AN INTEGRATED MULTI-CRITERIA SCREENING FRAMEWORK TO ANALYZE FLEXIBILITY IN ENGINEERING SYSTEMS DESIGN: APPLICATIONS IN LNG INFRASTRUCTURES

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DECLARATION

I hereby declare that this thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has also not been submitted for any degree in any university previously.

Mehdi Ranjbar-Bourani

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Table of Contents

AN INTEGRATED MULTI-CRITERIA SCREENING FRAMEWORK TO ANALYZE FLEXIBILITY IN ENGINEERING SYSTEMS DESIGN: APPLICATIONS IN LNG INFRASTRUCTURES

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Summary

This thesis presents a novel integrated multi-criteria screening framework to analyze flexibility in the conceptual design of complex engineering systems. The proposed methodology aims to address two main issues in the evaluation of flexible systems design: 1) the computational intensity of exhaustively exploring the flexible design solutions because of different types of flexibility inherent in the systems design and 2) the multiple and possibly conflicting criteria inherent in the collaborative decision-making process of the design. The proposed screening framework based on meta-modelling and computing budget allocation is applied to real-world capital-intensive projects in on-shore LNG supply chain systems design. Results indicate that the screening models offers better performance than a full exhaustive search of the design space in terms of the number of evaluations and simulation runtime, while providing adequate design solutions in terms of lifecycle performance with respect to decision-makers' preferences. This work provides insights on how to analyze flexibility in the conceptual design of complex systems, especially when computational resources are limited and the design must include multiple decision-making criteria.

Thesis supervisor: Michel-Alexandre Cardin

Title: Assistant Professor of Industrial and Systems Engineering

List of Tables

List of Figures

List of Abbreviations

AF	Allocation factor
ATCF	After tax cash flow
BIR	Budget incremental rate
BOCBA	Bi-objective computing budget allocation
BTCF	Before tax cash flow
CAPEX	Capital expenditure
CAPM	Capital asset pricing model
CBA	Computing budget allocation
CCD	Central composite design
CDF	Cumulative density function
CNG	Compressed natural gas
Cover	Coverage distance
DAKR	Design archive keep rate
DACE	Design and analysis for computer experiments
DCF	Discounted cash flow
DM	Decision maker
DoE	Design of experiment
DRMEXP	Decision rule for capacity expansion at the main production site
DRFCD	Decision rule for the first capacity deployment at demand sites
DRDEXP	Decision rule for capacity expansion at demand sites
DsiteTV	Demand site capacity expansion threshold value
EE	Exhaustive enumeration
EGO	Efficient global optimization
EI	Expected improvement

EoS	Economies of scale
EEA	Epoch era analysis
ENPV	Expected net present value
FLNG	Floating liquefied natural gas
HCBA	Heuristic computing budget allocation
InCap	Initial capacity
IBR	Initial budget rate
LHD	Latin hypercube sampling design
LNG	Liquefied natural gas
MARR	Minimum attractive (acceptable) rate of return
MsiteTV	Main production site capacity expansion threshold value
MCDM	Multi-criteria decision-making
MDC	Modular design capacity
MLE	Maximum likelihood estimation
MB	Maximum budget
MDAS	Minimum design archive size
MM	Meta-model
MOCBA	Multi-objective computing budget allocation
MoveTV	Moving threshold value
NPV	Net present value
OCBA	Optimal computing budget allocation
OPEX	Operational expenditure
PDF	Probability density function
RSM	Response surface method
Std.	Standard deviation

tpd	Ton per day
UMD	Unmet demand
USC	Unused capacity
VASC	Valuation approach for strategic changeability
VaG	Value at gain
VaR	Value at risk
VBA	Visual basic for applications

