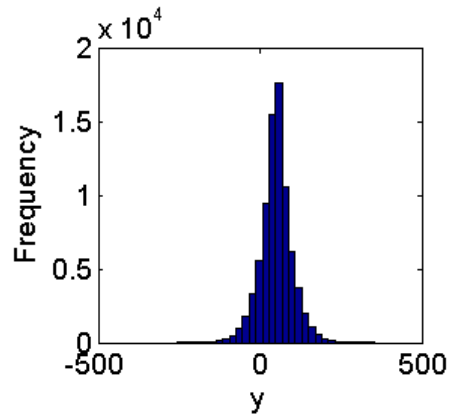
#### 4.4.1. Mean and Variance based Decision Criterion

In this section I consider a decision criterion which is based on both the mean and the variance of the posterior distribution. The specific decision criterion considered in this section is shown by equation (4.31). The value of the variable  $k$  in (4.31) is considered to be equal to 1 for all the examples this section.

##### 4.4.1.1. Example 1

Consider the model structure in equation (4.51). Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.11). The *GSA* results show that both the uncertainties are equally important. Further  $cGSA^{up}$  suggests that  $x_1$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_2$  is the key uncertainty. Results for two different *cutoff* values of 12 and 88 are shown in Table 4.4 and 4.5 respectively. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to higher lower false rejection and higher false acceptance.

$$y = 50 + x_1 - x_2 \tag{4.51}$$



**Figure 4.11:** Frequency distribution of model output  $y$  for example 1

**Table 4.4:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example1 for *cutoff* value of 12

	$x_1$	$x_2$
<b><i>GSA</i></b>	0.5	0.5
<b><i>cGSA<sup>up</sup></i></b>	0.88	0.00
<b><i>cGSA<sup>down</sup></i></b>	0.01	0.76
<b>False Rejection (%)</b>	0	0
<b>False Acceptance (%)</b>	7	41

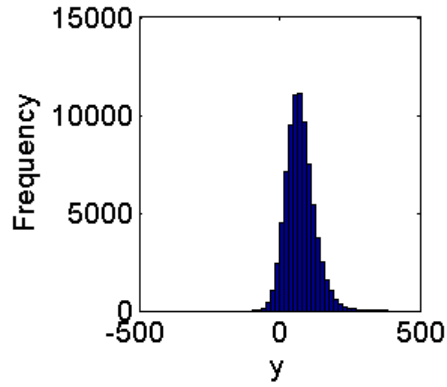
**Table 4.5:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example1 for *cutoff* value of 88

	$x_1$	$x_2$
<b>GSA</b>	0.5	0.5
<b><math>cGSA^{up}</math></b>	0.88	0.00
<b><math>cGSA^{down}</math></b>	0.01	0.76
<b>False Rejection (%)</b>	41	7
<b>False Acceptance (%)</b>	0	0

#### 4.4.1.2. Example 2

Consider the model structure in (4.52). The model output consists of the positively skewed uncertainty  $x_1$  and non-skewed uncertainty  $h_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.12). The *GSA* results show that both the uncertainties are equally important. Further  $cGSA^{up}$  suggests that  $x_1$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_2$  is the key uncertainty. Results for two different *cutoff* values of 112 and 37 are shown in Table 4.6 and 4.7 respectively. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to higher lower false rejection and higher false acceptance.

$$y = 150 + x_1 - 11h_2 \tag{4.52}$$



**Figure 4.12:** Frequency distribution of model output  $y$  for example 2

**Table 4.6:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 2 for *cutoff* value of 112

	$x_1$	$h_2$
<b><i>GSA</i></b>	0.5	0.5
<b><i>cGSA<sup>up</sup></i></b>	0.51	0.13
<b><i>cGSA<sup>down</sup></i></b>	0.09	0.57
<b>False Rejection (%)</b>	47	24
<b>False Acceptance (%)</b>	0	0

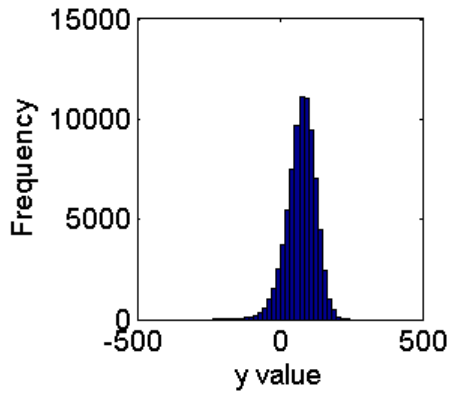
**Table 4.7:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 2 for *cutoff* value of 37

	$x_1$	$h_2$
<b>GSA</b>	0.5	0.5
<b><math>cGSA^{up}</math></b>	0.51	0.13
<b><math>cGSA^{down}</math></b>	0.09	0.57
<b>False Rejection (%)</b>	0	0
<b>False Acceptance (%)</b>	3	6

#### 4.4.1.3. Example 3

Consider the model structure in (4.53). The model output consists of the negatively skewed uncertainty  $-x_1$  and non-skewed uncertainty  $h_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.13). The *GSA* results show that both the uncertainties are equally important. Further  $cGSA^{up}$  suggests that  $x_2$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_1$  is the key uncertainty. Results for two different *cutoff* values of -37.5 and -112.7 are shown in Table 4.8 and 4.9 respectively. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to higher lower false rejection and higher false acceptance.

$$y = -x_1 + 11h_2 \tag{4.53}$$



**Figure 4.13:** Frequency distribution of model output  $y$  for example 3

**Table 4.8:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 3 for *cutoff* value of 37.5

	$x_1$	$h_2$
<b><i>GSA</i></b>	0.5	0.5
<b><i>cGSA<sup>up</sup></i></b>	0.09	0.57
<b><i>cGSA<sup>down</sup></i></b>	0.51	0.13
<b>False Rejection (%)</b>	0	0
<b>False Acceptance (%)</b>	48	24

**Table 4.9:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 3 for *cutoff* value of 112.7

	$x_1$	$h_2$
<b>GSA</b>	0.5	0.5
<b><math>cGSA^{up}</math></b>	0.09	0.57
<b><math>cGSA^{down}</math></b>	0.51	0.13
<b>False Rejection (%)</b>	3	6
<b>False Acceptance (%)</b>	0	0

#### 4.4.2. CVaR based Decision Criterion

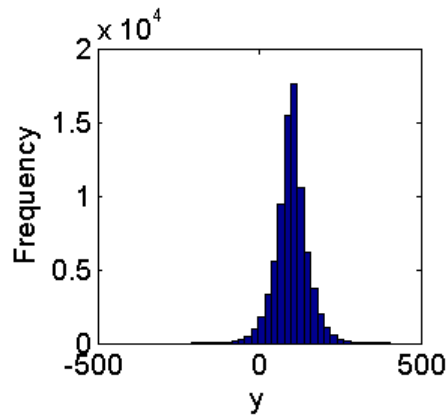
In this section I consider a decision criterion which is based on the conditional value at risk of the posterior distribution of the model output  $y$ . The specific decision criterion considered in this section is shown by equation (4.32).

##### 4.4.2.1. Example 4

Consider the model structure in equation (4.54). The model output consists of two skewed uncertainties, positively skewed  $x_1$  and negatively skewed uncertainty  $-x_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.14). The *GSA* results show that both the uncertainties are equally important. Further  $cGSA^{up}$  suggests that  $x_1$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_2$  is the key uncertainty. Results for two different *cutoff* values of 0 and 50 are shown in Table 4.10

and 4.11 respectively. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to higher lower false rejection and higher false acceptance.

$$y = 100 + x_1 - x_2 \tag{4.54}$$



**Figure 4.14:** Frequency distribution of model output  $y$  for example 4

**Table 4.10:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 4 for *cutoff* value 0

	$x_1$	$x_2$
<b>GSA</b>	0.50	0.50
<b><math>cGSA^{up}</math></b>	0.76	0.01
<b><math>cGSA^{down}</math></b>	0.01	0.76
<b>False Rejection (%)</b>	77	0
<b>False Acceptance (%)</b>	4	100

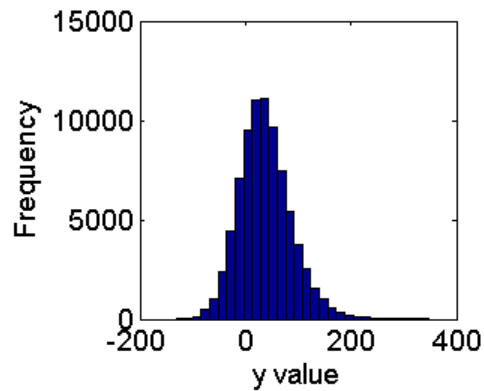
**Table 4.11:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 4 for *cutoff* value 50

	$x_1$	$x_2$
<b>GSA</b>	0.50	0.50
<b><math>cGSA^{up}</math></b>	0.76	0.01
<b><math>cGSA^{down}</math></b>	0.01	0.76
<b>False Rejection (%)</b>	100	0.7
<b>False Acceptance (%)</b>	0	69

#### 4.4.2.2. Example 5

Consider the model structure in equation (4.55). The model output consists of positively skewed uncertainty  $x_1$  and symmetric uncertainty  $h_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.15). The *GSA* results show that both the uncertainties are equally important. Further  $cGSA^{up}$  suggests that  $x_1$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_2$  is the key uncertainty. Result for *cutoff* value of 0 is shown in Table 4.12. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to lower false rejection and higher false acceptance.

$$y = 112.7 + x_1 - 11h_2 \quad (4.55)$$



**Figure 4.15:** Frequency distribution of model output  $y$  for example 5

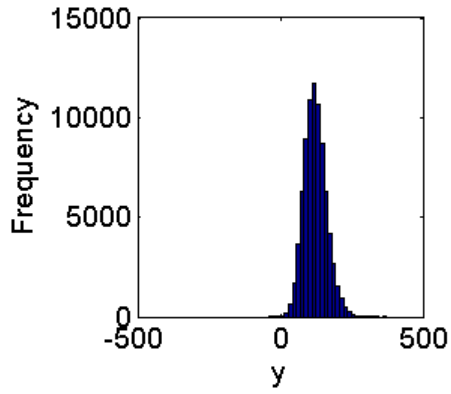
**Table 4.12:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 5 for *cutoff* value of 0

	$x_1$	$h_2$
<b>GSA</b>	0.50	0.50
<b><math>cGSA^{up}</math></b>	0.51	0.13
<b><math>cGSA^{down}</math></b>	0.09	0.57
<b>False Rejection (%)</b>	99	35
<b>False Acceptance (%)</b>	0	2

#### 4.4.2.3. Example 6

Consider the model structure in (4.56). The model output consists of positively skewed uncertainty  $x_1$  and symmetric uncertainty  $h_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.16). The *GSA* results show that both the uncertainties are very close in importance. Further  $cGSA^{up}$  suggests that  $x_1$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_2$  is the key uncertainty. Result for *cutoff* value of 61.4 is shown in Table 4.13. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to higher lower false rejection and higher false acceptance.

$$y = x_1 + 9.48h_2 - 0.02x_1h_2 \quad (4.56)$$



**Figure 4.16:** Frequency distribution of model output  $y$  for example 6

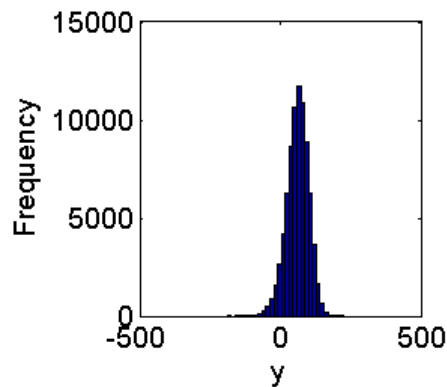
**Table 4.13:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 6 for *cutoff* value of 61.4

	$x_1$	$h_2$
<b><i>GSA</i></b>	0.47	0.50
<b><i>cGSA<sup>up</sup></i></b>	0.49	0.45
<b><i>cGSA<sup>down</sup></i></b>	0.01	0.58
<b>False Rejection (%)</b>	68	0
<b>False Acceptance (%)</b>	1	97

#### 4.4.2.4. Example 7

Consider the model structure in equation (4.57). The model output consists of positively skewed uncertainty  $x_1$  and symmetric uncertainty  $h_2$ . Given the input uncertainties the distribution of the model output  $y$  is shown in figure (4.17). The *GSA* results show that both the uncertainties are very close in importance. Further  $cGSA^{up}$  suggests that  $x_2$  is the main uncertainty while  $cGSA^{down}$  suggests that  $x_1$  is the key uncertainty. Result for *cutoff* value of 0 is shown in Table 4.14. Results support the argument that the uncertainty reduction in the key  $cGSA^{up}$  uncertainty leads to higher false rejection and lower false acceptance, while reduction in key  $cGSA^{down}$  uncertainty leads to lower false rejection and higher false acceptance.

$$y = 184.2 - x_1 - 9.48h_2 + 0.02x_1h_2 \quad (4.57)$$



**Figure 4.17:** Frequency distribution of model output  $y$  for example 7

**Table 4.14:** Comparison of  $cGSA^{up}$  and  $cGSA^{down}$  for example 7 for *cutoff* value of 0

	$x_1$	$h_2$
<b>GSA</b>	0.47	0.50
<b><math>cGSA^{up}</math></b>	0.32	0.55
<b><math>cGSA^{down}</math></b>	0.58	0.03
<b>False Rejection (%)</b>	6	99
<b>False Acceptance (%)</b>	30	0

Further, since the reduction in key  $cGSA^{up}$  leads to negatively skewed distribution and negatively skewed distribution has higher distance between the posterior CVaR and posterior Mean value, this would intuitively give higher FALSE REJECTION and lower FALSE ACCEPTANCE. Hence it should not matter if the number of variables is two or more. Similarly for  $cGSA^{down}$  based results. It important to note here, that since CVaR based decision criterion just focuses on the lower tail of the distribution and does not have the option of no-decision, makes it a very sensitive decision criterion. Hence CVaR decision criterion based cases show significantly higher rates of false rejections or false acceptance.

## 4.5 Conclusions

In this chapter, a new approach conditional global sensitivity analysis,  $cGSA$ , is introduced for the identification of the key uncertainty contributors, when  $GSA$  fails to do so. The two  $cGSA$  based approaches  $cGSA^{up}$  and  $cGSA^{down}$  support two different types of decision makers.  $cGSA^{up}$  is useful for a decision maker who is relatively more concerned about the R&D cost and less about the probability of success, as it leads to lower false acceptance and higher false rejection. This would be a scenario, where the decision maker has large number of alternatives, which have potentially low probability of success but decision maker still wants to screen them, in case there is some good alternative in them.

Alternatively  $cGSA^{down}$  is useful for a decision maker who is relatively more concerned about the success probability and not so much about the R&D cost, as it leads to lower false rejection and higher false acceptance. This would be a scenario, where the potential alternatives demonstrate fair chance of success, and the decision maker wants to take no risk in falsely rejecting these alternatives.

# CHAPTER V

## DECISION ORIENTED DESIGN OF EXPERIMENTS

Traditional ‘Design of Experiment’ (DOE) approaches focus on minimization of parameter error variance. In this work, we propose a new “decision-oriented” DOE approach that takes into account how the generated data, and subsequently, the model developed based on them will be used in decision making. By doing so, the parameter variances get distributed in a manner such that its adverse impact on the targeted decision making is minimal. Our results show that the new decision-oriented DPE approach significantly outperforms the standard D-optimal design approach. The new design method should be a valuable tool when experiments are conducted for the purpose of making R&D decisions.

### **5.1. Introduction**

Design of experiments (DOE) as a field has evolved over the period of last few decades. Its importance has grown significantly because of the increasing need to reduce the resource requirements for achieving a target. Typically scientists performing experiments have been driven towards understanding underlying phenomena or estimating parameters. Consequently, the traditional DOE tools have been geared towards maximization of some measure of information or towards the minimization of variances in the parameter estimates.

It is my opinion that this way of thinking over a long period of time has led the field to lose sight on the ultimate purpose of experiments in many applications. If one

looks back into the history of the evolution of design of experiments one finds the answers: “*Scientists typically does not have, nor can be normally expected to have, a clear idea of the utility of his results. An alternative is to design an experiment to maximize the expected information to be gained from it.*” ((Bernardo 1979), p 686). (Bernardo 1979) further goes on proving that any  $f$  (function of the parameters,  $\theta$ ), in informational theoretical terms, is ‘*garbling of  $\theta$* ’. Hence follows the conclusion that maximization of information of  $\theta$  is better than maximizing information on  $f$ .

This practice, while seeming logical, does not fit today’s industrial situations, where experiments are oftentimes conducted with a specific objective in mind. For example, experiments can be conducted to aid decisions for the maximization of a revenue function when investigating a new process or for the selection of a few processes among the large alternatives. In such scenarios, following the traditional route for design of experiments can be significantly suboptimal.

In this chapter we develop two decision oriented design of experiment strategies, which are focussed on the decision making rather than uncertainty reduction in parameter estimates. In developing these two methodologies, we take into consideration that after the experiments are conducted based on an experimental design strategy, one will always perform an optimization to estimate the optimal operating conditions. This key aspect is mostly left out in the traditional approaches, due to technical challenges.

The rest of the chapter is structured as follows: Section 5.2 provides the background about the fundamental idea behind the traditional design of experiment strategies, Section 5.3 discusses in more detail the setup and algorithm for the decision

oriented designs, Section 5.4 presents the numerical results, and Section 5.5 concludes the chapter.

## 5. 2. Background

Traditionally there have been two major classes for the design of experiments (DOE) approaches: Classical approach and Bayesian approach. Historically, Classical DOE approaches like the factorial design have been more popular due to the computational complexities associated with the Bayesian approach. However, recent developments in sampling techniques such as Markov Chain Monte Carlo (MCMC) ((Kass, Carlin et al. 1998), (Cowles and Carlin 1996)) have rejuvenated the interest in Bayesian approaches. In addition, the Bayesian approaches provide an added advantage of enabling the designer to incorporate the prior knowledge, which is critical when the resource or opportunity for obtaining information is limited. In this chapter, we focus on the Bayesian approaches for design of experiments.

To elaborate on the traditional Bayesian design strategies, we follow the approach of (Chaloner and Verdinelli 1995), as it does justice to the inherent, but not always transparent, decision aspect of the Bayesian approach. The idea of Bayesian DOE has evolved from information acquisition concepts in decision theory. (Raiffa and Schlaifer 1961) presented a decision theoretic approach for optimal information acquisition strategy using Expected Value of Information (*EVOI*) approach for investment decision problems. *EVOI* is defined as the expected difference between the expected posterior and prior utility, if one is to acquire the information in question. (Lindley 1956) introduced his seminal work on the use of Shannon information as a measure of information provided by an experiment. Following this, several authors ((Stone 1959), (DeGroot

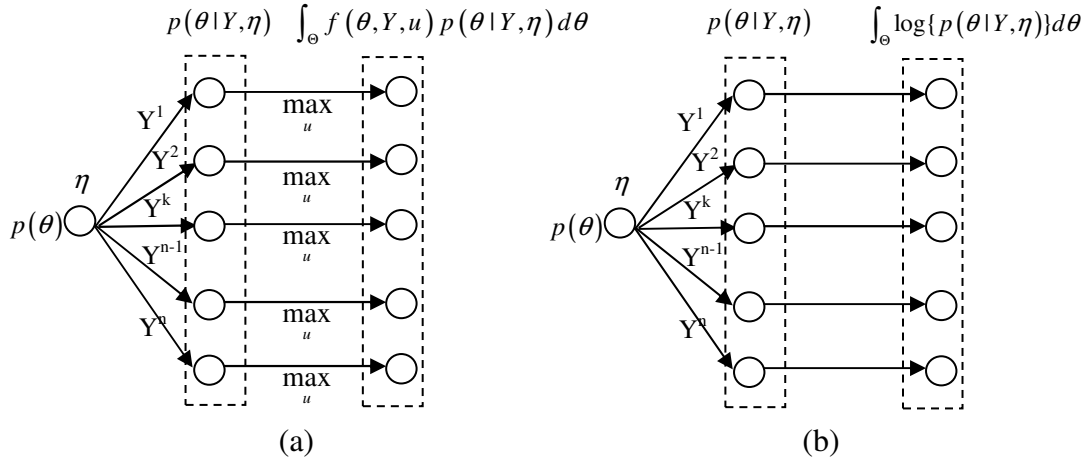
1962) and (Bernardo 1979)) presented a decision theoretic approach to experimental design, which was basically the maximization of *EVOI* with the utility function being replaced by Shannon information.

Consider a utility function ( $f$ ), optimal decision ( $u$ ) under posterior distribution, design matrix ( $\eta$ ), parameters ( $\theta$ ) and observations ( $Y$ ). Application of Lindley's *EVOI* maximization approach results in the maximization of expected pre-posterior utility as the expected value of the prior utility function is constant. The optimal expected pre-posterior utility is given in (5.1). Figure 5.1 demonstrates how (5.1) can be solved numerically. Based on a given design ( $\eta$ ) and the prior distribution of the parameters ( $p(\theta)$ ), potential observations ( $Y$ ) are found via Monte Carlo simulation. For each of these potential realizations, posterior distribution (e.g., mean and covariances) for the parameters (denoted by  $p(\theta|Y, \eta)$ ) are obtained. Here the symbol  $\eta$  is added in the expression to emphasize the dependence of the distribution on it but we note that this is with some abuse of notation as  $\eta$  is a deterministic variable in a strict sense. In addition, based on these posterior parameter estimates, optimal posterior decision variable ( $u$ ) is estimated, which is shown as 'max over  $u$ ' in the figure. Next step is to calculate, for each of these potential realizations ( $Y$ ), the posterior expected utility value  $E_{\theta|Y}[f]$  corresponding to the optimally chosen  $u$ . The average of the posterior expected utility values for all the potential realizations ( $Y$ ) gives a score of the design ( $\eta$ ). The design that maximizes this average value is the optimal design ( $\eta^*$ ).

$$\eta^* = \arg \max_{\eta} \left[ \Omega(\eta) \triangleq \int_Y \max_u \int_{\Theta} f(\theta, Y, u) p(\theta|Y, \eta) p(Y|\eta) d\theta dY \right] \quad (5.1)$$

Now, if one considers the Shannon information as the utility function, as suggested by Lindley, the above simplifies to (5.2). As both Fig. 5.1(b) and (5.2) show, the calculations become much simpler as the ‘max’ step drops out.

$$\eta^* = \arg \max_{\eta} \left[ \Omega(\eta) \triangleq \int_{\Theta} \int_{\Theta} \log\{p(\theta|Y, \eta)\} p(Y, \theta|\eta) d\theta dY \right] \quad (5.2)$$



**Figure 5.1:** Demonstrating the calculation of optimal design based on (a) Lindley’s *EVOI* concept and (b) Shannon information criterion.