List of Variables and Symbols

a	Translation parameter in S-curve function
α	Economies of scale factor
Av	Annual demand volatility, percent
b^D	Sharpness parameter in deterministic demand model
Δ_b	Volatility of sharpness parameter, percent
b^U	Sharpness parameter in stochastic demand model
B	Slope of learning effect
C_{ij}	Cost of transporting one unit of LNG (i.e., one ton) from i^{th} supply site to j^{th} demand site
$Cover$	The coverage distance from the main production site where demand sites located beyond this coverage distance are considered for the first capacity deployment in the relevant decision rule embedded at each demand site (%)
$CAP_{Msite,t,s}$	Capacity of LNG at the main production in year *t* under demand scenario *s* (tpd)
$CAP_{l,t,s}$	Capacity of LNG at the demand site *l* in year *t* under demand scenario *s* (tpd)
d_t	Sum of all noncash, or book, costs during year t, such as depreciation
D_t^D	Deterministic LNG demand in year t
D_t^U	LNG demand under uncertainty in year t
D_0^D	Deterministic demand in year 0, ton per day
Δ_{D_0}	Volatility of realized demand in year 0, percent
D_0^U	Demand under uncertainty in year 0, ton per day

$DsiteTV$ Percentage of the modular design capacity for capacity expansion decision rule used at the demand site with installed capacity (%)

$ESCF$ Escalation factor for gas purchase and LNG selling price

G_t Annual LNG demand growth rate

$InCap_l$ Initial capacity of LNG at demand site *l* (tpd)

$InCap_{Msite}$ Initial capacity of LNG at the main production site (tpd)

L Total number of demand points

LR Learning rate, percent

M_T^D Forecast limit of deterministic demand in year T, ton per day

Δ_{M_T} Volatility of realized demand in year T, percent

M_T^U Forecast limit of demand under uncertainty in year T, ton per day

MDC Modular design capacity of LNG used in the system design (tpd)

$MsiteTV$ Percentage of the modular design capacity for capacity expansion decision rule used at the main production site (%)

$MoveTV$ Percentage of the modular design capacity to consider the time for the first capacity deployment at demand sites in the relevant decision rule embedded at each demand site (%)

O_i^U Utopia point for objective function *i*

O_i^N Nadir point for objective function *i*

$\bar{O}_i$ Normalized objective function *i*

r Discount rate, after-tax MARR

$RD_{l,t,s}$ Realized demand at demand site *l* in year *t* under scenario *s* (tpd)

$SQ_{l,t,s}$ Sale quantity of LNG facility for the demand site *l* in year *t* under demand scenario *s* (tpd)

$SDF_{l,t,s}$ Short-term forward looking demand forecast at demand site *l* in year *t* under scenario *s* (tpd)

T	Project lifetime/study period, year
Tax	Effective income tax on ordinary income
TV_l	Percentage of the modular design capacity for capacity expansion decision rule used at demand site *l* (%)
$TRSC_{t,s}$	Total transportation cost incurred by enabling operational flexibility in year *t* under scenarios *s*
$TRO_{t,s}$	Total revenue generated by enabling operational flexibility in year *t* under scenario *s*
$TCO_{t,s}$	Total cost incurred by enabling operational flexibility, comprising gas purchase cost and transportation cost, in year *t* under scenario *s*
U_1 , U_i	Capex required for building the first and the i-th, respectively, LNG modular plant, \$M
$USC_{l,t,s}$	Unused capacity at demand site *l* in year *t* under scenario *s* (tpd)
$UMD_{l,t,s}$	Unmet demand at demand site *l* in year *t* under scenario *s* (ton)
$VAO_{t,s}$	The value added by enabling operational flexibility in year *t* under demand scenario *s*
WS_k	Weighted-sum value for flexible design *k*
$x_{i,j,t,s}$	Amount of LNG to be transferred from demand site *i* with unused capacity to demand site *j* with unmet demand in year *t* under scenario *s* (tpd)

Chapter 1 Introduction

1.1 Background

The conceptual design phase of complex and capital-intensive engineering systems is very important as crucial decisions need to be made at this stage. These systems generally require a significant amount of capital investment and are subject to various sources of uncertainty throughout the system lifetime (Allen, Mcgowan et al. 2002; Lin, de Weck et al. 2009). Hence, in the design and management of these systems, literature shows that the notion of flexibility is at the center of attention for improving economic performance under uncertainty. Due to the importance of evaluating flexibility in engineering designs, various evaluation methods have been developed (Nilchiani and Hastings 2007; Mikaelian, Nightingale et al. 2011; Cardin 2014). Of these methods, a quantitative performance model based on the simulation approach, first developed by de Neufville, Scholtes et al. (2006), for the evaluation of flexibility under uncertainty has gained wide attention from academia and industry.