Other Bayesian DOE methodologies follow a similar line as (5.2) with the main difference being the choice of the utility function. In a broad sense, there exist three categories of Bayesian DOE approaches. First is the information maximization approach, which consists of maximizing the Kullback - Leibler distance between the prior and the posterior distribution. This approach includes the well-known D-optimal and Ds-optimal designs. The second category is the set of designs with the objective is to obtain a point estimate of the parameter values. The A-optimal and C-optimal designs belong to this category. The third category is the mini-max type of designs, where the objective is to minimize the maximum possible variance for all the linear combinations of the

parameters under consideration. E-optimal and G-optimal designs fall into this category. These various designs are further explained in details as follows:

**D - Optimal:** Maximize information gain for the parameters (Uses Kullback-Leibler distance between the prior and posterior distribution as a measure of gain in information).

**Ds-optimality:** Maximize gain in Shannon information of  $\Psi (= s^T\theta)$ , where ‘s’ is a known constant vector.

**A- Optimal:** The objective of the experiment is to obtain a point estimate of the parameters. A design is chosen to maximize the following objective function:

$$\Omega(\eta) = -\int (\theta - \hat{\theta})^T A(\theta - \hat{\theta}) p(y, \theta | \eta) d\theta dY \quad (5.3)$$

Here ‘A’ is a symmetric positive semi-definite matrix. This design minimizes expected squared error of loss for estimating  $c^T\theta$  or minimizing squared error for predicting  $c^T\theta$ , where  $c$  is an arbitrary vector of appropriate dimension.

A special case of A-optimality is when  $c$  is a specific, known vector. This case is referred to as **C-optimal design**.

**E- Optimal:** This is a mini-max approach for variance. The maximum posterior variance of all possible normalized linear combinations of parameter estimates is minimized. An E-optimal design minimizes:

$$\sup_{\|c\|=\omega} c^T (\eta^T \eta + R)^{-1} c = \omega^2 \lambda_{\max} \left[ (\eta^T \eta + R)^{-1} \right] \quad (5.4)$$

where ‘ $\eta$ ’ is the design matrix,  $\sigma^2 R^{-1}$  is the covariance matrix for the parameter ‘ $\theta$ ’ and  $\sigma^2$  is the variance of the known noise.

**G- Optimal:** Closely related to E-optimal design is G-optimal design, which minimizes  $\sup_{x \in D} x^T (\eta^T \eta + R)^{-1} x$ .

It is important to note that, among the above mentioned designs, D-, Ds-, A- and C-optimal design have a corresponding utility function, which justifies its decision theoretic sense. On the other hand, E- and G-optimal designs, though considered Bayesian designs, do not correspond to any specific utility function (Chaloner and Verdinelli 1995).

### **5.3. Decision – oriented design criterions**

As elaborated in the previous section the traditional design criterions either try to maximize the information gain or minimize the variance. Consider the following two objectives of experimentation:

- a) To evaluate the true potential of the process, i.e. the maximum of the revenue function value for the process.
- b) To select/reject processes from a large set of candidate processes

In either of the above scenarios, the traditional parameter variance minimization design techniques may not give the best chance of making a correct decision. For example, assume that the selection criterion is based on a cut-off value of operating profit margins, say \$10M/yr, and processes that have operating profit margins equal or above the cut-off are worth pursuing. The question then may be: Should one be more focused towards reducing the overall parameter uncertainty or towards designing experiment strategies that directly target this objective?

In order to design experiments focused on the above mentioned two objectives, we propose the following two design criteria:

- a) Design experiments that **Maximize** the expected operating **Profit Margin** (*MPM*).

- b) Design experiments that **Maximize the Probability of Decision** (either Acceptance or Rejection) for a process (*MPD*).

The premise for *MPM* is that the designs that try to obtain the maximum operating profit margins would inherently be able to obtain values closer to the true optimal operating profit margin values. In order to obtain such a DOE, we substitute the operating profit margin function in place of the utility function  $f^*$  in (5.1).

Contrary to *MPM*, in *MPD* the decision maker is not only concerned about the posterior mean value of the operating profit margins but also about the variance of the posterior operating profit margins. The idea for optimal selection of a design matrix for *MPD* is to select the one that maximizes the probability of decision, either acceptance or rejection. Such an objective function may be degenerate and may give multiple optimal design choices. In order to avoid such circumstances, we introduce an additional negatively weighted term in the objective function, corresponding to normalized variance of the posterior expected optimal objective operating profit margins.

### **5.3.1 Problem formulation**

Assume that an initial model structure and prior estimates for the model parameters are available from earlier experimental results or expert knowledge. The decision-maker wants to perform additional experiments to select the few processes with the most potential.

Assume the yield ( $y_1$ ) of the process has a linear model,  $y_1 = \eta^T \theta_1 + \varepsilon_1$  where  $\eta$  is the vector of the operating conditions to be optimized and  $\varepsilon_1$  is the Gaussian noise,  $N(0, \sigma)$  with known variance ( $\sigma^2$ ). In this example,  $\eta$  represents both the experiment design

variables and operating variables to be optimized a posteriori. To avoid confusion, we will use the notation  $\eta_{ex}$  (denoted ‘ $\eta$ ’ previously) and  $\eta_{op}$  (denoted by ‘ $u$ ’ previously) respectively whenever the distinction is needed. We assume that the quality of the product ( $y_2$ ) also varies linearly,  $y_2 = \eta^T \theta_2 + \varepsilon_2$ , with the operating conditions and the target quality is  $\mu$ . We consider the operating profit margin function ‘ $f$ ’ in (5.5), which depends linearly on the yield value, and also includes a quadratic penalty for the quality deviation and a quadratic penalty for higher operating conditions.

$$f = \alpha \cdot y_1 - \beta \cdot (y_2 - \mu)^2 - \frac{1}{2} \eta_{op}^T \cdot Q \cdot \eta_{op} \quad (5.5)$$

To evaluate the new design criterion, we consider ‘ $\eta$ ’ to be a two dimensional vector and hence both the prior parameter estimates  $\theta_1 = [\theta_{1,1}, \theta_{1,2}]^T$  &  $\theta_2 = [\theta_{2,1}, \theta_{2,2}]^T$  are also two dimensional vectors. We consider the range of the operating conditions to be in the range of  $[1e^{-5}, 10]$ . We consider the prior estimates of the parameters ( $\theta_1$  and  $\theta_2$ ) to be normal distributions with mean  $\bar{\theta}_1 = [\bar{\theta}_{1,1}, \bar{\theta}_{1,2}]^T$ ,  $\bar{\theta}_2 = [\bar{\theta}_{2,1}, \bar{\theta}_{2,2}]^T$  and covariance matrices  $\Sigma_{\theta_1}$  and  $\Sigma_{\theta_2}$  respectively.

In order to statistically evaluate the performance of our DOE approach against the traditional D-optimal DOE approach, we consider the distributions for the parameter values as shown in (5.6) - (5.15) as follows:

$$\bar{\theta}_{1,1} \sim U[-100, 100] \quad (5.6)$$

$$\bar{\theta}_{1,2} \sim U[\max(-100, -\bar{\theta}_{1,1}), 100] \quad (5.7)$$

$$\bar{\theta}_{2,1} \sim U[-100, 100] \quad (5.8)$$

$$\bar{\theta}_{2,2} \sim U \left[ \max(-100, -\bar{\theta}_{2,1}), 100 \right] \quad (5.9)$$

$$\Sigma_{\theta_1} = \begin{bmatrix} (0.1 * \bar{\theta}_{1,1})^2 & 0 \\ 0 & (0.1 * \bar{\theta}_{1,2})^2 \end{bmatrix} \quad (5.10)$$

$$\Sigma_{\theta_2} = \begin{bmatrix} (0.1 * \bar{\theta}_{2,1})^2 & 0 \\ 0 & (0.1 * \bar{\theta}_{2,2})^2 \end{bmatrix} \quad (5.11)$$

$$\sigma = 5 * \sqrt{\min \left( (0.1 * \bar{\theta}_{1,1})^2, (0.1 * \bar{\theta}_{1,2})^2 \right)} \quad (5.12)$$

$$\mu \sim U \left[ 0.5 * 1e^{-5} * \min(\bar{\theta}_{2,1}, \bar{\theta}_{2,2}), 1.5 * 10 * \max(\bar{\theta}_{2,1}, \bar{\theta}_{2,2}) \right] \quad (5.13)$$

$$\alpha \sim U \left[ 1e^{-5}, 10 \right] \quad (5.14)$$

$$\beta \sim U \left[ 1e^{-5}, 10 \right] \quad (5.15)$$

In the above equations,  $U[a, b]$  represents the uniform distribution spanning the range between ‘ $a$ ’ and ‘ $b$ ’. The idea behind choosing the above parameter space is not only to have a sufficiently broad range of the parameter space but also to have some realistically sensible parameter values. The noise to signal ratio is approximately maintained at 10%, as shown in (5.12). Since the yield values depend on the operating conditions, which are not decided a priori, an average value (‘5’ to be specific) of the operating conditions is assumed, in order to determine the noise to signal ratio. This results in a higher noise to signal ratio at a low signal value, which is consistent with the most real situations. The quadratic penalty matrix ‘ $Q$ ’ is sampled appropriately (using (5.16) – (5.20)) so that it is positive definite and represents a practically reasonable value.

$$Q = \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix}, \text{ where} \quad (5.16)$$

$$q_{11} \sim U \left[ 1e^{-5}, \alpha^* | (\bar{\theta}_{1,1} + \bar{\theta}_{1,2}) / 2 | \right] \quad (5.17)$$

$$q_{22} \sim U \left[ 1e^{-5}, \alpha^* | (\bar{\theta}_{2,1} + \bar{\theta}_{2,2}) / 2 | \right] \quad (5.18)$$

$$q_{12} \sim U \left[ 1e^{-5}, \sqrt{q_{11} * q_{22}} \right] \quad (5.19)$$

$$q_{21} \sim U \left[ 1e^{-5}, q_{11} * q_{22} / q_{12} \right] \quad (5.20)$$

The user defined cut-off value, needed for *MPD*, is defined as follows:

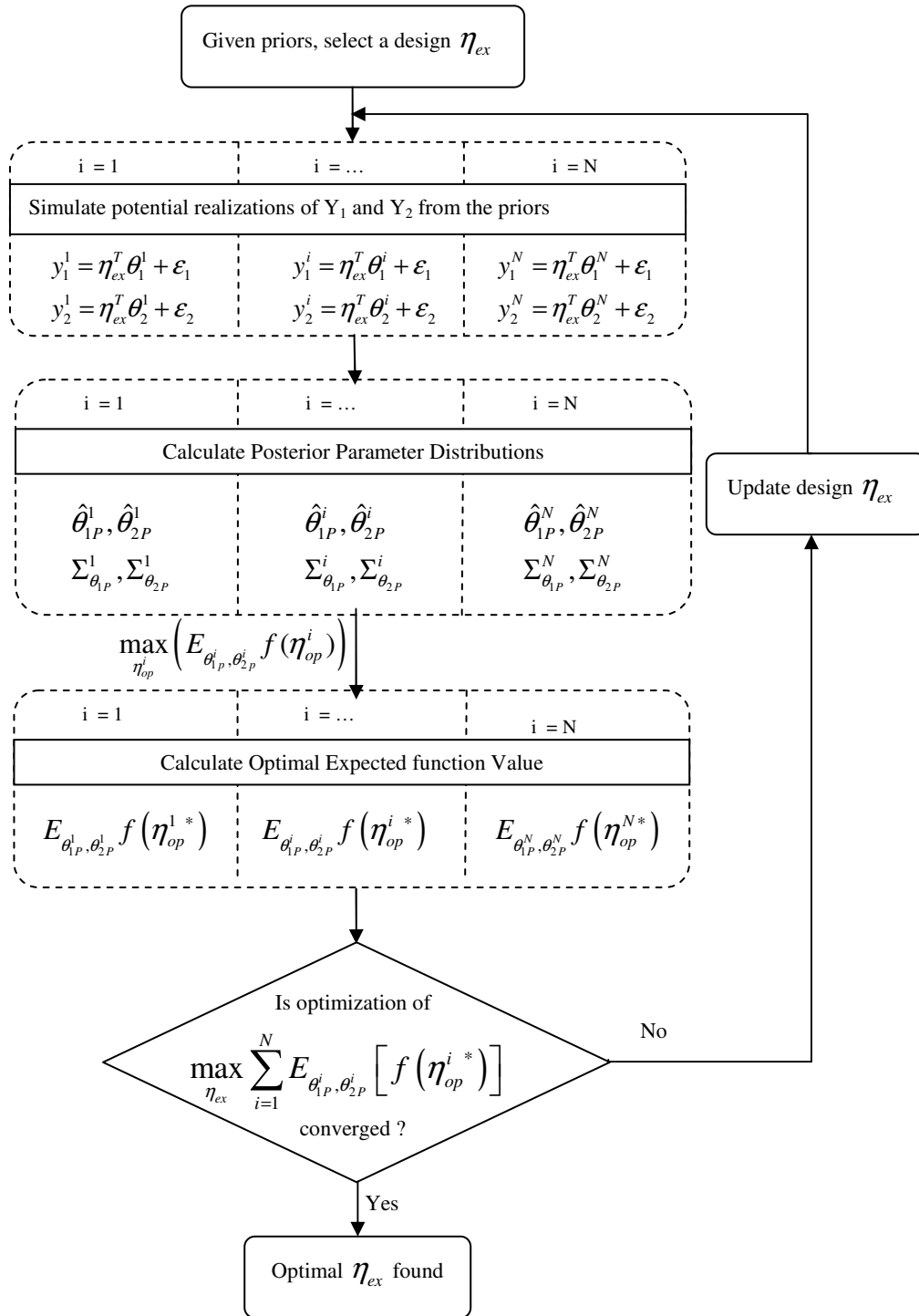
$$cutoff = \max \left( 0, \max_{\eta_{op}} \left( \alpha^* \eta_{op}^T \bar{\theta}_1 - \beta^* (\eta_{op}^T \bar{\theta}_2 - \mu)^2 - \frac{1}{2} \eta_{op}^T * Q^* \eta_{op} \right) \right) \quad (5.21)$$

For the purpose of evaluating the performance, we need to assume some true parameter values, which are unknown to the decision-maker. They will be drawn randomly from the prior parameter distributions.

### 5.3.2 Solution approach for *MPM*

To obtain the optimal design solution for the above mentioned problem, we need to solve equation (5.22). In (5.22)  $Y$  is the two dimensional vector  $[y_1, y_2]^T$ , corresponding to the yield and the quality value. And  $\Theta$  is the vector of the corresponding parameters for the yield ( $\theta_1 = [\theta_{1,1}, \theta_{1,2}]^T$ ) and quality ( $\theta_2 = [\theta_{2,1}, \theta_{2,2}]^T$ ) respectively. The algorithm to calculate the optimal design via (5.21) is shown in figure (5.2).

$$\eta_{ex}^* = \arg \max_{\eta_{ex}} \left[ \Omega(\eta) \triangleq \int_Y \max_{\eta_{ex}} \int_{\Theta} f(\theta, Y, \eta_{op}) p(\theta | Y, \eta_{ex}) p(Y | \eta_{ex}) d\theta dY \right] \quad (5.22)$$



**Figure 5.2:** Algorithm to calculate the optimal decision oriented design of experiment for *MPM*. (Note: The posterior covariance matrix is independent of the sampled data, so the posterior covariance matrix would be the same for all the realizations)

The calculation algorithm consists of two stages of optimization. The outer optimization is for selecting the optimal design and the inner optimization is for obtaining the optimal posterior operating conditions. The details for evaluating a given design ‘ $\eta$ ’ are explained as follows:

Step 0: Assume an initial design ‘ $\eta_{ex}$ ’

Step 1: Based on the given design and the prior distributions for the parameters  $\theta_1 = [\theta_{1,1}, \theta_{1,2}]^T$  and  $\theta_2 = [\theta_{2,1}, \theta_{2,2}]^T$  generate potential realizations of  $y_1^i$  and  $y_2^i$  for  $i = 1, 2, \dots, N$  (we consider  $N = 500$ ).

Step 2: For each given realization, calculate the posterior mean values and covariance matrices for the parameters  $\theta_1$  and  $\theta_2$ , denoted as  $\hat{\theta}_{1,p}$  and  $\hat{\theta}_{2,p}$  and  $\Sigma_{\theta_{1,p}}$  and  $\Sigma_{\theta_{2,p}}$  respectively.

Step 3: For each posterior distribution, obtain the optimal operating condition  $\eta_{op}^*$ .

Step 4: Calculate the expected value of the function ‘ $f$ ’ value with  $\eta_{op} = \eta_{op}^*$  for each of the distributions.

Step 5: Calculate the average of all the optimal expected function values calculated in Step 4.

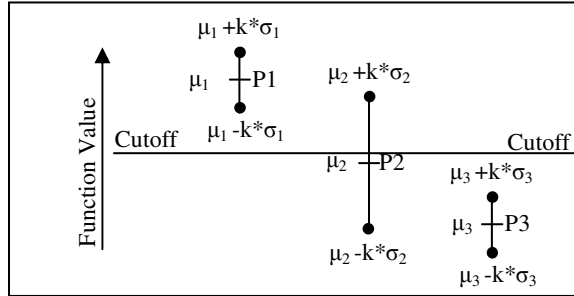
The value obtained in Step 5 is the score value signifying the potential of the given design ‘ $\eta_{ex}$ ’. In order to obtain the optimal design, maximization is performed over the experimental design variable space. This maximization is performed using the inbuilt function ‘*fmincon*’ in MATLAB.

### 5.3.3 Solution approach for MPD

Contrary to *MPM*, where we only take into consideration the posterior expected value of the operating profit margin, for this criterion we consider both the posterior

mean and variance of the posterior operating profit margin,  $f(\eta_{op}^*)$ . To elucidate further on this, consider the three processes (P1, P2 and P3) shown in Fig 5.3.

The selection criterion of the decision maker for these processes is that  $\mu - k^*\sigma$  be greater than the ‘Cut-off’ value and the rejection criterion being that  $\mu + k^*\sigma$  be less than the ‘Cut-off’, where  $\mu$  is the posterior mean and  $\sigma$  is the posterior standard deviation of the objective function ‘ $f$ ’ corresponding to the optimally chosen operating variable  $\eta_{op} = \eta_{op}^*$ . So, according to Figure 5.3, Process P1 is selected (as  $\mu_1 - k^*\sigma_1 > \text{‘Cut-off’}$ ), process P3 is rejected (as  $\mu_3 + k^*\sigma_3 < \text{‘Cut-off’}$ ) and process P2 is undecided (as neither  $\mu_2 - k^*\sigma_2 > \text{‘Cut-off’}$  nor  $\mu_2 + k^*\sigma_2 < \text{‘Cut-off’}$ ).



**Figure 5.3:** Acceptance/Rejection criterion

Design experiments for selection/rejection of processes based on this type of criterion can be done by maximising  $|\sum \delta_i|$ , where  $\delta_i$  is defined as follows:

$$\delta_i = \begin{cases} +1, & \text{if } \mu_i - k^* \sigma_i > \text{Cutoff} \\ -1, & \text{if } \mu_i + k^* \sigma_i < \text{Cutoff} \\ 0, & \text{Otherwise} \end{cases} \quad (5.23)$$

The subscript ‘ $i$ ’ represents the potential random samples with value ranging form  $i = 1, 2, \dots, N$ , as explained earlier in Section 5.3.2. The above criterion essentially measures how often the decision is reached and how consistently, since the (+1,-1) will

cancel. The calculation algorithm for *MPD* also consists of two stages of optimization. The outer optimization is for selecting the optimal design and the inner optimization is for obtaining the posterior optimal operating conditions. The algorithm to obtain an optimal *MPD* criterion is shown in figure 5.4. Further details for evaluating a given design ‘ $\eta$ ’ are explained as follows:

Step 0: Assume an initial design ‘ $\eta_{ex}$ ’

Step 1: Based on the given design and the prior distributions for the parameters  $\theta_1 = [\theta_{1,1}, \theta_{1,2}]^T$  and  $\theta_2 = [\theta_{2,1}, \theta_{2,2}]^T$  generate potential realizations of  $y_1^i$  and  $y_2^i$  for  $i = 1, 2, \dots, N$  (we consider  $N = 500$ ).

Step 2: For each given realization, calculate the posterior mean values and covariance matrices for the parameters  $\theta_1$  and  $\theta_2$ , denoted as  $\hat{\theta}_{1,p}$  and  $\hat{\theta}_{2,p}$  and  $\Sigma_{\theta_1,p}$  and  $\Sigma_{\theta_2,p}$  respectively.

Step 3: For each posterior distribution, obtain the optimal operating condition  $\eta_{op}^*$  and also the expected value of the function  $f(\eta_{op}^*)$ .

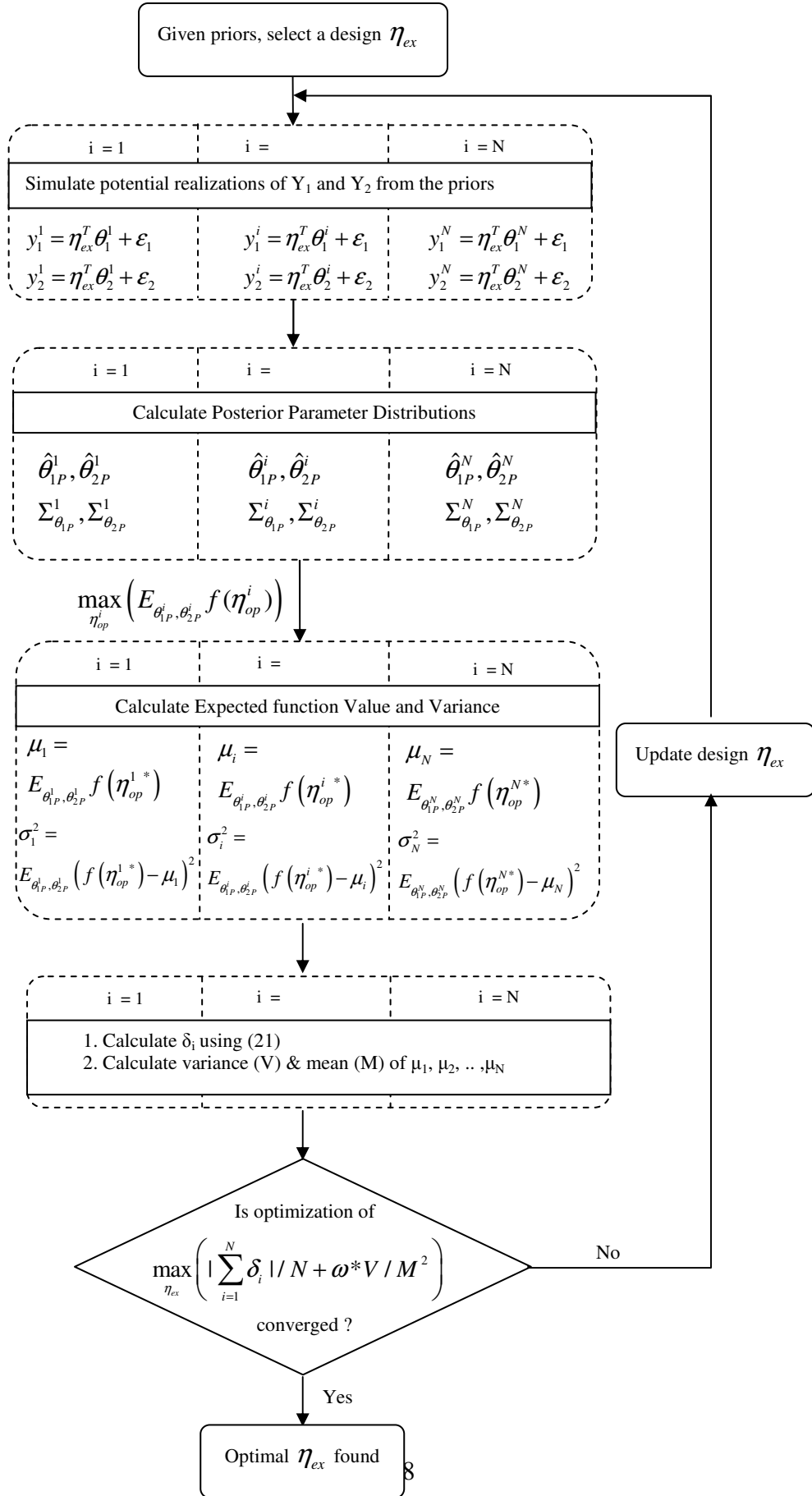
Step 4: Calculate both the expected value ( $\mu_i$ ) and the variance ( $\sigma_i$ ) of the optimal function ‘ $f$ ’ value for each of the distributions.

Step 5: Based on the estimated mean ( $\mu_i$ ) and variance ( $\sigma_i$ ) values calculate  $\delta_i$ .

Step 6: Find the weighted sum of the following two quantities:

- a) Normalized absolute value of the sum of all  $\delta_i$  for  $i = 1, 2, \dots, N$ , i.e.  $|\Sigma \delta_i|/N$
- b) Normalized variance of the posterior mean values ( $\mu_i$ )

$$MPD = |\Sigma \delta_i|/N + w * \text{variance}(\mu_i / (\Sigma \mu_i / N)) \quad (5.24)$$



**Figure 5.4:** Algorithm to calculate the optimal decision oriented design of experiment for *MPD*

The value obtained in Step 6 or (5.24) is the score value signifying the potential of the given design ‘ $\eta$ ’. In order to obtain the optimal design, maximization is performed over the design space. This maximization is performed using the inbuilt function ‘*fmincon*’ in MATLAB.

## 5.4. Results

### 5.4.1 Maximize Operating Profit Margins (*MPM*)

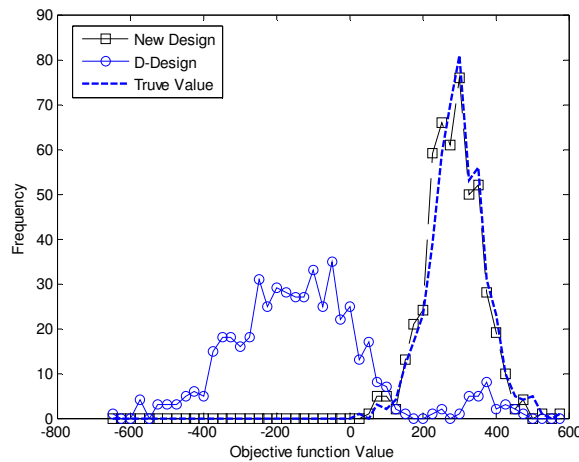
To compare the performance of our new design approach with that of the D-optimal design approach, we generated 200 scenarios of nominal parameter values ( $\bar{\theta}_1, \bar{\theta}_2, \mu, \alpha, \beta$  and  $Q$  through random sampling) and performed the two types of design for each scenario. Then, to evaluate the performance for each design for each of the 200 scenario, 500 samples of the “true” parameter values, unknown to the decision-maker, are randomly sampled from the given prior distributions. Each of these true parameter values are used to generate the experimental data using the given DOE, which in turn are used to calculate the parameter estimates and then the optimal value of operating condition  $\eta$  based on them, denoted hereafter by  $\eta_{pred}^*$ . Then, the profit margin values corresponding to the predicted optimal operating condition  $\eta_{pred}^*$  as well as the true optimal operating condition  $\eta_{true}^*$  (calculated based on the true parameter values) are calculated.

For performance measure, we used the closeness of the predicted operating profit margin value (*i.e.*, the profit margin corresponding to  $\eta_{pred}^*$ ) to the true optimal operating profit margin value (*i.e.*, the profit margin value corresponding to  $\eta_{true}^*$ ). Then, the

percentage of times (out of  $200 * 500 = 100,000$  cases) a particular design gives a predicted value closer to the true value than the other design is reported as the ‘Performance Index’ of that design.

**Table 5.1:** Comparison of performance of new decision oriented (*MPM*) and D-optimal designs for the 10% noise case.

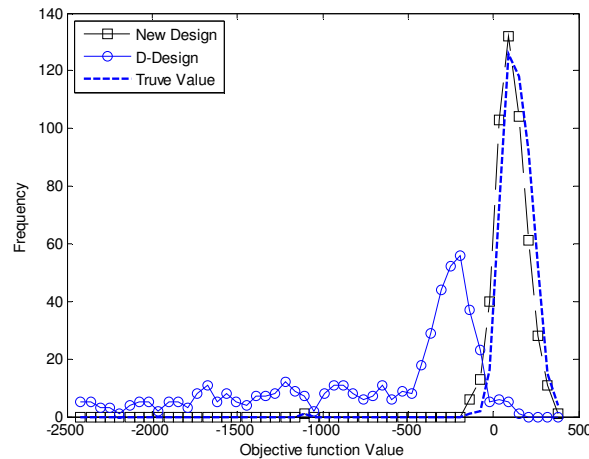
Type of Prior Distribution	‘Performance Index’	
	New Design	D Design
<i>Strongly Informative</i>	45.23	25.99
<i>Informative</i>	53.51	22.81
<i>Mildly Informative</i>	58.22	21.11
<i>Un-Informative</i>	63.57	17.30



**Figure 5.5:** Histogram comparing the predictions of the maximum profit margin from the new decision oriented (*MPM*) design and D-optimal design to the true value for ‘*Mildly Informative*’ prior distribution.

**Table 5.2:** Comparison of performance of the new decision oriented (*MPM*) design and the D-optimal designs for the 5% noise case

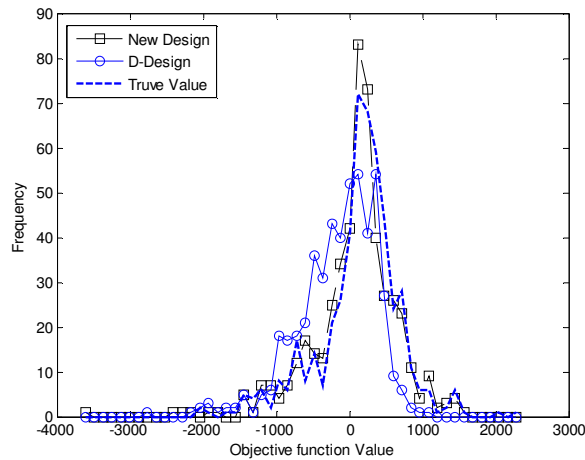
Type of Prior Distribution	'Performance Index'	
	New Design	D Design
<i>Strongly Informative</i>	52.83	23.37
<i>Informative</i>	60.51	18.29
<i>Mildly Informative</i>	63.96	16.43
<i>Un-Informative</i>	67.30	14.09



**Figure 5.6:** Histogram comparing the predictions of the maximum profit margin from the new decision oriented (*MPM*) design and D-optimal design to the true value for '*Informative*' prior distribution.

In order to check if the kind of prior distribution has an effect on the relative performance of the new-design approach to the D-optimal design, we tried four different levels of prior information. '*Informative*' prior distribution represents the one with the square root of the diagonal elements of the prior covariance matrix being 10% of the

prior mean of the respective parameter, as shown in (5.10) and (5.11). ‘*Strongly Informative*’ prior distribution has smaller variances and is obtained by replacing the 0.1 values by 0.05 in (5.10) and (5.11). On the other hand, ‘*Mildly Informative*’ prior distribution has somewhat larger variances and is obtained by replacing 0.1 values by 0.15 in (5.10) and (5.11). Finally, ‘*Un-Informative*’ prior distribution has highest variances and is obtained by replacing 0.1 values by 0.30 in (5.10) and (5.11). The comparison of the performance measure for our decision-oriented (*MPM*) and the D-optimal design is shown in Table 5.1. The above results clearly show ~20-35% improvement in the prediction power of the model obtained from the decision-oriented design compared to the D-optimal design of experiments.



**Figure 5.7:** Histogram comparing the predictions of the maximum profit margin from the new decision oriented (*MPM*) design and D-optimal design to the true value for ‘*Strongly Informative*’ prior distribution.

**Table 5.3:** Comparison of performance of the new decision oriented (*MPM*) design and the D-optimal designs for the 15% noise case

Type of Prior Distribution	'Performance Index'	
	New Design	D Design
<i>Strongly Informative</i>	39.52	25.40
<i>Informative</i>	49.31	24.81
<i>Mildly Informative</i>	53.54	22.66
<i>Un-Informative</i>	60.26	19.12

To give more insight into the results we plot the histogram of the optimal operating margin values for the decision oriented (*MPM*) and D-optimal design along with the true optimal operating margin values (determined assuming that the 'true' parameter values are known), for a particular set of parameter values with 500 different 'true' parameter values being sampled from the prior distribution. To be precise, these are the operating margins for the 'true' plant (with 'true' parameter values) with the optimal operating conditions determined based on the parameter estimates resulting from the respective DOEs. Figure 5.5 shows the histogram for '*Mildly Informative*' prior distribution, with 500 'true' parameter values sampled from the prior distribution. The histograms for the '*Informative*' and '*Strongly Informative*' are shown in Figure 5.6 and figure 5.7 respectively. They clearly demonstrate the better performance of the decision-oriented DOE strategy compared to traditional D-optimal design strategy.

In order to check if noise has any significant impact on the performance of the decision-oriented designs, we vary the noise measured by the variance of the Gaussian noise in (5.12). In comparison to the initial noise of 10% as specified by the value 0.1 in

(5.12), we test two other levels of noise, 5% and 15% , which correspond to changing ‘0.1 value in (5.12) to 0.05 and 0.15 respectively. The results for the 5% and the 15% noise cases are shown in the Table 5.2 and Table 5.3 respectively. The results clearly demonstrate that the decision-optimal design outperforms the D-optimal design regardless of the noise level.

#### **5.4.2 Maximize Probability of Decision (*MPD*)**

To compare the results given by our new design approach designed to maximize the probability of decision and the D-optimal design approach, we tested 400 scenarios for different nominal parameter values. To measure the performances of the different designs, we measure the frequency of both correct and incorrect decisions, out of 200,000 (400\*500) cases. The percentage of times the design choice reports a correct/incorrect decision is reported as ‘Performance Index – Correct/Incorrect Decision’, denoted by  $PI_{CD}/PI_{ID}$ , of that design.

Similar to the cases in *MPM*, we test four levels of prior knowledge. As mentioned in Section 5.3.2, we consider a weight constant  $w$  in the *MPD* decision criterion. Since, the secondary term (normalized variance of the expected value of the posterior optimal operating profit margins) is introduced in order to reduce the degeneracy in the optimization, we keep the value of  $w$  to be of small magnitude ( $w = 0.001$ ). The results for the *MPD* design and the D-optimal design are compared in Table 5.4. The results ( $PI_{CD}$  values) indicate that the *MPD* design outperforms the D-optimal design and the relative improvement of the *MPD* criterion is more for the less informative priors. The results also indicate an increase in the  $PI_{CD}$  (probability of correct decision) values is accompanied by a small increase in the  $PI_{ID}$  (probability of incorrect decision)

values. This signifies that the *MPD* approach is relatively more aggressive, in terms of giving decisions, compared to the D-optimal design.

**Table 5.4:** Comparison of performance of the new decision oriented (*MPD*) design and the D-optimal designs for the 10% noise case ( $w = -0.001$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	44.43	0.74	43.14	0.57
<i>Informative</i>	44.29	0.98	38.84	0.51
<i>Mildly Informative</i>	43.99	1.04	36.28	0.58
<i>Un-Informative</i>	36.48	1.17	31.08	0.69

**Table 5.5:** Comparison of performance of the new decision oriented (*MPD*) design and the D-optimal designs for the 5% noise case ( $w = -0.001$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	50.23	0.88	47.68	0.64
<i>Informative</i>	49.67	1.06	42.32	0.58
<i>Mildly Informative</i>	48.03	1.12	39.16	0.69
<i>Un-Informative</i>	39.76	1.25	32.75	0.72

**Table 5.6:** Comparison of performance of the new decision-oriented (*MPD*) design and the D-optimal designs for the 15% noise case ( $w = -0.001$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	40.98	0.63	40.07	0.54
<i>Informative</i>	41.97	0.93	36.72	0.49
<i>Mildly Informative</i>	41.42	1.02	33.99	0.52
<i>Un-Informative</i>	34.65	1.07	29.44	0.63

To evaluate the effect of the level of noise on the performance of the *MPD* criterion, we again tested two other levels of noise, 5% and 15%. The results for the 5% and 15% noise level cases are presented in Tables 5.5 and 5.6, respectively. The results for these two additional levels demonstrate that the *MPD* design outperforms the D-optimal design irrespective of the noise level.

**Table 5.7:** Comparison of performance of the new decision oriented (*MPD*) design and the D-optimal designs for the 10% noise case ( $w = -0.005$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	44.29	0.71	43.14	0.57
<i>Informative</i>	44.68	1.10	38.84	0.50
<i>Mildly Informative</i>	44.18	1.15	36.29	0.58
<i>Un-Informative</i>	37.90	1.28	31.10	0.67

**Table 5.8:** Comparison of performance of the decision oriented (*MPD*), design and the D-optimal designs for the 5% noise case ( $w = -0.005$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	50.04	0.88	47.68	0.64
<i>Informative</i>	49.72	1.10	42.30	0.61
<i>Mildly Informative</i>	48.25	1.17	39.20	0.66
<i>Un-Informative</i>	42.16	1.27	32.70	0.77

**Table 5.9:** Comparison of performance of the new decision-oriented (*MPD*) design and the D-optimal designs for the 15% noise case ( $w = -0.005$ )

Type of Prior Distribution	'Performance Index'			
	New Design		D Design	
	PI <sub>CD</sub>	PI <sub>ID</sub>	PI <sub>CD</sub>	PI <sub>ID</sub>
<i>Strongly Informative</i>	41.28	0.65	40.07	0.54
<i>Informative</i>	41.92	0.97	36.73	0.49
<i>Mildly Informative</i>	41.50	1.20	34.01	0.50
<i>Un-Informative</i>	35.84	1.24	29.43	0.63

As explained earlier, the idea is to keep a small value of  $w$  and to do so we assigned the value of  $w = -0.001$ . To evaluate whether a specific (small) choice of value has any significant effect on the performance of the *MPD* design, we evaluated the relative performance of the design criteria for the  $w$  value of  $-0.005$ . The results for the new value of ' $w$ ' (see Table 5.7, 5.8 and 5.9) are similar. The results show that the choice

of 'w' value does not have a significant effect on the result for the case of well informed priors. But there might exist, some potential benefits in the choice of  $w$  values for the case of ill-informed priors.

## **5.5 Conclusions**

We introduced two new decision oriented design of experiment strategies, which significantly improve decision-making compared to the D-optimal or other traditional optimal design strategies. The *MPM* criterion, which is mainly based on the mean value of the optimal operating profit margin, shows an improvement of 25-30% in the prediction of the true optimal profit margin. Moreover the *MPD* criterion, which is based on both the mean and the variance of the optimal operating profit margin, is used for the Acceptance/Rejection of candidates. The use of *MPD* criterion led to a smaller improvement compared to the D-optimal designs for a relatively informed prior though the performance improvement was more significant for less informed priors. Overall the both decision-oriented designs demonstrate significant improvements over the traditional D-optimal design of experiment strategy, as they directly address the ultimate objective of the experiment.

# **CHAPTER VI**

## **HIEARCHICAL BAYESESIAN FRAMEWORK FOR IMPROVED R&D DECISIONS**

Decisions during the early stages of R&D are made under uncertainty. Evaluation of R&D alternatives under uncertainty generally does not provide a clear choice that is best under all possible scenarios. In such cases, the decision maker may either make the selection based on a user defined utility function, or conduct more experiments to further reduce uncertainty in the most promising alternatives, so that a better decision can be reached. The latter option has more intrinsic appeal, but conducting experiments to reduce uncertainty can be both time consuming and expensive. Hence, it is important to have a systematic approach and accompanying design of experiment (DOE) strategies that are geared towards a particular selection criterion adopted.

In this chapter, we present the integration of the previous three chapters' contributions: a hierarchical Bayesian approach to improve R&D decision-making. To recap, the hierarchical Bayesian approach consists of three major components. The first component quantifies the uncertainties as probability distributions. The second component provides information about the contribution of various uncertainty factors to the downside risk. The third component addresses the allocation of resources and design of experiments which have the aim of making the best selection among the alternatives under a given criterion. This is in contrast to the traditional design of experiments approaches that are geared towards minimizing some measure of the parameter uncertainty. The utility of the hierarchical approach is demonstrated using a real case

study (Hemi-cellulose pre-extraction to produce ethanol in a thermo mechanical pulp producing mill)

## **6.1 Introduction**

Development of new and improved processes and products through investment in research is a key driving force in the competitiveness of any industry. Investment in research and development (R&D) is considered high risk and high return. Hence, the systematic reduction of uncertainty in R&D options is undeniably an important problem. This has led to a significant body of research in the field of optimal R&D investment decision-making with the main focus on R&D portfolio optimization or the optimal timing of adoption or investment in R&D (Grenadier and Weiss 1997; Sampson 1998; Doraszelski 2004). This line of research addresses the key issues when the objective is to select a portfolio of non-competing processes and products or select the optimal timing of R&D investment.

Once the portfolio is selected, the second stage of the problem is to make R&D investment decisions within an individual R&D project. Alternatively, another class of problems is the selection of the best alternative among many R&D alternatives. A systematic method to optimally resolve the uncertainties is needed to address such problems.

Though this problem is intrinsically very important by itself, limited literature exists addressing this problem. To the authors' knowledge, there has been only one previous publication: Bode (2006) addresses the problem of decision making in development projects. Bode (2006) introduced a methodology to address risk in a

development project but they did not go into details on how to address various individual issues quantitatively. Some of the key issues in such problems are:

- a. *Lack of quantitative information*: This makes it very difficult for the decision maker to compare various R&D alternatives and to evaluate the true potentials of the alternatives. For example, the decision maker cannot calculate the utility (e.g. Net present value, (NPV)) distributions for the various alternatives. Due to the lack of quantitative information, optimization over the operating conditions is not possible and hence it is not possible to evaluate the optimal utility distributions. The lack of quantitative information makes it hard to quantify the performance of the R&D investment plan and further limits the scope of optimizing R&D investment.
- b. *Key Uncertainties*: Generally multiple sources of epistemic/technical uncertainties exist in a R&D project. Tools such as GSA (Global Sensitivity Analysis) can be used by the decision maker to find the major uncertainty contributors. However, often GSA is unable to differentiate among the various uncertainties, i.e. it often assigns equal or similar global sensitivity indices to two or more uncertainties.
- c. *Optimal Design of Experiment*: Once the main uncertainty contributing factors are known, one can perform experiments to reduce uncertainty. The traditional approaches to the design of experiment focus towards the uncertainty reduction in the parameter estimates of the underlying model, whereas during the initial stages of R&D investigations the main focus is towards the ‘invest’/‘don’t invest’ type of decision.

In this chapter we will present a hierarchical Bayesian approach that addresses all the above mentioned key issues and provides the decision maker with a systematic

procedure to address R&D investment decision problems. The hierarchical framework consists of various tools that address different parts of the problem. When integrated together, they are capable of addressing the overall R&D investment decision problem.

In order to demonstrate the value of the introduced Bayesian framework in a real problem setting, we consider a case-study involving biofuel production. The rest of the chapter is structured as follows: In section 6.2, the ‘Bayesian Framework’ is introduced. Section 6.3 introduces the biofuel case study and the results of the application of the ‘Bayesian Framework’ to the case study are presented in Section 6.4. Finally section 6.5 concludes the chapter.

## **6.2 Hierarchical bayesian framework**

The key challenge that a decision maker faces during the evaluation of R&D alternatives is the lack of quantitative information. This is driven by either the complete absence of experimental data or lack of sufficient experimental data to quantify the uncertainty. R&D alternatives or ideas are based on intuitions and insights of experts and this knowledge of experts is often qualitative in nature. Hence a methodology is needed to translate the qualitative knowledge of experts into quantitative information.

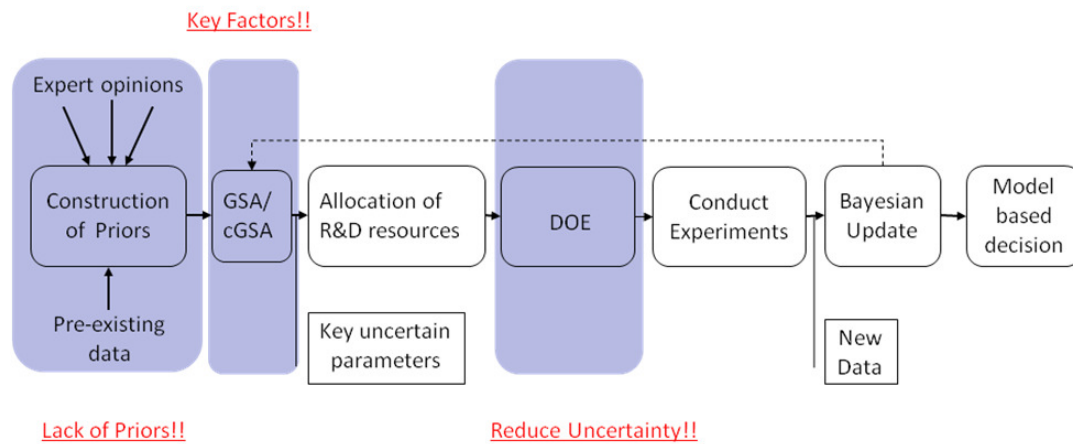
Quantification of expert’s knowledge can be in terms of model structures and/or parameter estimates. Furthermore, the parameter estimates can be a point estimate or a distribution. Since point estimates do not account for the uncertainty whereas parameter distributions account for both uncertainty and experts’ confidence (confidence can be measured in terms of the spread of the distribution), distributions are preferred way to quantify uncertainty. Furthermore, similar to design of experiment where more than one

experiment is conducted, knowledge from multiple experts can be quantified and integrated to obtain a more balanced estimate of uncertainty.

Once the technical uncertainty is quantified, the decision maker can perform Monte Carlo analysis to evaluate revenue/profit distributions for the various alternatives. If any alternative demonstrates a stochastic dominance over the rest of the alternatives the decision maker's job is complete and the scientists can pursue that alternative. Generally, this is not the case and none of the R&D alternatives shows complete stochastic dominance over the rest of the alternatives. In such scenarios the decision maker is left with two choices: Select an alternative based on a user defined utility function or conduct additional experiments to further reduce uncertainty for the most promising alternatives, so that a decision can be reached. The latter choice has more scientific appeal, but conducting experiments to reduce uncertainty can be both time consuming and expensive. Hence, an approach is needed that both reduces the experimental effort and directs the design of experiment efforts towards the chosen decision criterion, i.e. the objective of the selection of the best alternative.