Flexibility is a fundamental approach to systems design. Flexibility in design (also referred in this thesis as a real option) provides “the right, but not the obligation to change a system in the face of uncertainty”, and aims to improve the expected value of system performance over time as compared to standard design and project evaluation methods (e.g. discounted cash flow analysis). It does so by limiting exposure to downside losses (like an insurance policy), while positioning the system to capture possible additional gains (like a call option on a stock). For instance, a “flexible modular” Liquefied Natural Gas (LNG) plant may outperform an "optimal" fixed LNG plant. The reason is that instead of building a large capacity LNG plant right away, systems operators may initially build a smaller plant, reducing initial capital expenditure, and therefore exposure to potential losses in the face of uncertainty capacity demand. A flexible modular design, however, enables may position the system to capture more upside, deploying capacity when and if it is needed, thus providing contingencies to capitalize on upside opportunities and profits, should more demand arise than originally planned (de Neufville and Scholtes 2011). Part of the work presented in this thesis focusing on tradeoffs between the time-value of money and economies of scale in the context of uncertainty and flexibility analysis have been published in a recent research paper. More details can be found in Cardin, Ranjbar-Bourani et al. (2015).

Flexibility in engineering design has been widely used in different domains such as aerospace, airport design, the automotive industry, defense, energy, healthcare, mining, public infrastructure and management. Several examples of flexibility in engineering design, including urban infrastructures (de Neufville, Scholtes et al. 2006), real estate (Guma, Pearson et al. 2009), satellite systems (de Weck, de Neufville et al. 2004), water resource systems (Wang 2005), automotive manufacturing systems (Yang 2009) and petroleum exploration and production systems (Lin 2009), have been summarized by de Neufville and Scholtes (2011) in their book. The emerging literature on flexibility in engineering design has shown that flexibility can improve the economic performance of a project from 10% to 30% as compared to standard methods (de Neufville and Scholtes 2011; Cardin 2014).

1.2 Motivation

Taking uncertainty into account in the design evaluation process is not prevalent in industry (de Neufville and Scholtes 2011). According to Savage's (2009) "Flaw of Averages", relying on the most likely or average scenario may lead to incorrect design selection and investment decisions. This is because the output from an upside scenario (e.g. high LNG demand growth) does not necessarily balance the output from a downside scenario (e.g. low LNG demand growth). Equation 1.1 captures this formally:

$$f(E[x]) \neq E[f(x)] \tag{1.1}$$

Here, *E[x]* represents for instance expected LNG demand, and *f(E[x])* the Net Present Value (NPV) (the sum of all cash flows discounted back to present time t = 0) associated to the most likely or expected demand scenario (i.e. the time discounted value of the cash flows generated by the project). What equation 1.1 means is that a design evaluation based on the average or expected demand scenario – as captured by *f(E[x])* – does not lead to the same value as an evaluation relying on individual system responses from different demand scenarios, and then taking the average of the responses – as captured by *E[f(x)]*. If one chooses a systems design based on the left hand side – as often done in standard design and evaluation – a better design that can adapt to each scenario and provide better average NPV may be ignored altogether. Also, the right hand side of the scenario requires calculating the NPV over several scenarios, thus being a more realistic assessment that accounts for uncertainty.

For example, suppose a hypothetical LNG production facility at 1.0 ton per day (tpd) based on the expected or average demand forecast (referred as "Medium" demand) has $f_M(x) = NPV_M(1.0) = \$1.0$ million. Suppose also using the same economic model a low demand forecast at 0.5 tpd leads to $f_L(x) = NPV_L(0.5) = \$0.5$ million with equal 1/3 probability. Now consider with equal probability a forecast where demand is higher at 1.5 tpd than installed capacity. The latter would lead to $f_H(x) = NPV_H(1.5) = \$1.0$ million as well, because the maximum production capacity of 1.0 tpd is already reached. Considering that $E[x] = 1/3(0.5 + 1.0 + 1.5) = 1.0$ tpd, $f(E[x]) = NPV(1.0) = NPV_M(1.0) = \$1.0$ million based on the average forecast, but in reality the average NPV outcome should be $E[f(x)] = 1/3(NPV_L) + 1/3(NPV_M) + 1/3(NPV_H) = 1/3(0.5 + 1.0 + 1.0) = \$0.83$ million. This is lower than the anticipated \$1.0 million by 17%. Therefore, a design decision based on deterministic analysis may lead to incorrect production capacity and project selection, given that the real expected return of a system cannot be measured via standard evaluation methods (i.e. like NPV based on discounted cash flow or DCF analysis). A different approach is needed to capture the full value of LNG production infrastructure systems, and different approach to systems design recognizing both uncertainty and flexibility is needed.