In order to reduce the experimental efforts, the decision maker needs to estimate and understand the various sources of uncertainties. Each alternative consists of both technical uncertainties (i.e., epistemic uncertainties, which can be reduced by further experimentation, e.g. model/parameter uncertainty) and financial uncertainties (i.e., aleatory uncertainties, which cannot be reduced via further experimentation, e.g. product demand, raw material price, etc.). It is the epistemic uncertainties over which the decision maker has some control and needs to devise a strategy to optimally channel the available resources to reduce them.

As a first step to reduce the experimental efforts, the decision maker needs to identify the key sources of uncertainties. Traditionally, for such type of analysis one would use the Global Sensitivity Analysis (GSA), which accounts for the variance each uncertain factor contributes to the overall variance. However, GSA often times fails to give a clear order among the various uncertainties, i.e. it assigns equal global sensitivity index (GSI) to some uncertainties. For such scenarios, we consider conditional global sensitivity analysis, c-GSA, which compares the upside and downside risk contributed by the various uncertainties in order to further sort out the key uncertainties. (See Chapter 4 for more details).



**Figure 6.1:** Hierarchical Bayesian framework for improved R&D decisions

Once the key uncertainty contributors are found, the decision maker allocates the available resources to reducing them. As a next step, it is important to channel the resources to design of experiments, in a manner directly geared towards resolution of the decision maker's dilemma, which in this case is the selection of a most appropriate alternative in terms of the expected profit and risk. In order to achieve this goal, we

adopt the Bayesian decision oriented design of experiments (See Chapter 5 for more details).

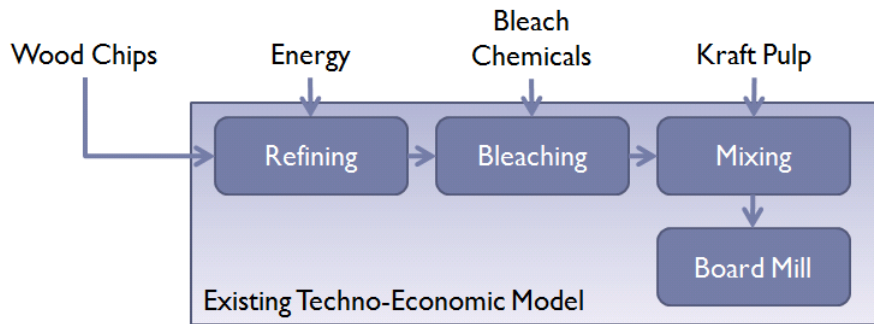
After the design of experiment strategy is devised, experiments can be conducted. The new experimental observations can be integrated with the prior distribution of the model parameters to obtain the posterior distributions. Using these posterior distributions one can again evaluate the various R&D alternatives. If an acceptable alternative is found, the decision maker's job is complete, but if not, the decision maker must return to perform the second and the third steps as mentioned above, starting with recalculation of the c-GSA indices.

The overall summary of the Bayesian framework is given in Figure 6.1. The first step is to quantify uncertainty by integrating all the available a priori information (pre-existing data, expert knowledge, etc.). Next, global sensitivity analysis (GSA) or/and c-GSA is performed to ascertain the key uncertainty contributing factors. Then the R&D resources are appropriately allocated to the identified sources of uncertainty to reduce the variance of the outcome. Given the above information, decision oriented design of experiment strategies are performed and experiments are conducted with the resulting design. The last step is to update the prior distribution to obtain the posterior distribution based on the observed data.

### **6.3. Case study (Hemicellulose Pre-Extraction in a Thermo Mechanical Pulping Mill)**

To demonstrate the importance of the developed hierarchical framework, we consider a biofuel related case study. Figure 6.2, shows a block diagram of a 'thermo-

mechanical pulping’ process. It is composed of three main unit operations ‘Refining’, ‘Bleaching’ and ‘Mixing’. In refining, a mechanical force is applied to the wood chips in a crushing or grinding action which, generates heat and water vapour and softens the lignin, thus separating the individual fibres. This process gives a high yield of fibre from the timber (around 95%) and as the lignin has not been removed, the fibres are hard and rigid. The refining is followed by bleaching, where bleach chemicals are used to improve the brightness of the pulp. Finally, the thermo mechanical pulp is mixed with the Kraft pulp. Each of these unit operations, refining, bleaching and mixing, determines the target product properties of ‘Runnability’, ‘Brightness’ and ‘Strength’, respectively. Thermo mechanical pulping is a well known process and we use a proprietary Microsoft excel/VBA based techno-economic model.



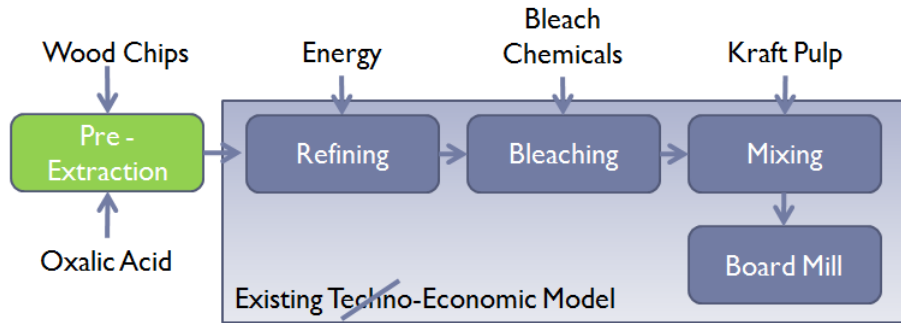
**Figure 6.2:** Block diagram of a traditional Thermo Mechanical pulping

As a bio-refinery option the R&D alternative under consideration is to introduce a pre-extraction stage before the wood is sent for refining (See figure 6.3). During the pre-extraction, significant fraction of hemi-cellulose can be extracted, from which ethanol can be produced via fermentation, and the rest of the woody biomass can be sent to the refining process. This potential option produces an additional value added product (ethanol) along with the traditional product paper. Introduction of pre-extraction prior to

the three unit operations leads to modifications in the technical models for each unit operation. In addition, a technical model for the pre-extraction is also required. Hence the introduction of the pre-extraction stage transforms the existing techno-economic models to an effectively economic model.

**Table 6.1:** List of technical and economic uncertainties for the TMP based biofuel alternative

	<b>Factors</b>	<b>Units</b>	<b>Uncertainty</b>	<b>Group</b>
Epistemic Uncertainty	Oxalic Acid Loading	%	U(0.5,3)	1
	Pretreatment Temperature	<sup>o</sup> C	U(120,150)	
	Hemicellulose Removed (Pre-treatment)	%	N(20,10)	2
	Extractives Removed(Pre-treatment)	%	N(50,10)	
	Cellulose Removed (Pre-treatment)	%	U(0,0.01)	
	Primary Refiner Specific Energy	MWhr/mt	N(0.9,0.1)	3
	Secondary Refiner Specific Energy	MWhr/mt	N(0.55,0.2)	
	Rejects specific energy	MWhr/mt	N(0.55,0.3)	
	Hydrogen Peroxide	%	U(1.5,2.5)	4
	Sodium Bisulphite	%	U(0.4,0.6)	
	Kraft Pulp	%	N(30,5)	5
Conversion Monosaccharide's to Ethanol	%	N(46,2)	6	
Conversion Oligomers to ethanol	%	N(20,1)		
Aleatory Uncertainty	Ground wood pulp <sup>1</sup>	%	N(27,5)	7
	LWC coating weight	%	N(15,5)	
	Wood chips price	\$/mt	N(68.2,4.54)	
	Electricity price	\$/MWhr	N(59.125,6)	
	Oxalic acid price	\$/kg	N(1,0.06)	
	Lime price	\$/kg	N(0.083,0.0775)	
	Hydrogen Peroxide price	\$/kg	U(0.74,0.86)	
	Sodium Hydroxide price	\$/kg	U(0.21,0.25)	
	Bisulfite price	\$/kg	U(0.59,0.61)	
	Kraft pulp price	\$/mt	N(880,126)	
	Groundwood pulp price	\$/mt	N(400,69)	
	Water treatment price	\$/mt	N(1,0.1)	
	Solid waste disposal price	\$/mt	N(40,5)	
	TMP mill process labor	\$/worker/day	U(198,218)	
	Ethanol plant process labor	\$/worker/day	U(198,218)	
	Other TMP mill variable operating costs	\$/mt	U(250,350)	
	Other Ethanol plant variable operating costs	\$/kg	U(0.05,0.15)	
	Ethanol price	\$/kg	N(0.736,0.19)	
	Acetic acid price	\$/kg	N(1.2,0.06)	
	Process steam (cost and price)	\$/mt	N(24.3,5.03)	
	TMP mill capital cost (\$/OD ton/yr)	\$/OD ton/yr	N(1953,200)	
	Ethanol plant capital cost (\$/gallon/yr)	\$/OD ton/yr	N(2,0.4)	
	Pretreatment capital cost (\$/OD ton/yr)	\$/gallon/yr	N(2.15,0.05)	



**Figure 6.3:** Block diagram of the alternative with biofuel production options in a Thermo Mechanical pulping mill

#### 6.4. Results

As a first step of the hierarchical approach, one needs to quantify the technical and economic uncertainty. List of the various uncertainties based on initial discussions with the experts are provided in the Table 6.1. The technical uncertainties are grouped according to the unit operation they belong to. Group 1 consists of the factors related to the operating conditions of the pre-extraction unit. Similarly group 2, 3, 4, 5, 6 and 7 consist of factors related to the pre-extraction yield, refining energy requirement, bleaching, pulp strength, fractional conversion of sugars to ethanol and the aleatory uncertainties, respectively.

Next more rigorous methods for elicitation of uncertainty are used, wherever possible. The elicited technical model for the pre-extraction yield of hemi-cellulose, cellulose and extractives is given by (6.1), (6.2) and (6.3), respectively. Further, the technical model for the brightness, runnability and pulp strength are given by (6.4), (6.5) and (6.6) respectively. The vector  $X$  is given by (6.7) and the variables  $T$ ,  $OA$ ,  $H_2O_2$ ,  $K$  and  $E$  represent the pre-extraction temperature, oxalic acid concentration in the pre-

extraction model, peroxide concentration in the bleaching process, percent mix of kraft pulp in the thermo-mechanical pulp mix, and the energy supplied for the refining process, respectively.

$$y_h = X^T \theta_h + \varepsilon_h \quad (6.1)$$

$$y_c = X^T \theta_c + \varepsilon_c \quad (6.2)$$

$$y_e = X^T \theta_e + \varepsilon_e \quad (6.3)$$

$$y_b = X^T \theta_b + \varepsilon_b \quad (6.4)$$

$$y_r = X^T \theta_r + \varepsilon_r \quad (6.5)$$

$$y_s = X^T \theta_s + \varepsilon_s \quad (6.6)$$

$$X = \begin{bmatrix} 1 & T & OA & OA^2 & H_2O_2 & (H_2O_2)^2 & K & E & E^2 & T*K & OA*K & OA^2*K \end{bmatrix} \quad (6.7)$$

Since the elicited models are linear with respect to the parameters as shown in (6.1) – (6.6), and standard methods (Wolfson 1995) exist for elicitation of parameter uncertainty exist (application of which has already been demonstrated in Chapter 3). Hence, we use mean and correlation matrices for various parameters ( $\theta_h, \theta_c, \theta_e, \theta_b, \theta_r$  and  $\theta_s$ ), which are assumed to be already assessable. The mean values are based on some preliminary experimental data, which is proprietary and hence those values are not reported here. The covariance matrices are assumed to be a diagonal matrix, with the magnitude of the diagonal element being square of the one tenth of the corresponding mean value. To account for the noise in the experimental observations, a 10% noise to signal ratio is assumed. Given these uncertainties, global sensitivity analysis is performed on the various uncertainties and the results are presented in Table 6.2.

**Table 6.2:** Global sensitivity analysis and conditional-global sensitivity analysis results

<b>Group</b>	<b>Main Effect</b>	<b>cGSA<sup>up</sup></b>	<b>cGSA<sup>down</sup></b>
<b>1.</b>	0.005	0.2445	0.013
<b>2.</b>	0.012	0.254	0.022
<b>3.</b>	0.004	0.227	0.002
<b>4.</b>	0.004	0.232	0.005
<b>5.</b>	0.000	0.258	0.001
<b>6.</b>	0.004	0.232	0.006

The hierarchy of the importance of the various uncertainties based on the global sensitivity analysis and conditional global sensitivity analysis is as follows:

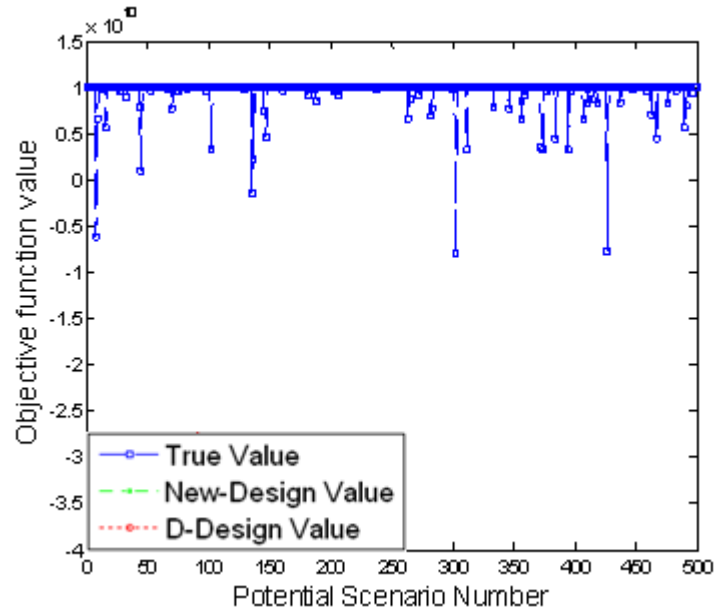
- a. Group – 2 (Pre-extraction yield)
- b. Group – 1 (Pre-extraction operating conditions)
- c. Group – 6 (Fraction conversion of sugars to ethanol)
- d. Group – 4 (Bleaching)
- e. Group – 3 (Refiner)
- f. Group – 5 (Pulp Strength)

The next step is the design of experiment, but the computation of optimal design of experiment based on the available Microsoft excel based model would be computationally infeasible. Hence, a meta-model for the objective function ' $f$ ' is developed from the existing excel/VBA based model for the biofuel producing TMP mill and is given by (6.8).

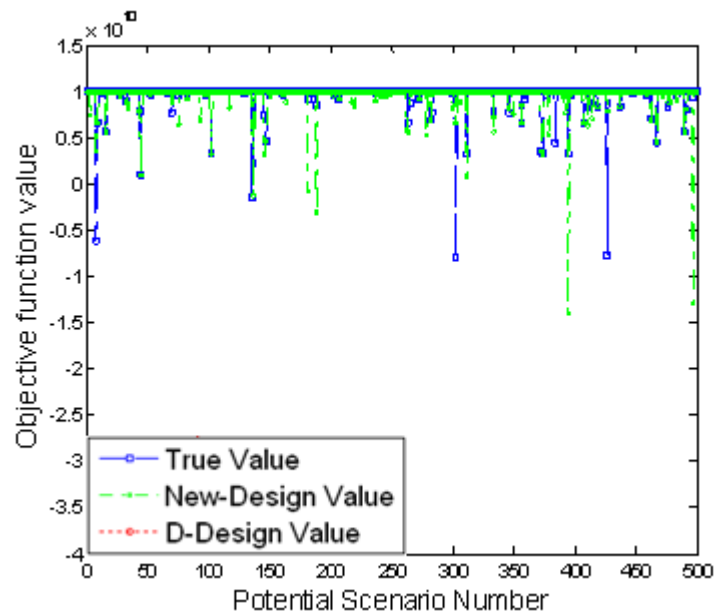
$$f = \alpha_h y_h + \alpha_c y_c + \alpha_e y_e - \beta (y_b - T_b)^2 - \gamma (y_r - T_r)^2 - \delta (y_s - T_s)^2 - W^T X - 1/2 X^T Q X \quad (6.8)$$

In (6.8),  $f$  is the net present value of the alternative and  $\alpha_h$ ,  $\alpha_c$  and  $\alpha_e$  are the scaling parameters for the economic values of hemicellulose yield, cellulose yield and the extractive yield. Similarly  $\beta$ ,  $\delta$  and  $\gamma$  are the scaling parameters for the quadratic penalties on the deviation from the target quality values ( $T_b$  for brightness,  $T_r$  for runnability and  $T_s$  for pulp strength) for brightness, runnability and pulp strength. Additionally ‘W’ and ‘Q’ represent the linear and quadratic penalties for higher operating conditions. Here the target values,  $T_b$ ,  $T_r$  and  $T_s$ , are selected after discussion with the experts and the scaling parameters  $\beta$ ,  $\delta$  and  $\gamma$  are assigned appropriately. Since the parameter values for the meta-model are based on proprietary data and model, those values are not shared here.

Given the objective function  $f$  and the underlying uncertainty in the various technical models, we perform the optimal decision oriented DOE design and D-optimal design. To compare the performance of the two design-of-experiment strategies, it is assumed that one experiment for each unit operation is performed using the respective design strategy. This is followed by updating of the parameter distributions and then the optimal objective function value is reported.

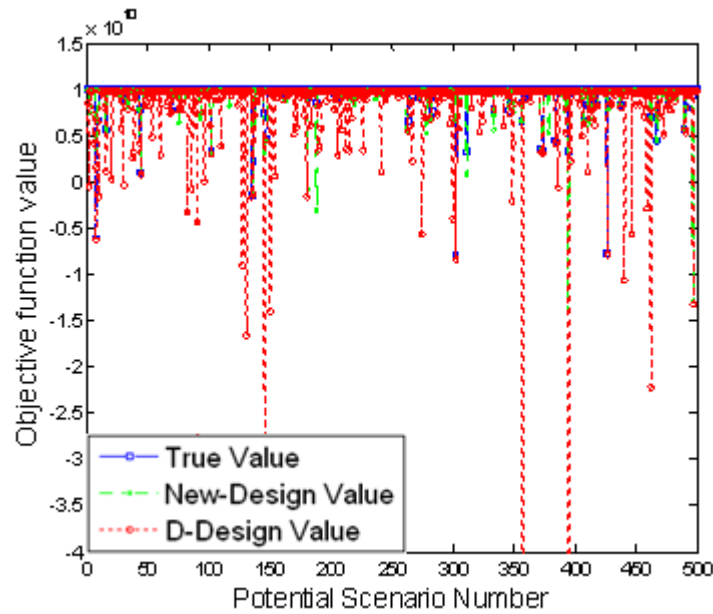


**Figure 6.4:** The true objective function values for the 500 potential scenarios



**Figure 6.5:** True optimal objective function values along with the corresponding predicted optimal objective function values based on decision oriented design (i.e. new design) of experiment

In order to compare the performance of the two design approaches, we take 500 samples from the prior distributions of the model parameter uncertainties and consider them as the potential 500 true values for the parameters. The true optimal objective function value for these 500 potential cases is shown in figure 6.4. The optimal objective function values predicted by the decision oriented DOE strategy and the true optimal objective function values are compared in the figure 6.5.



**Figure 6.6:** The true objective function value along with the corresponding predicted optimal objective function values based on decision oriented and D-optimal based design of experiment strategy

Figure 6.6 compares the true objective function value with the values predicted by both an optimal decision oriented and a D-optimal design of experiment strategy. The comparison indicates the superior performance of the decision oriented DOE strategy compared to D-optimal DOE strategy. Further comparison of the prediction by the two approaches reveals that decision oriented DOE strategy leads to a predicted value which

is 90% of the times closer to the true value in comparison to the predicted value based on D-optimal DOE strategy.

## **6.5 Conclusions**

In this chapter, we have presented a hierarchical framework to improve R&D decisions. The hierarchical framework consists of mainly three methods, expert opinion elicitation, conditional global sensitivity analysis and decision oriented design of experiment. The motivation of this work has been the challenges in the R&D decisions with regard to bio-refinery options and in order to demonstrate the value of the hierarchical framework we apply the hierarchical framework on a bio-refinery case study (Hemi-cellulose pre-extraction in a Thermo-mechanical pulp mill).

As shown in Chapter 4, experimentation on the key uncertainty (identified by c-GSA) leads to higher expected value of sample information. Moreover, as shown in Chapter 5, the decision oriented design of experiment which is basically based on expected value of information maximization criterion leads to better prediction of the optimal objective function values. It can be concluded that both c-GSA and decision oriented design of experiment are in synergy.

The number of key uncertainties on which experimentation should be conducted is driven by the availability of the resources. The higher the number of key uncertainties on which the experimentation is conducted the better would be the expected value of sample information (since no uncertainty gives negative expected value of information) and better would be the predicted result.

To consider one of the extreme cases, for the case study in this chapter, we assume that one experiment is conducted for each unit operations. The results based on both decision oriented and D-optimal DOE strategy reveal that after conducting one experiment for each unit operation, 90% of the times the decision maker is able to predict a value closer to the true value based on the decision oriented DOE approach in comparison to the D-optimal approach.

# CHAPTER VII

## CONTRIBUTIONS & FUTURE RESEARCH

### 7.1 Summary of contributions

The main contribution of this thesis is the integrated Bayesian framework along with new tools, which can be used as a systematic method to improve R&D decisions. Though the integrated Bayesian framework is based on a very intuitive approach, this type of systematic approach does not exist in the literature. The Bayesian framework provides the benefit of integrating the knowledge of the R&D managers and technical experts in developing a systematic strategy and hence commands more confidence. The Bayesian framework consists of three steps: elicitation of experts' knowledge, estimation of key uncertainty and estimation of decision oriented design of experiment strategies.

For elicitation of the experts knowledge an existing elicitation method (Wolfson 1995) was used and applied to a biofuel related case-study in Chapter 3. To our knowledge, this is the first application of the methodology to a real chemical engineering case-study and introduces the methodology to the chemical engineering domain. Quantification of technical uncertainty using experts' knowledge is useful in both developing an efficient R&D investment strategy and an optimal design of experiment strategy.

To identify the key uncertainty, one can use global sensitivity analysis (GSA). As shown in Chapter 4, reduction in uncertainty in the key uncertainty factor leads to higher expected value of information (*EVOI*). In Chapter 4, a new method, conditional global sensitivity analysis (c-GSA), is built upon the existing GSA method. Conditional global

sensitivity analysis demonstrates the ability to supersede the performance of global sensitivity analysis, as it is able to identify the key uncertainty contributors even when global sensitivity analysis fails to do so.