Because the economic response from complex systems is highly nonlinear, long-term decisions should not be made considering only the expected or most likely scenario. The NPV of projects based on optimization for the most likely demand scenario is not the same as the expected NPV resulting from different demand scenarios, as captured by equation 1.1. A system may appear more or less valuable than it is, as compared to other mutually exclusive design alternatives.

Flexibility enables a system to capture the potential value associated with different scenarios. It might enable, for instance, capturing more demand in the high demand cases, thus increasing the expected economic value (i.e. like a call option). It might reduce the financial losses in a downside demand scenario (i.e. like an insurance policy).

Figure 1.1 illustrates conceptually the effects of embedding flexibility into the design of engineering systems. Flexibility enables the system to change its configuration (i.e. by acquiring more capacity as needed) over time and thus leads to a shift in the cumulative density function of the system design to the right, with higher value outcomes. The figure exemplifies conceptually an observation that is routinely made in flexibility studies, which is that a flexible design offers better expected economic performance metrics by shifting the distribution of outcomes towards better value, leading to improved expected NPV, value at risk ($VaR_{10\%}$), and value at gain ($VaG_{90\%}$) as compared to a more rigid, and fixed design (de Neufville and Scholtes 2011).

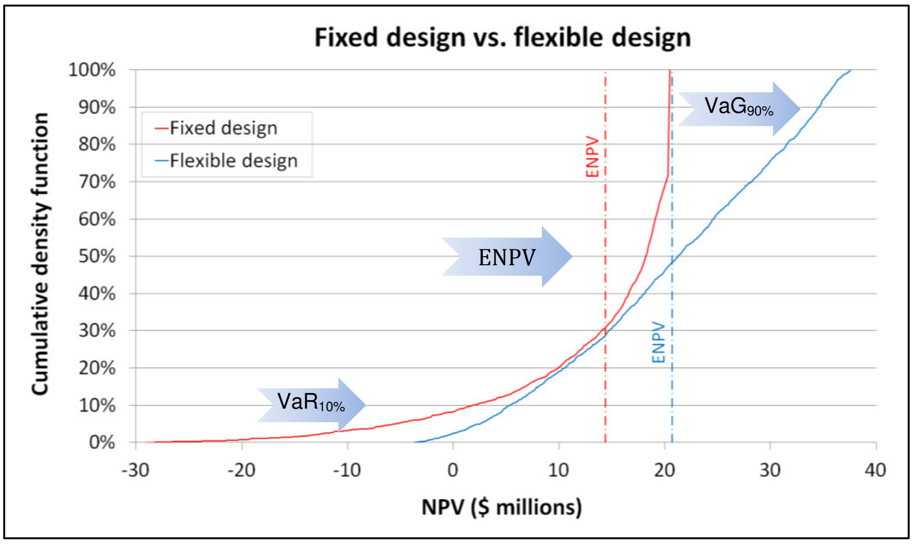


Figure 1.1: Fixed design versus flexible design

Although flexibility in engineering systems design has multiple advantages, the evaluation of flexible designs can be a challenging task. Exploring the flexible design space may require substantial computational effort due to the large number of design variables and parameters that usually need to be evaluated and optimized in performance models of complex engineering systems. Such systems are already difficult to analyze due to their sizes and complexity, analyzing flexibility (which adds even more in terms of design variables, parameters, and uncertainty scenarios) certainly exacerbates the computational problem, and may result in an intractable challenge if considered exhaustively. Screening models, as proposed by de Neufville and Scholtes (2011), can be used to quickly explore the solution space of flexible designs and efficiently provide good-enough flexible solutions before the detailed design evaluation process. To address the computational challenge, several researchers have recently developed various forms of innovative screening model methodologies to explore flexible design strategies in infrastructure, off-shore petroleum, automotive manufacturing and space tug systems (Cardin 2007; Lin 2009; Yang 2009; Fitzgerald, Ross et al. 2012).