Traditional ‘Design of Experiment’ (DOE) approaches focus on minimization of parameter error variance. In Chapter 5, we propose a new “decision-oriented” DOE approach that takes into account how the generated data, and subsequently, the model developed based on them will be used in decision making. Two new decision oriented design of experiment strategies are introduced, which significantly improve decision-making compared to the traditional optimal design strategies. The *MPM* (Maximize Profit Margins) criterion, which is mainly based on the mean value of the optimal operating profit margin, shows an improvement of 25-30% in the prediction of the true optimal profit margin. Moreover the *MPD* (Maximize Probability of Decision) criterion, which is based on both the mean and the variance of the optimal operating profit margin, is used for the Acceptance/Rejection of candidates. The use of *MPD* criterion led to a smaller improvement compared to the D-optimal designs for a relatively informed prior though the performance improvement was more significant for less informed priors. Overall the both decision-oriented designs demonstrate significant improvements over the traditional D-optimal design of experiment strategy, as they directly address the ultimate objective of the experiment.

## **7.2. Future work**

The future work mentioned in the following sections, is the additional work which can be done to extend the work in this thesis.

### **7.2. 1. Elicitation of expert knowledge**

The expert knowledge elicitation method (Wolfson 1995) used in this thesis is mainly valid for linear models and is the only generic enough model which is practically possible to apply to real chemical engineering problem. It would be very helpful to develop an elicitation model, which assist in elicitation of experts' knowledge for a certain class of nonlinear models, for example the uncertainty quantification in monod kinetics models.

### **7.2. 2. Identification of key uncertainty contributors**

In this thesis, for the identification of the key uncertainties a new approach c-GSA was introduced. Though c-GSA is a variance based approach, it would be important to look into new methods which account for the other measures of risk. Additionally, though the performance of c-GSA was evaluated for many examples, it would be ideal to extend the evaluation to wide range of non-linear models to ascertain if the model structure has significant effect on the performance of c-GSA.

### **7.2. 3. Design of experiment**

To evaluate the performance of the newly developed decision oriented design of experiment strategies (MPM and MPD), it was considered that only one experiment is conducted. The above strategy is good for sequential design of experiment strategy as both the MPM and MPD strategies demonstrated benefit over the traditional D-optimal

design approaches. For the future, it would be interesting to evaluate the performance of the MPM and MPD approach for multiple parallel experiments.

The underlying model was assumed to be linear for the evaluation for the two new strategies (MPM and MPD) in Chapter 5. The model structure under consideration in Chapter 6 is linear in parameters. The results for the model structures presented the advantage of the new strategies. The two strategies are also applicable when the model structure is not linear in parameters and it would be an interesting exercise. The challenge with this problem would be the increased computational time especially due to the posterior optimization of the operating conditions at each node.

Additionally the prior and likelihood distributions assumed in both the Chapter 5 and Chapter 6 are conjugates, specifically Gaussian distributions. Bayesian update of the model parameters is analytical if the prior and likelihood are conjugate, which is true for Gaussian priors and likelihood. Though it is common to have Gaussian priors and likelihood, but sometimes one might have non-Gaussian or non-conjugate priors. The challenge with the non conjugate priors would be the Bayesian update. The Bayesian update for non-conjugate priors though analytically not possible is computationally possible using Markov Chain Monte Carlo (MCMC) (Cowles and Carlin 1996; Brooks 1998; Kass, Carlin et al. 1998).

## **APPENDIX A**

### **EVALUATING BIOREFINERY OPTIONS IN A PULP & PAPER**

#### **MILL – CARBON BALANCES**

Concerns over the reliance of the U.S. economy on crude oil, the reliance on foreign sources for the majority of this commodity, and the recent high volatility of crude oil prices have led to an increased interest in diversifying the U.S. energy base. The higher crude oil prices make processes that utilize renewable energy sources such as biomass, wind and solar power competitive in the marketplace. Biorefineries, integrated production systems for materials and energy from agricultural or silvicultural inputs, are considered capable of meeting part of the need for renewable resources. Pulp and paper mills have existing infrastructure to receive, store, and handle woody biomass residuals, which can be used to produce fuels, and thus they have an initial capital base for a biorefinery and a potential leverage for increased value from these inputs. However, there are many different configurations for such biorefineries, and it is important to analyze the alternatives systematically to uncover their different strengths and weaknesses before major research and development and capital expenditures are made.

We have considered the following significantly different technological alternatives for the expansion of pulp and paper mills: first, the pre-extraction of hemicellulose from the wood to produce ethanol through fermentation route and second, the replacement of Kraft cycle by polysulphide pulping, followed by black liquor gasification, which leads to the opportunity to produce various transportation fuels. The

above mentioned technological alternatives lead to four scenarios to be considered as the possible alternatives for biorefineries. In order to make rational comparisons without detailed design calculations, we have evaluated the various alternatives on the basis of carbon yield. The results of the above mentioned four cases indicate that hemicellulose extraction increases pulp wood conversion to alcohols, but the flow and yield of carbon may be too low to justify the capital expenditure and warrants further investigation.

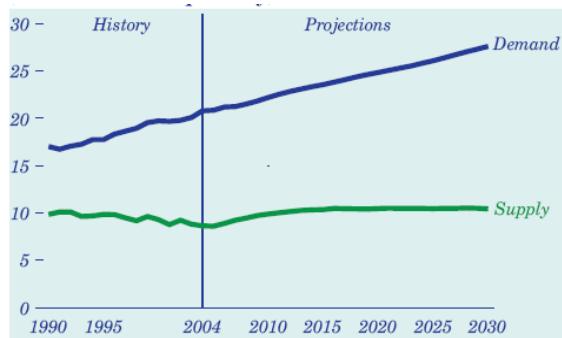
### **A.1 Introduction**

The widening gap between US petroleum product demand and domestic petroleum supply (see Figure A.1)(2006) has led to a greater interest in the production of alternate/substitute transportation fuels. Ethanol and MTBE (methyl tertiary butyl ether) are the only two economically feasible oxygenates used by the industry. In the light of repeal of oxygenate requirement for federally reformulated gasoline according to the Energy Policy Act of 2005, refiners see an increasing liability with pollution of water by MTBE (MTBE readily contaminates groundwater when blended gasoline is spilled)(2006). On the contrary, demand for ethanol is expected to continue as it is a clean, high-octane blending component and a good substitute for MTBE. Moreover it is expected that as crude oil prices increase, so will the demand for ethanol as it can be a substitute for hydrocarbons (see Figure A.2).

At present time, corn is the main source of ethanol production. The production of ethanol by corn can be regarded a mature technology that is not likely to see significant reductions in production costs (DiPardo 2006). Moreover the supply of corn is relatively small compared to the U.S. gasoline demand (Collins August 26,2006). In addition, the

higher future ethanol demand makes it inevitable to evaluate other options for ethanol production. Production of ethanol from cellulose-based feedstocks is such an option and it is gaining importance because of the low cost and easy availability of the raw material (DiPardo 2006).

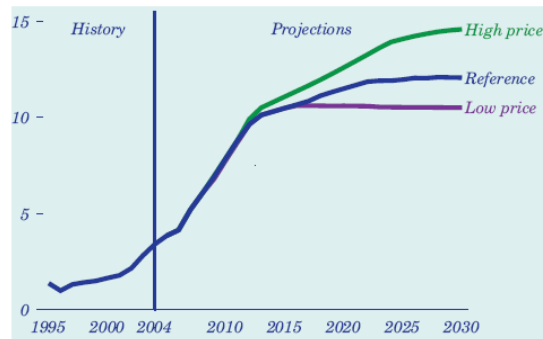
Ethanol can be produced from woody biomass through two different routes, biochemical (sugar platform route) and thermochemical. The sugar platform route is already widely used for commercial production of ethanol from corn. The first plants for production of ethanol directly from cellulose-based feedstock have been announced. The thermochemical route (production of syngas) on the contrary is not currently used for ethanol production from biomass, as the process is still under evaluation for its economic viability (Wooley, Ruth et al. 1999).



**Figure A.1:** U.S. petroleum product demand and domestic petroleum supply, 1990-2030 (million barrels per day)(2006)

In order to support the growing future ethanol demand, a sustainable infrastructure is required. The U.S. pulp and paper industry, which is amongst the largest producers and users of woody biomass based renewable energy, has the capacity to provide such an infrastructure (Larson, Consonni et al. 2003). Recently, the pulp and paper industry has shown enthusiasm for the replacement of recovery boilers by gasifiers,

which increases the energy efficiency of the system(Larson, Consonni et al. 2003). If this technology becomes successful it will open another opportunity for the paper industry to operate biorefineries for the production of ethanol and various other alcohols. During gasification of woody biomass, organically bound carbon and hydrogen are released in the form of syngas ( $\text{CO}+\text{H}_2$ ) and this syngas can be used to produce ethanol and various other alcohols.



**Figure A.2:** U.S. ethanol fuel consumption in three oil price cases, 1995-2030 (billion gallons per year)(2006)

There is also a possibility to produce ethanol by the sugar platform route in the pulp and paper industry. The wood used for production of paper contains hemicellulose, a significant fraction of which is dissolved during the initial stages of chemical operations (pulping) and eventually burned in a recovery boiler for generation of heat and energy. It has been suggested that this is an inefficient way of recovering energy from hemicelluloses and a better way would be to separate out a significant fraction of hemicellulose prior to pulping and produce ethanol from it via fermentation (the sugar platform route).

Gasification creates greater flexibility for the paper industry to choose the chemical composition (pulping chemicals) used for chemical treatment of wood (pulping/cooking). During the gasification incoming sulfur splits into gas phase  $H_2S$  and condensed phase  $Na_2S$ . This offers a degree of freedom to convert the gas phase  $H_2S$  to the form of sulfur required; for example  $H_2S$  can be converted to elemental S for polysulphide cooking (Sanyer and Laundrie 1964; Kocurek 1989).

Here we have calculated carbon balances for four cases: polysulphide cooking and kraft cooking with high temperature gasification (Larson, Consonni et al. 2003) and mixed alcohol production, both with and without hemicellulose pre-extraction. Carbon yields to alcohol are considered here as a way to compare the different systems without having to develop detailed equipment and cost estimates and to identify the tradeoffs involved in the different design decisions. Carbon flow and yields are important indicators for whether a given configuration is likely to be economically viable. These flows are correlated with those for hydrogen, but the water gas shift can be used to generate additional hydrogen at the expense of carbon monoxide. We focus on carbon flows which are also important for understanding the impact of liquid fuel production on overall carbon utilization in fuels. Low flows and/or low yields will be associated with high capital or operating costs relative to other higher flow and yield options. The evaluation is based on southern pine (Loblolly pine) as it is the most important wood species pulped in the US.

## **A.2. Ethanol production via sugar platform route**

Ethanol production from corn is a well-known technology(Aden, Ruth et al. 2002) but ethanol production from woody biomass is still under evaluation(Wooley, Ruth et al. 1999). The information on the hemicellulose pre-extraction from wood chips prior to pulping is scarce and sufficient data required for the calculations in this study were available in the published literature(Oshima 1965). Unpublished experimental data(Ragauskas and Ho) about the sugar yield of loblolly pine wood with hemicellulose pre-extraction were used. Out of the various process conditions considered for experiments (0%, 0.2%, 0.5% H<sub>2</sub>SO<sub>4</sub> and 0.5,1 hr of pre-extraction)(Ragauskas and Ho), 0.2% H<sub>2</sub>SO<sub>4</sub> and 1 hour of pre-extraction is selected for this case study, with due consideration to the expected pulp strength after the pulping process.

Loblolly pine composition is given in Table A.1. The composition of the extracted sugar units and the wood composition after the extraction are given in Tables A.2 and A.3 respectively. It is considered that 10.0%(wt), of wood mass is lost during hemicellulose pre-extraction out of which 73.4% is recovered as sugars (Ragauskas and Ho ; Frederick, Lien et al. 2006).

In order to account for the ethanol production from the sugars, conversion values for the prehydrolysis and fermentation reactions are used from the NREL report on ethanol production from hardwood (Wooley, Ruth et al. 1999). Current level of technological achievement permits the conversion of only glucose and xylose units to ethanol. The oligomers formed during the prehydrolysis reactions cannot be converted to ethanol either. It is expected that in the near future it would be possible to ferment

oligomers and all C5, C6 sugar units. Hence Table A.4 reports the values of ethanol production per ton OD wood chips processed for hemicellulose pre-extraction, for fermentation of glucose and xylose only and for fermentation of all C5 and C6 sugars, along with each case where oligomers are fermented and not. It is evident from the values given in Table A.4, that ethanol production is almost three times higher if all C5 and C6 sugars can be fermented, whereas fermentation of oligomers is less significant.

**Table A.1:** Composition of Loblolly Pine wood(Frederick, Lien et al. 2006)

<b>Loblolly Pine Wood</b>	<b>Weight %</b>
Cellulose	46.6%
Hemicellulose	19.4%
Lignin	29.5%
Extractives	3.3%
Total	98.8%

**Table A.2:** Composition of extracted sugar units in the hemicellulose extraction slurry

<b>Composition of Extracted Sugar Units</b>	<b>Weight %</b>
Arabinose	12.0%
Galactose	12.3%
Glucose	9.5%
Xylose	22.4%
Mannose	43.8%
Total	100.0%

**Table A.3:** Composition of Loblolly pine wood after hemicellulose extraction

<b>Wood Composition after Hemicellulose Extraction</b>	<b>Weight % (of remaining wood)</b>
Cellulose	50.0%
Hemicellulose	15.5%
Lignin	32.0%
Extractives	2.5%
Total	100.0%

**Table A.4:** Moles ethanol produced by fermentation per ton of OD wood chips processed for pre-extraction.

	<b>From Glucose and Xylose Units only</b>		<b>From all C5 and C6 Sugar Units</b>	
<b>Oligomers (Fermented/Not Fermented)</b>	Not Fermented	Fermented	Not Fermented	Fermented
<b>Ethanol (moles)</b>	227	245	634	679

**Note:** For all C5 and C6 sugar units the conversion efficiency is considered the same as those of xylose and glucose (Wooley, Ruth et al. 1999)

### **A.3. Mixed Alcohol Production via the Thermo-chemical Route**

The adoption of gasification technology not only provides the benefit of higher energy efficiency to the pulp/paper industry but also offers the flexibility to adopt various other pulping technologies, such as polysulphide pulping in addition to Kraft. The choice of the above two pulping technologies is based on prior work by Iisa (Iisa, Courchene et al. 2005 ) on the evaluation of various pulping technologies suitable for gasification technology.

In the scenarios considering the extraction of hemicellulose prior to pulping it becomes very important to understand, how this extraction of hemicellulose will affect the pulp yield and black liquor composition. Due to the absence of published experimental data, we considered approximations taking into account the pulping chemistry and the information available for the various pulping methods in the literature. Moreover to measure all the scenarios on a common basis, all the scenarios are evaluated

for the pulp production of 1600 T/day, equivalent to Frederick's(Frederick, Lien et al. 2006) and Larson's(Larson, Consonni et al. 2003) case studies.

Kraft pulping, the base case in Larson's (Larson, Consonni et al. 2003) analysis of the benefits of the gasification technology was used here. We have considered the same pulping conditions as in Larson's case. Fredrick and Lien have developed a software for evaluating and optimizing the pulping and chemical recovery operations of a kraft pulp mill (BioRefinOpt<sup>TM</sup>)(Frederick, Lien et al. 2006). This software evaluates two options, kraft pulping and hemicellulose pre-extraction followed by kraft pulping. In order to calculate the black liquor composition, the above mentioned software was used. Moreover, since the software is based on Tomlinson recovery boilers, required changes were done to adopt the gasification and hence evaluate the syngas composition.

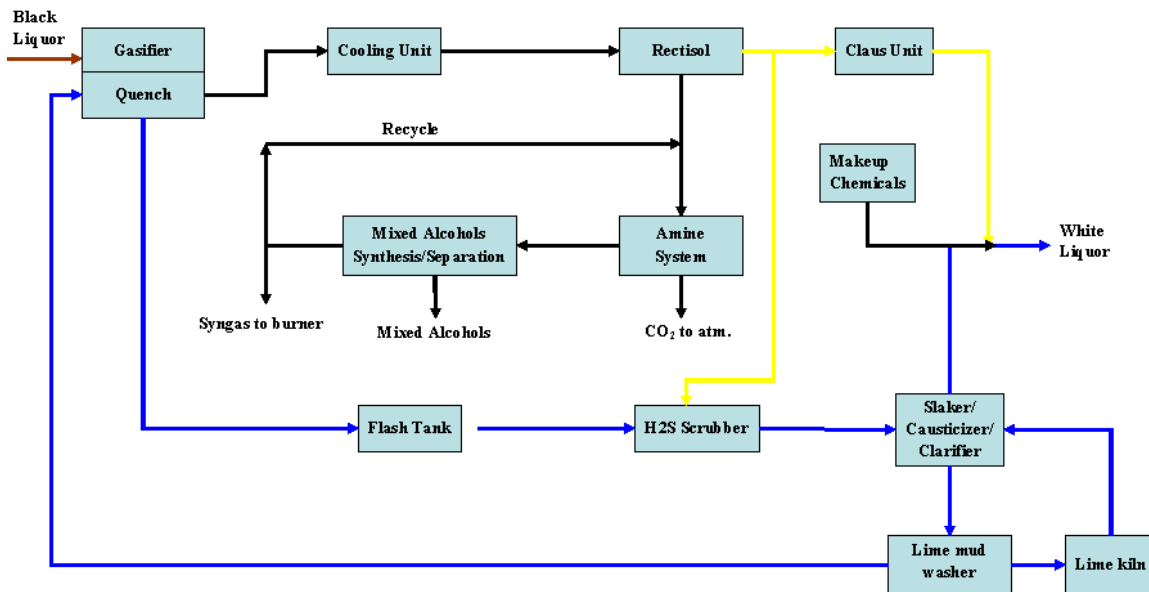
Polysulphide pulping is being considered as a future replacement of Kraft pulping as it offers the advantage of a higher pulp yield. The main difference in polysulphide pulping and kraft pulping cooking chemicals, is the addition of sulphur in polysulphide pulping chemicals. This addition of sulphur forms polysulphide in the liquor which increases the pulp yield, primarily due to protection of wood carbohydrates, probably by the oxidation of the carbohydrates reducing end groups and by decreasing peeling-off degradation in the presence of alkali(Sanyer and Laundrie 1964). The pulping conditions considered are the same as in Larson's report (Larson, Consonni et al. 2003) and the pulp yield for the softwood was considered. For the case where no pre-extraction of hemicellulose is done, reasonable information is available in the literature (Vaaler, Eriksen et al. ; Sanyer and Laundrie 1964) to determine the pulp composition. The black liquor composition can be easily calculated as the chemical charged and the original

composition of the chips is known. Under the realm of no prior knowledge available about the effect of hemicellulose extraction on the pulp yield, it was assumed that the fraction of each component converted to pulp is the same as in the base case (with no pre-extraction of hemicellulose).

We have evaluated the option of producing mixed alcohols within the framework of an integrated pulp and paper mill. Sufficient inputs are taken from the NREL review report (Spath and Dayton 2003) on assessment of syngas to various product processes (H<sub>2</sub>, MeOH, FTL, EtOH, mixed alcohols, etc.) and from another NREL report (Aden, Spath et al.), proposing efficient process design models for mixed alcohol production.

A general flow diagram of the integrated pulp/paper mill producing mixed alcohols is shown in Figure 3. The flow diagram is partly based on the high temperature gasification case in Larson's report (Larson, Consonni et al. 2003). A brief discussion about the flow diagram is as follows: Black liquor from the brown stock washer is fired in the high temperature gasifier, operating at 950°C and 35 bar pressure. The corrosive nature of the product gases at such a high temperature requires a quench so as to reduce the temperature of the outgoing syngas. Weak white wash from the lime mud washer is used in the quench. The gases leave the quench at temperature close to 250°C. Sulphur is mainly in the form of H<sub>2</sub>S, and in order to recover it from the syngas we use a one-stage Rectisol© unit. It operates at a temperature close to -20°C, so a cooling unit needs to be incorporated to reduce the syngas temperature. The hydrogen sulphide stream leaving the Rectisol unit consists of H<sub>2</sub>S and CO<sub>2</sub> in the ratio of 1:1. An appropriate amount of this stream is sent to the green liquor scrubber to recover sulphur in the form of Na<sub>2</sub>S and the rest is sent to the Claus unit to generate sulphur for polysulphide pulping. For kraft

pulping no part of the H<sub>2</sub>S stream is sent to the Claus unit as there is no sulphur requirement. The remaining syngas is sent for the mixed alcohol production.



**Figure A.3:** Integrated flow diagram of chemical recovery and mixed alcohol production.

The mixed alcohol production unit consists of an amine unit and a mixed alcohol synthesis unit. A modified Fischer-Tropsch catalyst system(MoS<sub>2</sub>-based) is considered for the mixed alcohol synthesis and the operating conditions considered are 300°C temperature, 2000 psia pressure, H<sub>2</sub>/CO ratio of 1.2 in a fixed bed reactor. The amine unit serves the purpose of keeping the CO<sub>2</sub> level in the syngas below 2 wt%, which is a requirement for good selectivity in the mixed alcohol synthesis unit(Aden, Spath et al.).

In the mixed alcohol synthesis unit the conversion of CO per pass is only 38%, so it is necessary to recycle this stream. The mixed alcohol reactor requires an H<sub>2</sub>: CO ratio of 1.2 for optimum selectivity and conversion. The incoming syngas has an H<sub>2</sub>: CO ratio lower than 1.2 and the stream leaving the mixed alcohol synthesis unit has an H<sub>2</sub>: CO ratio higher than the incoming stream and higher than 1.2. So, the product stream from

the mixed alcohol synthesizer is recycled after the mixed alcohols are separated. It is important to understand that it is this H<sub>2</sub>: CO ratio requirement, which forces the appropriate values of the recycle ratios (fraction of product stream leaving the alcohol separation unit) which are 0.92, 0.99, 0.68 and 0.75 for kraft, kraft with pre-extraction, polysulphide and polysulphide with pre-extraction, respectively.

The remainder of the flow diagram is very similar to the kraft recovery cycle. Smelt, mainly containing Na<sub>2</sub>S and Na<sub>2</sub>CO<sub>3</sub>, leaves the quench section, which also partly serves the purpose of a smelt dissolving tank at the gasifier's bottom. This green liquor stream is used in the scrubber to capture H<sub>2</sub>S from the H<sub>2</sub>S stream to recover sulphur in the form of Na<sub>2</sub>S. Followed by the scrubber is the slaker, causticizer and clarifier where slaking (formation of Ca(OH)<sub>2</sub> from CaO), causticizing (conversion of Na<sub>2</sub>CO<sub>3</sub> to NaOH) and clarification (separation of lime mud from the liquor stream) takes place respectively. The lime mud washer serves the purpose of removing any dissolved chemicals from the water associated with the lime mud captured from the clarifier and further increasing the solid content of the lime mud. The lime kiln serves the purpose of regenerating calcium oxide from calcium carbonate (lime mud). The production rate of the mixed alcohols from the thermo-chemical route per ton of wood chips processed is given in Table A.5. Larger quantities of mixed alcohols are produced in the case of pre-extraction followed by polysulphide than in the case of polysulphide pulping only. Moreover, there is no significant difference in mixed alcohol production for the kraft cooking and pre-extraction followed by kraft cooking, though it is evident that in the case of kraft and pre-extraction followed by kraft, significantly larger quantities of mixed alcohols are produced than for any case of polysulphide cooking.

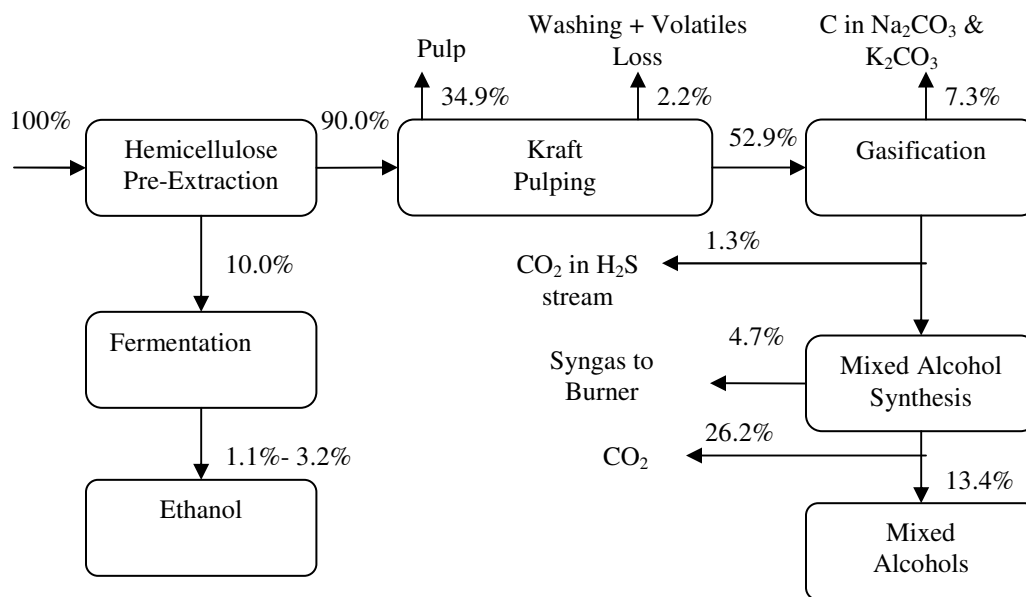
**Table A.5:** Moles alcohol produced from the thermo-chemical route, per ton of wood chips processed

<b>Unit : moles</b>	<b>Pre-extraction + Kraft</b>	<b>Kraft</b>	<b>Pre-extraction + Polysulphide</b>	<b>Polysulphide</b>
<b>Methanol</b>	1156	1117	828	841
<b>Ethanol</b>	1607	1553	1151	1169
<b>Propanol</b>	282	272	202	205
<b>Butanol</b>	70	68	51	51
<b>Pentanol</b>	14	14	10	10
<b>Hexanol</b>	12	11	8	9

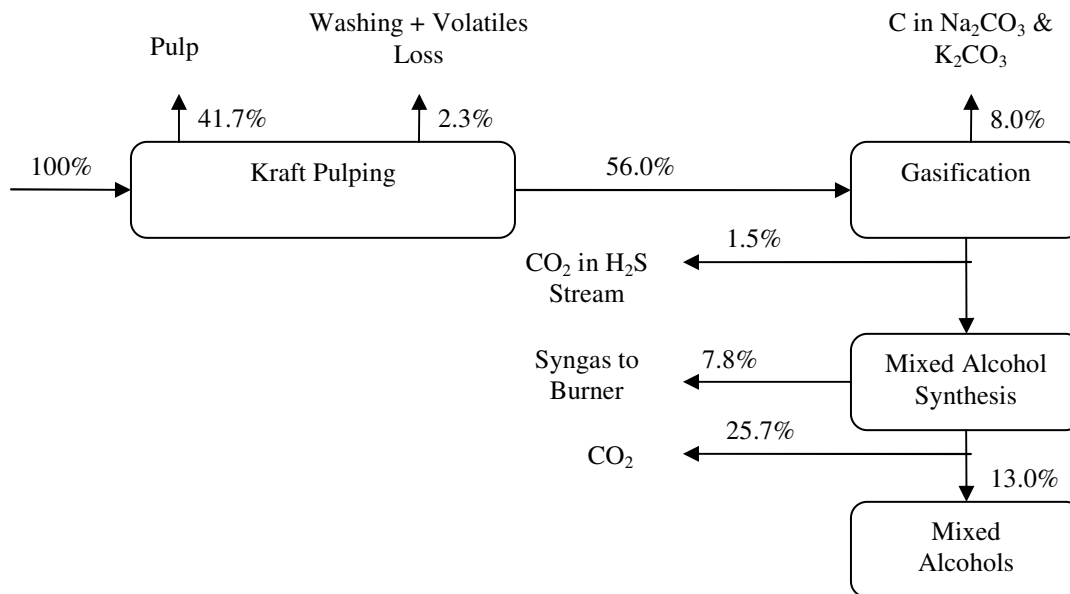
#### **A.4 Carbon Balances & Carbon Efficiencies**

Figures A.4, A.5, A.6, & A.7 give the carbon flows for ethanol and mixed alcohol production for kraft pulping with pre-extraction, kraft, polysulphide with pre-extraction and polysulphide respectively. The balances are based on the organic carbon content, i.e. carbon coming in with the wood and not any carbon due to the inorganic chemicals in the white liquor.

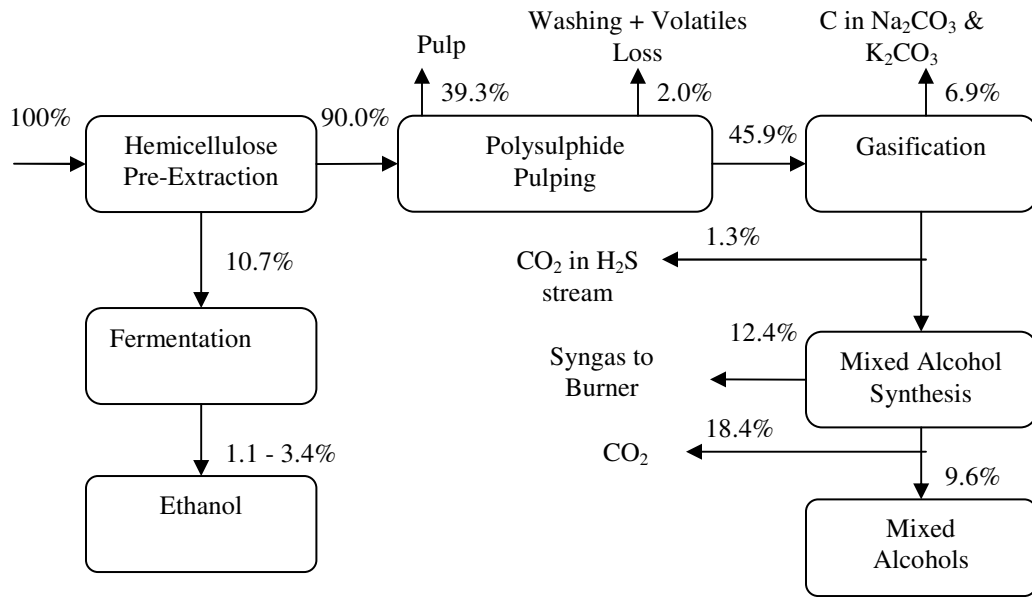
In the figures the carbon loss across the pulping section accounts for carbon converted to pulp, the washing loss and volatiles loss. The carbon lost as CO<sub>2</sub> in the H<sub>2</sub>S stream from the Rectisol unit and the loss of carbon due to the Na<sub>2</sub>CO<sub>3</sub> and K<sub>2</sub>CO<sub>3</sub> formation in the gasification account for the difference in the carbon flows of the outlet and inlet streams from the gasifier.



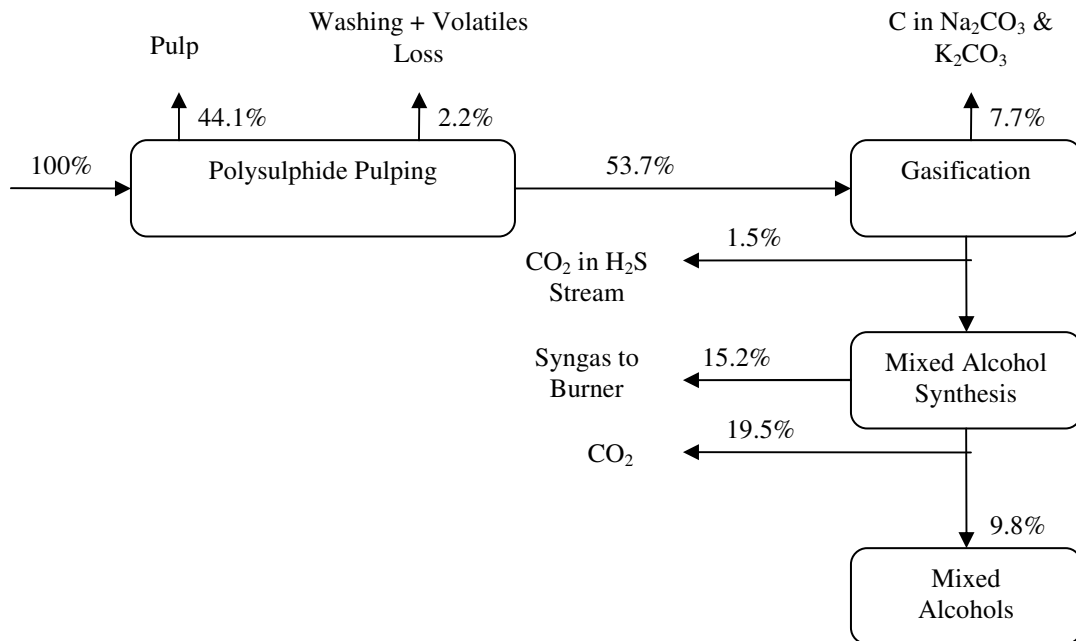
**Figure A.4.** Carbon balance for the case of hemicellulose pre-extraction followed by the kraft pulping



**Figure A.5.** Carbon balance for the case of simple kraft pulping



**Figure A.6.** Carbon balance for the case of hemicellulose pre-extraction followed by polysulphide cooking



**Figure A.7.** Carbon balance for the case of simple polysulphide cooking

For kraft pulping, a higher fraction of the incoming carbon is converted into mixed alcohols in the case of kraft without pre-extraction than with pre-extraction. However, the ethanol production in the pre-extraction case gives it an advantage in terms of overall carbon conversion to alcohol products. The design for the production of mixed - alcohols is based on maintaining an  $H_2:CO$  ratio of 1.2, a required condition for the mixed alcohol synthesis(Aden, Spath et al.),which changes the recycle ratio for each case and hence the amount of syngas sent to the burner. The syngas going to the burner can be used to provide for the heat requirement of the reboilers in the sugar platform route to increase the concentration of the ethanol produced or it can also be used to produce steam and power, required for the pulp/paper mill operations.

Figures A.6 & A.7 show a higher fraction of carbon converted to mixed alcohols in the case of hemicellulose pre-extraction followed by the polysulphide cooking than in the case of polysulphide cooking without pre-extraction. In addition, ethanol production from the extracted hemicellulose increases the alcohol production for the pre-extraction case in the case of polysulphide cooking.

The cases studied here show that from the point of efficiency of pulp wood carbon conversion to alcohols, it is advantageous to extract hemicellulose prior to pulping. However, we also need to understand that in the cases where hemicellulose extraction is not included a higher fraction of syngas is sent to the burner. Especially in the two cases considered for the polysulphide cooking, a significant fraction of the syngas is sent to the burner. This raises the additional question of the overall energy balance of the mill.

The figures above compare each case with respect to carbon entering with pulp wood but from the pulp/paper mills point of view it is important to compare the various cases for the same pulp production rate. Table A.6 compares the corresponding combined production rate for the various alcohols for a pulp production rate of 1600 short tons/day oven dry unbleached pulp.

Each of the above four cases has its own pros and cons, the two cases for the kraft suggest that a significant amount of alcohols can be produced from them but then one needs to rely on other resources for the production of steam and power to supply the mill requirements, whereas for the two cases of polysulphide cooking a significant fraction of incoming syngas goes to the burner, which indicates that in such cases there would be a lower requirement of other resources to fulfill the mill energy and power needs.

**Table A.6:** Total production of alcohols for 1600 T of pulp produced.

<b>Units: Ton</b>	<b>Pre-extraction + Kraft</b>	<b>Kraft</b>	<b>Pre-extraction + Polysulphide</b>	<b>Polysulphide</b>
<b>Methanol</b>	147.9	122.8	95.3	86.5
<b>Ethanol</b>	420.6	245.4	302.9	172.9
<b>Propanol</b>	67.7	56.1	43.6	39.6
<b>Butanol</b>	20.9	17.3	13.4	12.2
<b>Pentanol</b>	5.0	4.1	3.2	2.9
<b>Hexanol</b>	4.8	4.0	3.1	2.8

The above results are mainly dependent on the process design shown in Figure A.3, in which significant improvements can increase the alcohol production, but at the cost of increased energy demand, and this tradeoff needs to be further evaluated. A primary example of this is where one can recycle the CO<sub>2</sub> stream to the gasifier, in order to improve the overall product yield but this option needs to be carefully evaluated to check that the increment in product yield more than offsets the increment in energy

requirement. Another option to examine is whether one can recycle the syngas stream to the burner or to the gasifier, which would require an improved design of gasifier so one can both fire the black liquor and burn this syngas (rich in methane and ethane) in the same gasifier. Alternatively one can incorporate a steam reformer to burn this methane/ethane rich syngas and recover the carbon. Again the above two mentioned modifications would require a more detailed analysis in terms of marginal increment in energy and alcohol production, along with the increase in the cost of the equipment. However, the carbon yield analysis helps to focus the design decisions and tradeoffs without the overhead of more complex evaluations in the early flowsheet phases.

The above case-study shows that the production of mixed-alcohols is very sensitive to the wood composition used. As it is well known fact that there is a significant difference in the wood composition of the same species, the design one should be targeting for the production of mixed-alcohols should be robust enough to accommodate this variability of the wood composition. It also indicates the importance of accurately estimating the loss of individual components in the hemicellulose pre-extraction stage so that the uncertainty related to the composition of the extracted wood sent to the pulping is resolved.

In the absence of significant data on the effect of hemicellulose pre-extraction on pulp yield, simplified assumptions were made for the overall yield and the yield for each individual component. The black liquor composition is dependent on the amounts of individual components lost in the pulping which affects the syngas composition. This chain of effects on composition can make a significant difference in the alcohol production, which needs further investigation. One should investigate the effect of

hemicellulose extraction on the black liquor's HHV (Higher Heating Values), as it will affect the thermodynamic equilibrium in the gasification and hence, subsequently, the composition of the syngas produced.

### **A.5 Conclusions**

Pre-extraction of hemicellulose prior to pulping has higher yields of carbon for mixed alcohol production, but the overall increase in yield of alcohol through this route is a small percentage of the overall carbon entering the system. The carbon yield supports kraft pulping over polysulphide pulping for the production of mixed alcohols. Polysulphide and kraft pulping both have their own pros and cons if one considers the global level, as higher amounts of some other resources are needed to provide for the mills steam and power requirements in the case where a higher fraction of syngas is used for mixed alcohols production. So the tradeoff between the increase in alcohol production and the increase in the additional biomass requirement to maintain the required production of steam and power needs to be evaluated. This case-study also identifies key areas where research is required to reduce the level of uncertainty currently present in the system.

## **APPENDIX B**

### **PRELIMINARY BIOREFINERY ANALYSIS WITH LOW-TEMPERATURE BLACK LIQUOR GASIFICATION**

#### **B.1 Introduction**

A number of concepts for black liquor gasification have been proposed in the past (Consonni, Larson et al. 1998). Previous assessment of black liquor gasification combined cycle (BLGCC) systems by (Larson, Consonni et al. 2003) included detailed analysis of two different black liquor gasifier (BLG) designs, one (Chemrec design) operating at high temperature and pressure with the condensed phase leaving the gasifier as a molten liquid and one (MTCI design) operating at lower temperature and pressure, with the condensed phase leaving the gasifier as a solid.

A key objective in the current biorefinery assessment was to understand the relative costs/benefits of liquid fuels production vis-à-vis BLGCC electricity production. Accordingly, considering the limited resources available for the project, we made a tentative decision early in the project to focus the biorefinery analysis around a single black liquor gasifier design rather than carrying out parallel designs with two gasifiers, as done in (Larson, Consonni et al. 2003). The BLGCC work showed more favorable performance and economics for BLGCC systems designed around the high-temperature BLG (HTBLG) design, so this one was selected for the detailed kraft pulp mill biorefinery designs described in (D.Larson, Consonni et al. 2006).

However, because there was still considerable interest in the low-temperature BLG (LTBLG) design at the Department of Energy and in the pulp and paper industry, we pursued a preliminary analysis to evaluate the LTBLG in a biorefinery application to determine whether the more favorable performance and cost for the HTBLG in the BLGCC analysis would persist in biorefinery applications. This preliminary analysis, which is described in Section B.2 of this volume, confirmed that the HTBLG would likely give better results than the LTBLG in the biorefinery applications we were examining in our study.

This finding prompted discussion among project participants about what types of applications at pulp/paper mills would allow the unique features of the LTBLG technology to be best exploited. The unique features include the high hydrogen content of the synthesis gas and the nearly complete segregation of sulfur (to the gas phase) and sodium (to the condensed phase) that occurs due to the intrinsic thermodynamics of the LTBLG process.

One possibility is that applications involving the synthesis of products with a high hydrogen content, e.g., ammonia or pure hydrogen, might favor the LTBLG over the HTBLG because of the much higher H<sub>2</sub>:CO ratio that characterizes LTBLG product gas (H<sub>2</sub>:CO of 2.6 versus 1.1 on a molar basis in BLGCC study (Larson, Consonni et al. 2003)). There is some merit to this line of reasoning. However, relatively inexpensive commercial water-gas shift (WGS) reactors can be used to increase the H<sub>2</sub>:CO ratio of a synthesis gas to arbitrarily high values via the nearly-autothermal (The WGS reaction is only slightly exothermic, -41 kJ/mol) WGS reaction,  $\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{H}_2 + \text{CO}_2$ . Thus, the cost and energy efficiency penalties of including a WGS system in a HTBLG application

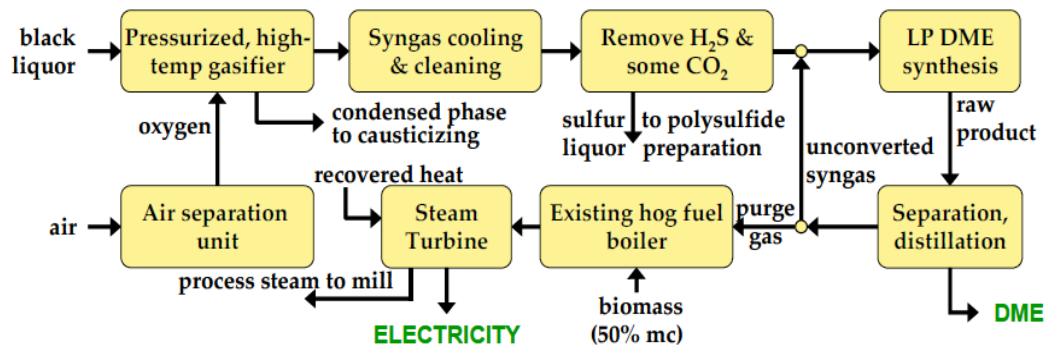
(to obtain a high hydrogen content syngas) are relatively minor, and there would appear to be little or no inherent advantage to be gained by the LTBLG technology because of its unique high-hydrogen content syngas production.

In contrast, there may be unique opportunities at a pulp mill to take advantage of the nearly complete segregation of sulfur and sodium that characterizes the LTBLG. Interestingly, this feature was one of the major factors contributing to the relatively unfavorable financial performance we predicted for the LTBLG in the BLGCC application at a pulp/paper mill using the kraft pulping process. The chemical segregation leads to a requirement that considerable additional causticizing capacity be installed at a kraft mill to enable the regeneration of the pulping liquor. If the concept of direct causticizing proves to be commercially viable, whereby the necessary pulping chemicals are largely regenerated directly by hydrolysis of the gasifier condensed phase (Nohlgren 2004), this might allow this limitation to be overcome at a kraft pulp mill. However, work on direct causticizing is still at the stage of laboratory investigations, and the most recent results from the Georgia Institute of Technology (Sinquefeld 2005) suggest that direct causticizing may not work at conditions of low-temperature gasification. This finding led us to assess alternative pulping strategies (non-kraft processes) that might be able to achieve higher pulp yields using different pulping chemistries that take advantage of having separate streams of sulfur and sodium in the chemical recovery area. Section B.3 in this appendix identifies some alternative pulping options and describes analysis aimed at better understanding the commercial implications of implementing the most promising of these. First we discuss analysis of a biorefinery application with the LTBLG using the

same polysulfide pulping strategy as used for biorefinery analyses in (Larson, Consonni et al. 2006).

## B.2 DME biorefinery design with low temperature BLG

The DME biorefinery design we selected for a preliminary analysis with the LTBLG at a kraft mill with polysulfide pulping uses a process configuration that parallels the DMEa configuration in the analysis in (Larson, Consonni et al. 2006). In DMEa, syngas from the HTBLG is processed through the synthesis reactor, with most of the unconverted syngas recycled to the synthesis reactor to maximize liquid DME production (Figure B.1). The resulting deficit in steam production is made up by burning hog fuel and some purchased residues in boilers, the steam from which is expanded through a back-pressure steam turbine before being delivered to the pulp/paper mill. The electricity generated by the turbine is sufficient only to meet all (or most) of the biorefinery's parasitic electricity demand. The pulp/paper mill's electricity needs would in this case need to be met by purchasing power from the grid.



**Figure B.1:** Schematic of biorefinery DMEa with high-temperature BLG.

Most of the syngas that is not converted to DME in a single pass through the synthesis reactor is recycled to increase DME production. Steam is generated for pulp/paper mill needs by burning hog fuel and some purchased residues. The back pressure steam turbine generates some electricity.

To assist in developing heat and mass balances for the LTBLG case, we undertook some detailed process design and simulation. These simulations were not as comprehensive and detailed as HTBLG simulations, but they are sufficiently detailed that one can be confident drawing conclusions regarding a comparison between the HTBLG and LTBLG in this application.

The LTBLG is an indirectly-heated fluidized bed that operates at near-atmospheric pressure. The heat needed for the endothermic gasification reactions is delivered to the gasifier through heat exchange tubes immersed in the fluidized bed and by fluidizing steam. Pulse combustors provide heat input by burning part of the syngas generated by the gasifier. The fluidizing steam is superheated to 540°C before injection. At the moderate temperature maintained in the reactor (~600°C), the condensed phase material is a dry solid.