Besides the computational challenge, the possibly conflicting flexible design performance measures necessary to support the design decision-making process is another issue. In the conceptual phase of engineering systems design, multi-criteria techniques can be used to capture existing tradeoffs, and satisfy different risk preference as well as profiles. The work on trade-space exploration is one example of such effort, based on utility and cost for flexibility in engineering systems design (Ross 2006; Viscito, Chattopadhyay et al. 2009; Viscito and Ross 2009).

In addition to the methodological motivation explained above, this thesis is also motivated by applications of ideas of flexibility in LNG infrastructure systems design. This is because the advantage of using natural gas products has increased over the last three decades, resulting in increasing demand growth for LNG products in some countries. On the other hand, there is much uncertainty on how such demand will evolve over the next decades in different areas of the world. Research has shown that by 2030 there is a possibility that the overall LNG demand worldwide will be more than three times higher than from where it was in 2011, and the regional distribution will significantly change accordingly (Kumar, Kwon et al. 2011). For example, gas product demand and supply forecasts in Australia indicate a potential shortfall of 300 to 600 TJ/day by 2015, and between zero and 600 TJ/day by 2020 (ECS 2011). A combination of growth and replacement production indicates there is a need to source at least 1,100 TJ/day of new production by 2020.

Over the past 20 years price differentials between fuel oil, gasoil/diesel and LNG have changed significantly. In 1997 oil prices hovered around \$20 per barrel (West Texas Intermediate - WTI) and around \$2.50 per Million British Thermal Unit (MMBtu) for Henry Hub natural gas in the United States. Today, these are around \$100 per barrel for oil and \$5 per MMBtu for natural gas (GLE 2011). Natural gas prices have only doubled in 20 years while WTI prices gone up 5 times in 20 years, making the price difference even more attractive.

In liquefied form, the volume of LNG is 600 times less than the same amount of natural gas at room temperatures while the volume of compressed natural gas (CNG) is 1% less of its original volume (GLE 2013). Hence, the energy density of LNG over CNG increases the driving range significantly. With one fuel tank, a road truck can go around 800-1,200 km distance (GLE 2011). New emissions control regulations are making LNG an increasingly attractive alternative for the shipping sector as well as for heavy road transport. Furthermore lower LNG tax compared to diesel tax is attractive for investors in this market. These advantages make LNG an excellent option for the heavy transportation sector.

Since LNG can be used reliably as on-road transport fuel, there are growing business opportunities for LNG production. Development of this business can be risky, however, as it requires substantial amount of initial investment. The project will be subject to different uncertainties such as LNG demand uncertainty, gas price, and facility availability. Hence the conceptual design stage of such projects is very important, as critical decisions need to be made as changing the configuration of the system later on might be too costly.

As a part of the motivation on the application domain, flexibility analysis is presented in this study as a practical procedure to improve (e.g., maximize expected net present value and minimize standard deviation) value of a system over its useful time. It enables developers to adapt the system for better performance as its requirements and opportunities evolve over its useful life by exploiting the notion of modularity in design (de Neufville and Scholtes 2011; Cardin 2014). It does so by addressing more specifically the computational challenges involved in the early phase analysis of design and project evaluation, considering explicitly uncertainty in the design decision-making process, and flexibility as an approach to improve expected lifecycle performance.

1.3 Research scope and objectives

Computational complexity of simulation based flexibility analysis and considering multiple objectives in the conceptual phase of design are the main research issues addressed in this thesis. So far, to the best of this author's knowledge, challenges of uncertainty, flexibility, computational complexity, and multi-criteria decision-making have not been addressed together in the context of engineering systems design. More specifically, there is currently no design framework and methodology that enables such an analysis in a structured and systematic manner. Therefore, to address these key issues simultaneously, this thesis proposes an integrated multi-criteria screening model to explore flexible design strategies efficiently and effectively under uncertainty. The proposed screening framework is then applied to two example real-world capital-intensive projects in on-shore LNG supply chain design. It is first to do this in the context of LNG production systems.