**Table B.1:** Composition of clean syngas in the BLGCC power/recovery system simulations.

	<b>LTBLG</b>	<b>HTBLG</b>
<b>Composition (vol%)</b>		
<b>Ar</b>	0.00	0.66
<b>CH4</b>	3.49	1.44
<b>CO</b>	23.47	26.09
<b>CO2</b>	10.50	11.27
<b>COS</b>	0.01	0.05
<b>H2</b>	61.91	27.51
<b>H2O</b>	0.34	32.73
<b>N2</b>	0.00	0.24



The overall performance results for the LTBLG refinery are shown in Table B.2, alongside the results from (D.Larson, Consonni et al. 2006) for the HTBLG refinery. An important difference shown in the table is in the H<sub>2</sub>:CO ratio of the syngas sent for synthesis. In the LTBLG case this ratio is much higher than in the HTBLG case due to the nature of the steam reforming reactions that occur in the LTBLG. The high H<sub>2</sub>:CO ratio means that there is an excess of H<sup>+</sup> for DME production (the stoichiometric H<sub>2</sub>:CO ratio is 1.0 for DME: 3CO + 3H<sub>2</sub> ↔ C<sub>2</sub>H<sub>6</sub>O + CO<sub>2</sub>), such that a considerable amount of H<sup>+</sup> cannot be converted to DME. This result in about 18% less DME being produced in the LTBLG case compared to the HTBLG case.

**Table B.2:** Comparison of heat and mass balances for a DME biorefinery using a high-temperature BLG (HTBLG) and one using a low-temperature BLG (LTBLG).

		HTBLG	LTBLG	Delta %	
FUEL INPUTS	<b>Black liquor (DS)</b>	kg/s	28.5	28.5	
		MWt LHV	350.7	350.7	
	% dry solids in black liquor	%	80.0	80.0	
	<b>Total woody biomass</b>	MWt LHV	131.5	177.8	<b>35%</b>
	Purchased residues	MWt LHV	77.4	123.7	<b>60%</b>
	<b>Lime kiln fuel oil</b>	MWt LHV	35.9	44.8	<b>25%</b>
STEAM TO MILL	MP steam to mill	kg/s	32.9	32.9	
	LP steam to mill	kg/s	64.1	64.1	
CLEAN SYNGAS	Mass flow	kg/s	13.3	7.7	
	Energy flow	MWt LHV	235.4	221.7	<b>-6%</b>
	H <sub>2</sub> /CO Ratio	mol/mol	1.05	2.85	
FUEL PRODUCTION	Recycle of unconverted syngas	%	97%	97%	
	Unconverted syngas to boiler	kg/s	7.00	1.07	
		MJ/kg	4.79	65.90	
		MWt LHV	33.5	71.0	<b>112%</b>
	DME mass flow	kg/s	5.9	4.8	
	DME energy flow	MWt LHV	168.0	137.4	<b>-18%</b>
HEAT FROM FS ISLAND	Heat for MP steam generation	MWt	22.3	24.9	<b>12%</b>
ELECTRIC POWER	Steam turbine gross output	MW <sub>el</sub>	32.9	46.6	
	Syngas expander (gasifier island)	MW <sub>el</sub>		5.0	
	Syngas expander (fuel synthesis island)	MW <sub>el</sub>	2.58	4.0	
	<b>Total gross power production</b>	<b>MW<sub>el</sub></b>	<b>35.5</b>	<b>55.6</b>	<b>57%</b>
	Boiler and steam cycle auxiliaries	MW <sub>el</sub>	3.1	4.5	
	Gasifier island auxiliaries	MW <sub>el</sub>	2.7	2.7	
	Air separation unit	MW <sub>el</sub>	15.2	0.0	
	Syngas compressor	MW <sub>el</sub>	2.0	23.3	
	Rectisol refrigeration	MW <sub>el</sub>	3.1	3.3	
	Recycle compressor	MW <sub>el</sub>	7.3	25.7	
	DME separation refrigeration	MW <sub>el</sub>	1.0	0.0	
	<b>Total parasitic power demand</b>	<b>MW<sub>el</sub></b>	<b>34.3</b>	<b>59.5</b>	<b>73%</b>
	Net Power Available for Mill	MW <sub>el</sub>	1.2	-8.9	
	Mill power demand	MW <sub>el</sub>	100.1	100.1	
<b>Grid Electricity Purchases required</b>	<b>MW<sub>el</sub></b>	<b>98.9</b>	<b>109.0</b>	<b>10%</b>	

The excess of H<sub>2</sub> also results in a much higher flow of unconverted syngas to the power boiler (more than double the HTBLG case), where process steam is generated from it. This might lead one to expect that the need for purchased residues (to meet process steam demands) might be lower. However, the LTBLG case actually requires more purchased woody residues as boiler fuel than the HTBLG case. This is due to the reduced heat recovery from the gasification island that is possible in the LTBLG case, as well as the steam requirements for the gasifier. The reduced heat recovery is due to a number of factors, including the lower temperature of the syngas leaving the gasifier (which enables less high grade heat to be recovered from syngas cooling) and rejection of all heat in the syngas below 250°C (to avoid tar condensation problems).

The larger consumption of fuel (unconverted syngas and wood residues) in the power boiler results in 64% more back-pressure steam turbine power production in the LTBLG case than in the HTBLG case. However, the greater power production is almost entirely offset by the higher power demand in the LTBLG case for compressing the clean syngas to synthesis reactor pressure and for running the recycle compressor in the downstream area. There is little potential for pressurizing the operation of the LTBLG (which would reduce or eliminate the need for downstream syngas compression) because the unique pulse-combustor-tube bundle heat transfer system does not lend itself to doing so.

In summary, based on the preliminary calculations, it appears that the LTBLG in a DME pulpmill biorefinery configuration would produce 15-20% less DME than in a HTBLG biorefinery, with both requiring some purchases of electricity to meet parasitic electricity demands and thus not having any power available to help offset pulpmill

electricity needs. Moreover, the LTBLG configuration would require the purchase of about double the wood residues that would need to be purchased with the HTBLG, and fuel oil purchases for the lime kiln would be some 25% higher. When these overall energy performance figures are taken into consideration, together with the likely higher capital investment required for a LTBLG biorefinery – a conclusion based on the comparison of LTBLG and HTBLG capital cost estimates developed for the BLGCC study – a pulpmill biorefinery based on LTBLG does not appear likely to show better financial performance for applications being targeted in the present work than one based on a HTBLG.

### **B.3 Low temperature BLG with alternative pulping chemistries**

The separation of sulfur and sodium during black liquor gasification enables the recovery of pulping chemicals for several high-yield sulfur-based pulping processes (Table B.3), (We have chosen to limit the analysis here to sulfur-based processes because these processes can be implemented now, without major changes in the pulp mill.). Polysulfide anthraquinone (PSAQ) pulping, which was the assumed pulping chemistry used in biorefinery analysis reported in (D.Larson, Consonni et al. 2006), requires approximately 60% of sulfur to leave the gasifier in the gas phase. This chemistry gives a two to four percentage point increase in yield of pulp from the digester. Alkaline sulfite pulping processes can increase pulp yields substantially more than PSAQ pulping, but these chemistries require a higher degree of sulfur-sodium separation in the recovery area – levels of separation achievable only with the LTBLG technology. Specific pulping chemistries in this category include alkaline sulfite anthraquinone (ASAQ) and mini-

sulfide sulfite anthraquinone (MSSAQ). Neither of these processes are commercially employed today primarily because there are no cost-effective means for recovering the pulping liquor with the Tomlinson recovery process.

**Table B.3:** Summary of some sulfur-based pulping options.

	<b>Kraft</b>	<b>PSAQ</b>	<b>MSSAQ</b>	<b>ASAQ</b>
<b>Applicability</b>	Soft or hardwood; unbleached or bleached products	Variant of kraft pulping. Same applicability.	Limited to unbleached grades (kappa # $\geq$ 50)	Soft or hardwood; unbleached or bleached products
<b>Pulping chemicals<sup>a</sup></b>	NaOH + Na <sub>2</sub> S	NaOH + Na <sub>2</sub> S <sub>x</sub> + AQ	Na <sub>2</sub> SO <sub>3</sub> + Na <sub>2</sub> S + AQ	NaOH + Na <sub>2</sub> SO <sub>3</sub> + AQ
<b>Rate</b>	Fastest delignification rate	Similar to or slightly slower than kraft (due to lower sulfidity).	Slower than kraft, but faster than ASAQ. Differences are small at high kappa #.	Somewhat slower than MSSAQ; needs longer time and higher temperature than kraft.
<b>Pulp yield</b>	Lowest yield: ~56% at kappa 100 and ~45% at kappa 30.	2 to 4 percentage points higher than kraft.	8 to 10 percentage points higher than kraft at high kappa #. Lower gain at lower kappa #.	3 to 7 percentage points higher than kraft, depending on kappa #.
<b>Brightness</b>	Low brightness	Same as kraft.	10 to 20 points higher than kraft.	10 to 20 points higher than kraft.
<b>Strength</b>	Highest tear strength	Somewhat lower tear than kraft, other properties similar.	Refining <sup>b</sup> 25-30% less than kraft; similar/slightly higher strength than kraft, except lower tear.	Less refining <sup>b</sup> than kraft; Similar/slightly higher strength than kraft, except lower tear.
<b>Sulfur needs for pulping</b>	100% of S needed as Na <sub>2</sub> S.	60% of S needed as elemental sulfur to mix with 40% of S in Na <sub>2</sub> S to form PS.	10-15% of S needed as Na <sub>2</sub> S and 85-90% as Na <sub>2</sub> SO <sub>3</sub> . Na <sub>2</sub> SO <sub>3</sub> can be made from H <sub>2</sub> S. <sup>c</sup>	100% of S needed as Na <sub>2</sub> SO <sub>3</sub> , which can be made from H <sub>2</sub> S.
<b>Best recovery system</b>	Tomlinson	HTBLG	LTBLG	LTBGL
<b>Causticizing demand with BLG</b>	Small $\uparrow$ with HTBLG Large $\uparrow$ with LTBLG	Small increase	Causticizing eliminated	Increase

(a) AQ = anthraquinone.

(b) Refining is a physico-mechanical process to increase the surface area available for inter-fiber bonding by defibrillation of fibers. It increases the strength properties of the fibers. Less refining means less electrical energy required.

(c)  $\text{H}_2\text{S} \rightarrow \text{SO}_2 \rightarrow \text{Na}_2\text{SO}_3$

### B.3.1 MSSAQ pulping

We have chosen MSSAQ pulping for further analysis for several reasons: (i) MSSAQ pulping gives the highest pulp yield increases (up to 10 percentage points), (ii) MSSAQ pulping can completely eliminate the need for causticizing and the associated lime kiln, and (iii) the high degree of sulfursodium segregation required in the recovery

process for MSSAQ makes it an especially good choice for integrating with a recovery system based on the LTBLG technology.

Among the pulping options shown in Table B.3, MSSAQ offers the greatest yield enhancement potential, but the level of yield improvement that can be achieved with bleached grades of pulp/paper is modest. The benefit of MSSAQ is best exploited in the production of unbleached grades of pulp (characterized by high kappa numbers), e.g., for linerboard manufacture. This limits somewhat the market potential for application of MSSAQ pulping, but unbleached pulp grades account for about 38% of total pulp production in the United States, so the potential market is not small.

Our detailed analysis here focuses on a reference mill utilizing MSSAQ pulping to make unbleached linerboard (LB). (This is a different product than the freesheet paper that is considered for a reference mill in the HTBLG analysis reported in (Larson, Consonni et al. 2006). A typical yield increase with MSSAQ pulping for this LB application (with kappa numbers of 90 to 100) is ten percentage points. For our analysis, we assume a pulping yield of 67% for MSSAQ pulping and 57% for conventional kraft cooking for unbleached linerboard. (For comparison, the digester yield at reference freesheet mill in (Larson, Consonni et al. 2003) was 46.2%.)

The assumptions for MSSAQ pulping conditions are compared against kraft pulping conditions in Table B.4 and the estimated black liquor elemental composition that would result with the MSSAQ option is given in Table B.5. Because of the high pulping yield and the high alkali charge the MSSAQ black liquor has a high inorganic content and a relatively low heating value compared to black liquor produced at a kraft pulp mill. The heating value per unit mass is only about 75% of that for a conventional

kraft mill. Moreover, as a consequence of the much higher pulp yield, the total energy content of the black liquor available at the recovery area of the mill is reduced by about one-third compared to the black liquor available at an unbleached LB mill using kraft pulping.

**Table B.4:** Pulping conditions for MSSAQ and reference kraft cook for linerboard quality pulping with kappa numbers of 90-100. Data based on (Teder, Olm et al. 1988) and (Naithani, Lindstrom et al. 2005).

<b>Pulping</b>	<b>Kraft</b>	<b>MSSAQ</b>
Pulp Yield	57%	67%
Liquor inorganic composition (Na <sub>2</sub> O equivalent basis)		
Na <sub>2</sub> SO <sub>3</sub>	-	83%
Na <sub>2</sub> S	21%	7%
Na <sub>2</sub> CO <sub>3</sub>	15%	10%
NaOH	61%	10%
Total alkali charge, kg Na <sub>2</sub> O/kg oven-dry wood	0.176	0.22
Anthraquinone charge	-	0.1% of oven-dry wood mass
Liquor to wood ratio	4	4
Max Temperature	160°C	160°C
H Factor <sup>a</sup>	700	700

(a) The H factor is the integral of the temperature-dependent delignification rate over the digestion period. A high H factor means a high temperature and/or long time indicating a high steam demand.

**Table B. 5:** Liquor elemental composition and higher heating value (HHV) for MSSAQ and for reference kraft cook for linerboard quality pulping with kappa numbers of 90-100.

	<b>Weight Percent</b>	
	<b>Kraft</b>	<b>MSSAQ</b>
<b>C</b>	37.0%	27.5%
<b>H</b>	4.2%	2.8%
<b>O</b>	33.3%	33.4%
<b>Na</b>	20.3%	21.0%
<b>S</b>	3.1%	13.2%
<b>K</b>	1.9%	2.0%
<b>Cl</b>	0.2%	0.2%
<b>HHV, kJ/kg BLS</b>	14,700	10,600

The conversion of an unbleached kraft linerboard mill to MSSAQ pulping may create significant operating cost savings for the mill. Increasing the pulp yield from 57% to 67% decreases wood consumption by 15% for the same level of pulp production. Another large source of savings is the complete elimination of the lime cycle and the associated savings in fuel cost. The anthraquinone would represent an important added operating cost. For pulp production of 1,580 short tons of oven dry pulp/day (the same level of unbleached pulp produced in the reference mill described in (D.Larson, Consonni et al. 2006)) the estimated cost of these items is shown in Table B.6 for an unbleached LB mill using either kraft or MSSAQ pulping. The capital investment and other operating cost changes that might be needed to achieve the indicated net savings of about \$11 million per year are discussed in Section B.3.3.

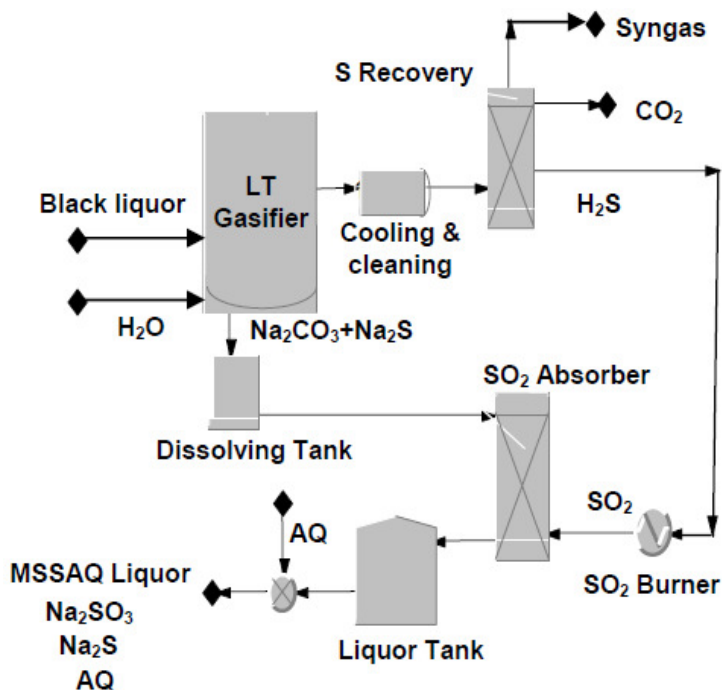
### **B.3.2 Integrating MSSAQ pulping with low-temperature BLG**

A simplified process diagram for LTBLG-based liquor recovery at a mill using the MSSAQ pulping process is shown in Figure B.3. The black liquor is reformed in steam in a LTBLG, after which the gas is cooled and cleaned of contaminants. Most of the sulfur in the black liquor (> 90%) appears as H<sub>2</sub>S in the clean syngas. The H<sub>2</sub>S is recovered using a conventional acid gas removal technology (e.g., 10 Rectisol or Selexol). This H<sub>2</sub>S is then oxidized to SO<sub>2</sub>, which in turn is absorbed into a sodium-rich green liquor stream (constituted by dissolving in water the condensed phase from the gasifier). This produces a white liquor stream to which anthraquinone is added before the liquor is recirculated to the digester.

**Table B.6:** Estimate for major operating cost changes (\$ per year) after converting a mill making 1,580 oven-dry short tons of unbleached linerboard pulp per day from Kraft to MSSAQ pulping.

	Kraft	MSSAQ	Cost Savings
<b>Pulpwood Purchases</b>	\$60,616,267	\$51,569,063	\$9,047,204
<b>Antraquinone</b>	-	\$2,813,000	\$ (2,813,000)
<b>Lime Kiln fuel(#6 oil)</b>	\$4,697,185	-	\$4,697,185
<b>Net Change</b>			\$ 10,931,389

Assumptions: pulpwood @ \$57.33 per dry short ton; AQ @ \$3.65/kg; lime kiln fuel @ \$5/MMBtu; 8,330 equivalent full-load operating hours/year.



**Figure B.3:** Schematic diagram of liquor recovery for MSSAQ pulping.

To gain some understanding of how this type of system might perform, we have carried out calculations to estimate on a preliminary basis the energy and mass balances for a LTBLG with input of MSSAQ black liquor generated at a kraft linerboard mill producing 1,580 short dry tons per day of unbleached pulp from the digester. We have

limited our detailed modeling to the gasification island, without simulating the whole integrated system comprising a gas clean-up island and further downstream syngas processing (e.g., power and/or liquid fuel production) at the same level of detail. Because the LTBLG is the most complicated element of the system from an energy balance perspective, it is the most critical area to model in detail for an assessment aimed at giving a preliminary indication of the potential of LTBLG in MSSAQ mill applications.

Our calculations use the black liquor properties for MSSAQ (Table B.5) as inputs to the LTBLG model as developed in BLGCC study (Larson, Consonni et al. 2003). We have made the same assumptions regarding carbon conversion, tars and Na<sub>2</sub>S as in BLGCC study (Table B.7). Our assumption of carbon conversion is high relative to what actually has been demonstrated to date. In particular, we assume 97% of the carbon input as black liquor is converted to light gases and 1.5% is converted to tars, for a total carbon conversion of 98.5%. (The remaining 1.5% carbon input leaves with the bed solids.) This level of overall carbon conversion using the low-temperature gasification technology has not yet been demonstrated at commercially-relevant scales. DeCarrera (DeCarrera ; DeCarrera January 2006) reports that measured carbon conversion to light gases plus tars at the pilot-scale low-temperature gasifier installed at a pulp mill in Big Island, Virginia, ranged from 60% to 80%, with the conversion to tars estimated to account for one-third to one-half of the converted carbon based on carbon balance closure. Measurements reported by researchers from the Institute of Paper Science and Technology for the Big Island gasifier (Iisa, Whitty et al. 2006) showed the following carbon distribution of carbon input with the black liquor: 65% to light gases, 23% to bed solids, 4.5% in heavy tars, and 6% missing. Analysis suggests that the missing fraction was light tars. Thus,

these measurements appear to be generally consistent with those reported by DeCarrera. Using our modeling assumptions, Table B.8 reports the calculated raw syngas composition at the gasifier exit.

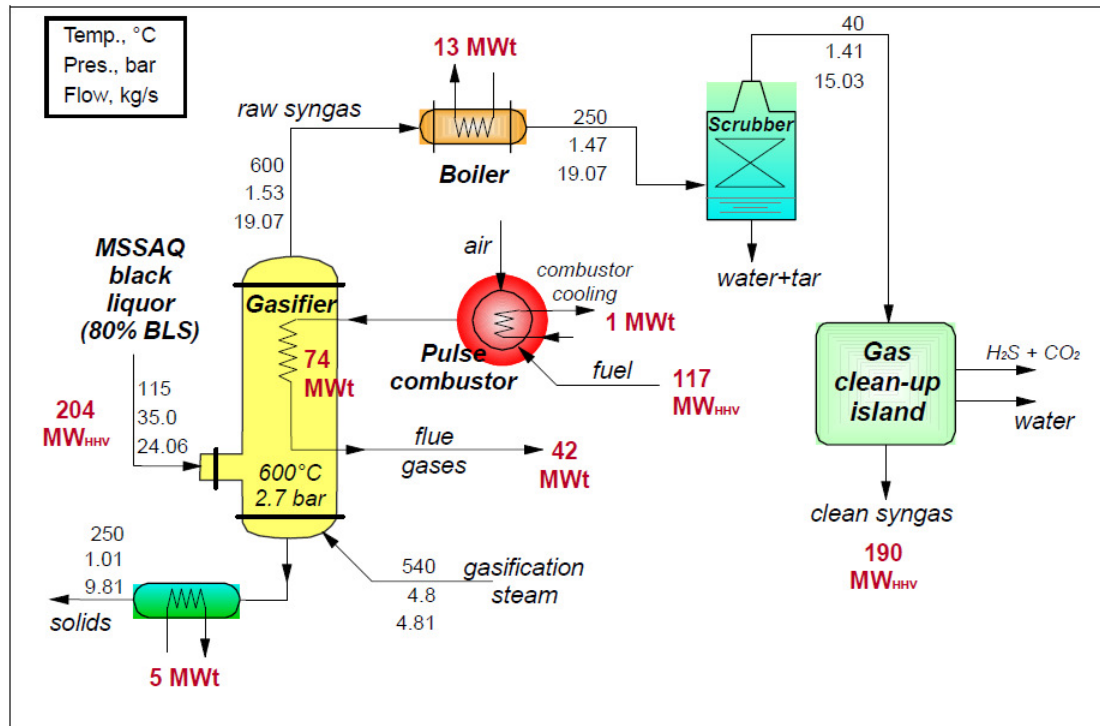
**Table B.7:** Assumptions adopted to evaluate the syngas composition and the heat/mass balances of the low temperature black liquor gasifier operating with black liquor from MSSAQ pulping.

Pressure	2.7 bar ( 25 psig)
Temperature	600°C (1112°F)
Gasification steam	0.25 kg/kg BLS
Heat loss to environment	1% of BL HHV
Carbon conversion	98.5% of total C in BL
Tar production	1.5% of total C in BL
Na <sub>2</sub> S production	7.8% of total S in BL
All other products (gas and condensed phases) assumed to be amixture at equilibrium	

**Table B.8:** Calculated molar composition of syngas at the gasifier exit.

H <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub> O	CO	CO <sub>2</sub>	H <sub>2</sub> S	COS
30.5%	9.3%	26.7%	8.1%	18.2%	7.0%	0.1%

As part of the gasifier island calculations, we also estimate the mass and energy balances for cooling of the raw syngas (from 600°C to 250°C) in a steam boiler, followed by scrubbing and cooling to 40°C to remove remaining alkali, tar and most of the water vapor. The cooled, dry syngas is then ready to be fed to the sulfur recovery unit (SRU), which would remove essentially all the H<sub>2</sub>S in the syngas and some portion of the CO<sub>2</sub>. The technology used in the SRU would be selected to achieve concentrations of H<sub>2</sub>S and CO<sub>2</sub> required by the downstream processing equipment. Commercially-established SRU options include Rectisol® and Selexol® systems (which were used in the simulation work reported in (D.Larson, Consonni et al. 2006)).



**Figure B.4:** Heat and mass balance of the low temperature gasifier serving a plant producing 1580 short tons/day of pulp by the MSSAQ pulping.

Figure B.4 shows the results of our mass/energy balance simulation. The available black liquor from the MSSAQ pulping represents a gasifier energy feed rate of 204 MW<sub>HHV</sub>. This energy input to the gasifier, together with heat supplied via the pulse-combustor, and heat carried in the fluidization steam, produce the following energy outputs:

- Chemical and thermal energy in the syngas leaving the gasifier at 600°C. Part of the thermal energy (13 MWt) is recovered as steam in the boiler that cools the syngas to 250°C, but the majority of it is lost in the scrubber used to remove tar and to cool the gas to a temperature suitable for feeding to the compressor needed to pressurize the syngas for the SRU.

- Thermal energy in the solids discharged by the gasifier. We assume that 5 MWt of this energy would be recoverable by cooling the green liquor to 250°C.
- Chemical energy in the removed tar, in the H<sub>2</sub>S, and in the sulfides in the condensed phase leaving the gasifier.

The chemical energy remaining in the clean, cooled syngas is 190 MW<sub>HHV</sub>. A significant amount of this (117 MW<sub>HHV</sub>) is needed for the pulse combustor, leaving 73 MW<sub>HHV</sub> available for further downstream processing, e.g. into electricity or liquid fuels. The ratio between the energy that must be supplied by the pulse combustors and the heating value of the input black liquor is much higher than with a conventional kraft black liquor because of the different properties of the MSSAQ black liquor, namely higher inert content and reduced heating value. Only about 35% of the heating value of the black liquor is transferred to heating value in the final syngas, corresponding to a cold-gas efficiency of 35%.

One of the most striking numbers in Figure B.4 is the amount of chemical energy contained in the MSSAQ black liquor: 204 MW<sub>HHV</sub>. For comparison, the estimate of the chemical energy in the black liquor at an unbleached kraft linerboard mill is 261 MW<sub>HHV</sub>. The low rate of black liquor energy input contributes significantly to a low net syngas production rate: 73 MW<sub>HHV</sub>, which can be compared with an estimated 194 MW<sub>HHV</sub> of clean syngas that could be produced at an unbleached kraft linerboard mill using a high-temperature BLG recovery system.

### **B.3.3 Some preliminary economics of MSSAQ pulping with LTBLG**

The relatively modest amount of net clean syngas per unit of pulp that can be produced with the LTBLG/MSSAQ system makes the attractiveness of further processing the syngas (into liquid fuel and/or electricity) uncertain (due to scale economies of synthesis and refining). The following high level economic analysis attempts to resolve some of this uncertainty.

Consider the conversion of an existing unbleached linerboard mill from conventional kraft pulping with Tomlinson power/recovery system to MSSAQ pulping with LTBLG power/recovery. We assume the rate of production of unbleached pulp is 1,580 short dry tons/day, the same rate as for the reference kraft uncoated freesheet pulp/paper mill used as the basis for analysis in (D.Larson, Consonni et al. 2006). For preliminary calculations, we will assume that the linerboard mill, both before and after conversion to MSSAQ, has the same process steam and electricity demands as the freesheet mill, namely:

- process steam demand of 212 MW,  $\frac{2}{3}$  of which is low-pressure (5 bar) and  $\frac{1}{3}$  of which is medium-pressure (13 bar) steam. (In reality, a linerboard mill with best available technology will have about 19% lower total process steam demand than a freesheet mill with best available technology (Jacobs Engineering Group). However, the steam demand for a linerboard mill using MSSAQ pulping will be approximately the same as one with the same output using kraft pulping.)
- process electricity demand of 100 MW. (In reality, a linerboard mill with best available technology will have about 8% lower electricity demand than a corresponding freesheet mill (Jacobs Engineering Group))

With these assumptions and the energy balance depicted in Figure B.4, we can estimate the amount of electricity that can be generated by the LTBLG system and the amount of purchased residues needed (to augment available hog fuel) to produce the requisite amount of process steam. Table B.9 shows our estimate of steam that can be produced from three sources: combustion of the clean syngas in a boiler, recovery of heat by syngas cooling and by cooling of the pulse combustor flue gases, and by combustion of hog fuel in a boiler. The amount of hog fuel is assumed to be 9% of the dry mass of pulpwood received at the mill (as for analysis in (D.Larson, Consonni et al. 2006)). The high digester yield with MSSAQ pulping reduces the amount of pulpwood needed to achieve the same pulp production rate as with conventional kraft pulping, leading to less hog fuel availability as well. The steam production amounts to 136 MWth, or  $\frac{2}{3}$  of the process steam needs of the mill (Table B.9).

**Table B.9:** Estimated steam production from clean syngas, hog fuel, and LTBLG heat sources.

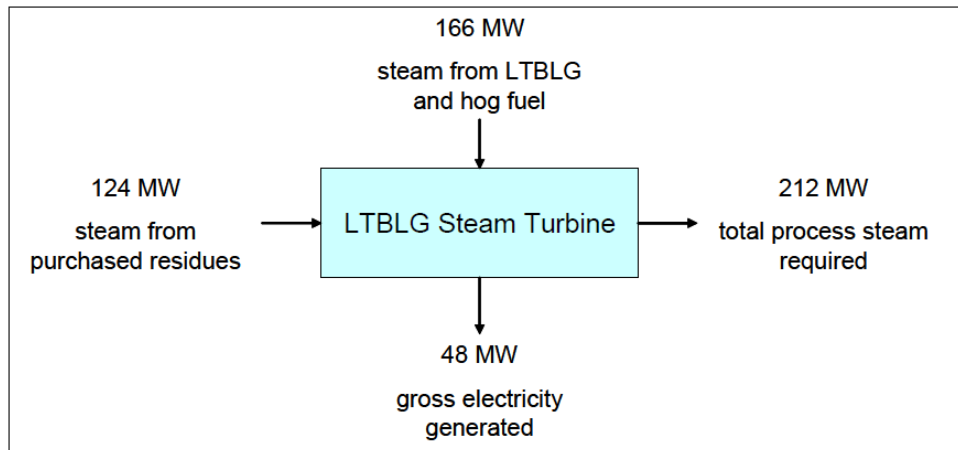
<b>LTBLG steam production</b>	<b>Available MWHHV</b>	<b>Approximate Steam MW</b>
Syngas (converted to steam @ 90% HHV efficiency)	73	65.7
Pulse combustor flue gas (84% heat exchanger efficiency)	42	35.4
Hog fuel (converted to steam @ 90% HHV efficiency)	24.5	22.0
Syngas cooling	13	13
<b>Total steam before use of purchased residues</b>		<b>136.2</b>

**Table B.10:** Estimate of electricity generation with LTBLG system using existing back-pressure steam turbine.

Total process steam required, MW	212
Delta-h of LP steam, MJ/kg	2.115
Approximate total process steam flow (assuming all LP), kg/s	100.2
Enthalpy of steam for expansion (from 78.5 bar, 475 C), MJ/kg	3.339
Enthalpy of LP steam (5 bar), assuming isentropic expansion, MJ/kg	2.678
Enthalpy of MP steam (13 bar), assuming isentropic expansion, MJ/kg	2.864
Delta-h for LP steam (isentropic), MJ/kg	0.661
Delta-h for MP steam (isentropic), MJ/kg	0.475
Fraction of total steam that is LP	0.667
Fraction of total steam that is MP	0.333
Average delta-h for steam expansion in steam turbine, MJ/kg	0.599
Assumed steam turbine efficiency	80%
<b>Gross electricity generated, MW</b>	<b>48.0</b>
LTBLG parasitic electricity load, MW	5.0
<b>Net electricity available for process use at the linerboard mill, MW</b>	<b>43.0</b>

Since 212 MWth of process steam are needed, the additional steam is generated by burning purchased residues in a boiler. To estimate the amount of purchased residues needed, we first estimate the amount of electricity that will be generated when 212 MWth of process steam are produced. This then enables an estimate of the amount of required purchased residues. Table B.10 details our calculation of electricity generation. We assume that steam is generated at 78.5 bar, 475°C and expanded through the existing back-pressure steam turbine at the mill. Two-thirds of the steam is expanded to 5 bar and one third of the steam is expanded to 13 bar. The gross electricity generation is 48 MW. The net electricity production (after accounting for an estimated 5 MW of parasitic electricity demand by the LTBLG system) is 43 MWe.

A simple energy balance around the steam turbine (Figure B.5) enables an estimate of 124 MWth of steam required to be generated using purchased residues. Assuming a biomass boiler efficiency of 90%, this corresponds to 138 MWHHV of purchased biomass residues.



**Figure B.5:** Approximate energy balance for LTBLG steam turbine island

From the above approximate energy balance, we are able to estimate the main annual operating costs for the MSSAQ/LTBLG process relative to a Kraft/Tomlinson alternative (Table B.11, which is an expanded version of Table B.6). Our estimate of the electricity generation with a new Tomlinson system at an unbleached kraft linerboard, 38.4 MWe, is calculated by linearly scaling (with black liquor energy flow rate<sup>7</sup>) the estimate in (D.Larson, Consonni et al. 2006) of the electricity generation for a Tomlinson system at a bleached kraft freesheet mill (64 MWe).

Table B.11 shows an estimated net annual savings of about \$6.6 million after converting the unbleached linerboard mill from kraft/Tomlinson to MSSAQ/LTBLG. This includes consideration of the operating and maintenance (O&M) costs for the LTBLG and Tomlinson systems. These annual O&M costs are estimated as 4% of the overnight installed capital cost of the recovery system in each case. Our net annual savings are lower than those estimated by (Naithani, Lindstrom et al. 2005) for a kraft-to-MSSAQ conversion.

**Table B.11:** Estimate of major operating costs (\$ per year) when converting a mill making 1,580 oven-dry short tons of pulp per day from Kraft/Tomlinson to MSSAQ/LTBLG.

	<b>Kraft</b>	<b>MSSAQ</b>	<b>Cost savings w/MSSAQ</b>
Pulpwood purchases	\$ 60,616,267	\$ 51,569,063	\$ 9,047,204
Anthraquinone	-	\$ 2,813,000	\$ (2,813,000)
Lime kiln fuel (#6 oil)	\$ 4,697,185	-	\$ 4,697,185
Electricity purchases	\$ 27,411,425	\$ 25,351,254	\$ 2,060,171
Purchased residues	-	\$ 3,911,855	\$ (3,911,855)
Recovery area O&M	\$ 3,796,129	\$ 6,260,606	\$ (2,464,477)
<b>Total savings / year</b>			<b>\$ 6,615,229</b>

Assumptions: pulpwood @ \$57.33 per dry short ton; AQ @ \$3.65/kg; lime kiln fuel @ \$5/MMBtu; electricity purchases @ 5 c/kWh; purchased residues @ \$1.53/MMBtu; 8,330 equivalent full-load operating hours per year. See text for discussion of recovery area O&M costs.

(Naithani, Lindstrom et al. 2005) estimated net operating cost savings of 30% (from 142 to 110 \$/oven dry ton pulp). For a mill producing 1580 oven dry short tons per day, this translates to a savings of \$17 million, which is substantially higher than our estimated \$6.6 million. The difference between our estimate and that of (Naithani, Lindstrom et al. 2005) is probably explained by the following factors:

- Assumes a 20 percentage point yield increase when converting from kraft to MSSAQ pulping (from 50% to 70%), compared to our more conservative 10 percentage points.
- Assumes a cost for anthraquinone that is approximately half of what we assume.
- Assumes a value for avoided lime kiln fuel use that is approximately double what we assume.

- Does not include recovery area O&M costs in their study.

Table B.12 details our estimate of the \$156 million installed capital cost estimate for the LTBLG system. The estimate is based on the capital cost for the LTBLG system in a BLGCC configuration (Larson, Consonni et al. 2003) serving a mill with the same pulp production rate as assumed here (1,580 short dry tons/day). The original cost estimate for the LT-BLGCC system includes H<sub>2</sub>S recovery equipment similar to that which would be needed for sulfur capture and conversion to SO<sub>2</sub> with the LTBLG/MSSAQ system. We have adjusted the original LT-BLGCC cost estimate to account for the following:

- We have removed the cost for the gas turbine combined cycle, since in our LTBLG/MSSAQ concept, electricity is generated using the steam turbine pre-existing at the mill.
- No syngas compressor and no syngas expander would be used in the LTBLG/MSSAQ concept (as is present in the LT-BLGCC system), since syngas pressurization is not part of our design.
- No lime kiln is required with the LTBLG/MSSAQ concept. In the prior LT-BLGCC analysis, additional lime kiln capacity was included in the cost estimate. This cost is removed. The black liquor flow with our LTBLG/MSSAQ concept is an estimated 204 MWHHV, compared to 391 MWHHV for the LT-BLGCC system. We have scaled the cost estimate (after the three above adjustments), using a 0.7 scaling exponent.
- We have escalated the cost from 2002\$ (used in the BLGCC analysis) to 2005\$. We have included the cost for some additional biomass boiler capacity. Consistent with

our BLGCC analysis (Larson, Consonni et al. 2003), we assume that the existing hog fuel/biomass boiler capacity available for use at the existing mill is 40% larger than the capacity required to handle the hog fuel generated at the kraft/Tomlinson linerboard mill. We have estimated that the existing boiler capacity is 40 MWHHV. Since the required capacity for the LTBLG/MSSAQ system is 162 MWHHV [24.5 MW of hog fuel (Table B.9) and 137.6 MW of purchased residues (noted in text above)], the new biomass boiler capacity required is 122 MWHHV. One of the biorefinery cases in (D.Larson, Consonni et al. 2006) (DMEa) included an installed capital cost of \$50.736 million for a biomass boiler with capacity of 50.5 MWLHV (corresponding to 62.2 MWHHV). We scaled this \$50.7 million by  $(122/62.2)^{0.7}$  to arrive at the estimate for the cost of additional biomass boiler capacity needed with the LTBLG/MSSAQ system.

**Table B.12:** Estimate of overnight installed capital cost for LTBLG system (million \$).

(a) Low-temperature BLGCC system from [2], 2002\$	252.51
(b) Remove cost of combined cycle -- 36% of (a)	162.48
(c) Remove cost of syngas compressor and expander	148.25
(d) Remove cost of additional lime kiln capacity included in (a)	106.15
(e) Scale to MSSAQ black liquor flow (0.7 scale exponent)	69.55
(f) Escalate to 2005\$	77.79
(g) Add cost of new biomass boiler capacity (122 MWHHV)	156.32
<b>Estimated overnight installed cost, million 2005\$</b>	<b>156.32</b>

Notes (corresponding to row lettering):

- (a) This is "TIC BEFORE ADJUSTMENTS" found in Table 12 of [2].
- (b) From Table 12 of [2], the combined cycle accounts for 36% of direct costs. We assumed this holds for installed costs as well.
- (c) The LT BLGCC system in [2] includes an 18.7 MW syngas compressor and a 5 MW syngas expander. These are not required for the LTBLG/MSSAQ system. We assume an average cost for these of \$600 per kW.
- (d) The figure in row (a) includes \$42.1 million for new lime kiln capacity (see note (d) of Table 12 in [2]). This \$42.1 million is removed since no lime kiln capacity is required with the MSSAQ process.
- (f) We escalate from 2002\$ to 2005\$ using a factor of 1.1185
- (g) We add the cost for new biomass boiler capacity, as described in the text.

We also estimate the cost for a new Tomlinson boiler at the unbleached kraft linerboard mill. We begin with the estimate in (Larson, Consonni et al. 2006) for a Tomlinson boiler at our reference kraft freesheet mill (\$136.15 million), and scale this (using 0.7 exponent) by the relative black liquor energy flows for these two types of mills. For the freesheet mill, the black liquor flow is 438 MW<sub>HHV</sub> (Larson, Consonni et al. 2003). Our estimate for the kraft linerboard mill is 261 MW<sub>HHV</sub>. Thus, the capital investment for the Tomlinson system at the linerboard mill is  $136.15 \times (261/438)^{0.7} = \$95$  million.

Thus, there is an incremental investment of about \$62 million required for the LTBLG/MSSAQ system in place of a new Tomlinson system, when the existing Tomlinson system reaches the end of its life. The annual operating cost savings of \$6.6 million (Table B.11) yields a 25-year IRR of about 10% on the incremental capital investment (assuming equity:debt = 100:0 and ignoring taxes).

#### **B.4 Conclusions**

Based on the preliminary analysis presented here, it appears likely that the low-temperature black liquor gasification technology designed into biorefineries similar to those evaluated in (Larson, Consonni et al. 2006) would yield lower energy efficiencies and less attractive financial performance than we found with the high temperature black liquor gasifier. Financial performance for application of the LTBLG may be better if unique features of the technology can be exploited. Our preliminary analysis of one such option – the LTBLG used in the recovery cycle at a pulp mill adopting the MSSAQ pulping process – indicates potentially viable financial performance, but more detailed

analysis is required to gain a more accurate estimate than we have presented here of the financial performance and to better understand how it might be improved.

## APPENDIX C

### ELICITATION PROCEDURE FOR MODEL PARAMETERS

To provide further details about the elicitation procedure the complete elicitation procedure for the ‘Arabinose’ sugar unit, is demonstrated in this appendix.

**Step 0:** Specify the minimum and maximum values for the appropriate operating conditions (See Fig.C.1).

	Time (min)	Temp (oC)
Min Value	15	130
Max Value	300	170

**Figure C.1:** User defined range of operating conditions for the elicitation procedure.

**Step 1:** Create or select a design matrix for operating conditions. A sample design matrix is shown in figure C.2.

Time(min)	Temp(oC)
300	170
300	150
300	130
100	170
15	170
15	130

**Figure C.2:** A sample design matrix for predictive elicitation of ‘Arabinose’ yield.

**Step 2/3:** Given the operating conditions in step 1, the expert is inquired about the most probable % yield values (i.e. the median value), 75<sup>th</sup> percentile\* and the 90<sup>th</sup> percentile\* values of yield for ‘Arabinose’. Fig.A.3. below shows a sample yield values for “Arabinose” sugars from a hypothetical expert.

Operating Conditions		Arabinose		
Time(min)	Temp(oC)	Median	75 Percentile	90 Percentile
300	170	89	92	93
300	150	40	42	43
300	130	15	17	18
100	170	65	67	70
15	170	10	11	12
15	130	5	7	8

**Figure C.3:** A sample of the elicited values from a virtual expert for the step.

**\*Note:** Percentiles basically represent the cumulative probabilities. Consider the yield values for “Arabinose” at Time (300 min) and Temp (170 °C). According to a hypothetical expert the most probable yield value is 89% and 75% of the time the value would be below 92% yield value and 90% of the time the yield value would be below 93% yield.

**Step 4:** Given the model structure in (3.1)-(3.3), the elicited data in step 3 is fitted to the model and the residuals are estimated. If the residuals are significantly higher for any operating conditions, it signifies deviation from the model structure and the expert is given the opportunity to revise the elicited value. The residuals for the elicited values from the hypothetical expert are shown in figure C.4.

Time (min)	Temp(oC)	Residuals
300	170	302.89
300	150	95.27
300	130	167.06
100	170	69.57
15	170	435.34
15	130	317.06

**Figure C.4:** Sample of the residuals for the predicted values from the virtual expert.

**Step 5:** Next, hypothetical experimental realizations are provided to the expert about his/her initial estimates of the yields. And they are asked to revise their opinions in the

light of the new hypothetical experimental data. This helps in capturing the confidence of the expert in their initial opinions and also quantifies their belief about level of external noise. For example, the expert is provided a virtual experimental data point of ‘Arabinose’ yield of 91.09 for the operating condition (300 min, 170 °C) and inquired to revise his/her 50<sup>th</sup> and 75<sup>th</sup> percentile values at various operating conditions (See figure C.5).

Operating Conditions		New Potential Observations	Conditional Assesments for Experiment No.									
Time (min)	Temp(°C)		1		2		3		4		5	
			50 <sup>th</sup>	75 <sup>th</sup>	50 <sup>th</sup>	75 <sup>th</sup>	50 <sup>th</sup>	75 <sup>th</sup>	50 <sup>th</sup>	75 <sup>th</sup>	50 <sup>th</sup>	75 <sup>th</sup>
300	170	91.09	91		45	47	17		67			
300	150	46.39			47		18	19	74			
300	130	18.70					18.5		75	76		
100	170	75.70							76		12	
15	170											

**Figure C.5:** Sample of the conditional assessments of a virtual expert.

So, for the operating condition set 1(i.e. Time = 300 min, Temp = 170 °C), experts prior Median value was 89% but his/her updated median value is 91%. Similarly for the operating condition set 2(i.e. Time = 300 min, Temp = 150 °C), experts prior Median and 75<sup>th</sup> percentile values were 40% and 42% respectively, but their updated median and 75<sup>th</sup> percentile values are 45% and 47% .

## APPENDIX D

### ELICITATION PROCEDURE FOR SUGAR YIELD CORRELATION

In this appendix, the procedure for elicitation of correlation between different sugar units is demonstrated. The procedure to capture the correlation between various sugars, again the predictive elicitation procedure is used. For example, as shown in Figure D.1, a hypothetical data point for ‘Arabinose’ yield 91.51% at operating conditions (300 min, 170<sup>o</sup>C) is provided to the expert and the Expert is inquired to update his/her estimate for the Median and 75<sup>th</sup> percentile estimates for the other sugar units at the same operating conditions. Given this potential experimental realization, for this example the expert provides the updated realization for galactose as 87% and 89% for the 50<sup>th</sup> and 75<sup>th</sup> realization respectively.

Operating Conditions		Arabinose			Galactose			
Time (min)	Temp(oC)	Initial Percentiles		Potential New Observation	Initial Percentiles		Updated Percentiles	
		50th	75'th		50th	75'th	50th	75'th
300	170	89	92	91.51	85	87	87	89
<b>Glucose</b>								
		Initial Percentiles			Updated Percentiles			
		50th	75'th		50th	75'th	50th	75'th
		4	5		4.1	5.1		
<b>Xylose</b>								
		Initial Percentiles			Updated Percentiles			
		50th	75'th		50th	75'th	50th	75'th
		85	88		87	89		
<b>Mannose</b>								
		Initial Percentiles			Updated Percentiles			
		50th	75'th		50th	75'th	50th	75'th
		45	50		46	48		

**Figure D.1:** Experts revised prediction for the 50<sup>th</sup> and 75<sup>th</sup> percentile yields for various sugar yields based on the conditional hypothetical yield of ‘Arabinose’ at (300min, 170oC).

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