1.4 Research opportunities and expected contributions

This section briefly summarizes the identified research gaps and the proposed integrated framework as the main contribution in this thesis. The more detailed explanations regarding research opportunities and expected contributions are explained in chapters 2 and 3 respectively.

In this thesis, relevant research studies are summarized in Chapter 2. Their limitations are summarized here to identify the main research gaps and contributions of the thesis. The identified research gaps are: 1) a lack of consideration of different types of flexibility in different domains of capital-intensive complex systems; 2) limitations in applying both design variables and decision rules in simulation-based evaluation models for flexibility and uncertainty; 3) the lack of a systematic approach for efficiently tuning decision rules and design variables simultaneously (i.e. a decision rule is a triggering mechanism that determines when it is appropriate to exercise a particular flexibility, based on some uncertainty observation); and 4) limitations in exploring flexible design solutions with different objectives and criteria. From a broader perspective, although considerable research has been devoted to evaluating flexibility in engineering systems design, little attention has been paid to considering screening models and multi-criteria decision-making techniques in an integrated design methodological framework. More specifically, although separate research has been done on each aspect, sometimes combining some of these aspects, there is currently no integrated framework to fill all of the identified gaps. Therefore, to address these research opportunities, this thesis develops an integrated multi-criteria screening framework to explore flexible design strategies for complex engineering systems efficiently and effectively.

This thesis, as a practical evaluation procedure, aims to facilitate the decision-making process, especially when computational resources are limited and the designer must consider multiple decision-making preferences and criteria. The proposed model can be applied to evaluate flexibility in complex engineering systems design. The proposed framework consists of: 1) developing a simulation model to evaluate flexibility in engineering systems design under uncertainty, accounting for both design variables and decision rules; 2) developing different types of flexibility to deliver value-added flexible designs by determining corresponding decisions; 3) developing a screening model based on a meta-modeling approach to lessen the computational effort of simulations by balancing exploration and exploitation of the design space; and 4) applying a multi-criteria model to provide distinct dominant flexible designs consistent with decision-makers' preferences.

1.5 Thesis outline

The remainder of this thesis is structured as follows:

- Chapter 2 provides a literature review of theories and methodologies of flexibility, screening models and multi-criteria decision-making techniques in the context of engineering systems design. Based on the literature review, research gaps for further contributions are identified.

- Chapter 3 focuses on the proposed screening methodology. In this chapter, the details of the proposed multi-criteria screening framework are presented step by step. Three approaches are investigated and explained in detail: 1) an exhaustive enumeration approach; 2) a meta-model based screening approach and; 3) a computing budget allocation based screening approach.

- Chapter 4 presents the first case study that is about a centralized on-shore LNG production system design. The problem is modeled for flexibility and uncertainty analysis and sensitivity analysis subject to the key parameter are conducted. Subsequently, the three above-mentioned screening approaches are applied as demonstration to the first case study.

- Chapter 5 demonstrates the application of the proposed methodology to a decentralized version of the on-shore LNG production system design. The problem is modeled for flexibility and uncertainty and is explained in detail. Subsequently three proposed screening approaches are applied to this case study. This case study aims to demonstrate that the method can be applied to different types of engineering systems, thereby further supporting external validation and generalizability of the proposed framework.

- Chapter 6 summarizes the major findings, provides conclusions, discusses the limitations and gives insights into further research.

Chapter 2 Literature Review

2.1 Introduction

This chapter provides a review on relevant academic and industrial literature and practice. Given that the identified research opportunity is multidisciplinary in nature, the literature review in this section is drawn from multiple domains: real options and flexibility, screening models, multi-criteria decision-making in conceptual design stage, as well as domain literature on LNG production system design. A thorough survey of research documents, including journal papers and theses, in the fields of systems engineering, engineering design, and real options analysis, was conducted. Of these research documents, some relevant research works were considered for further investigation.

The remainder of this review is organized as follows. Section 2.2 reviews real options in engineering design as a proactive way to deal with uncertainty in complex engineering systems. Section 2.3 provides a comparison of current methodologies on exploration of design space and of recently developed screening models. Section 2.4 reviews the methodologies for decision-making considering multiple criteria in the engineering systems design field. Section 2.5 reviews the domain literature on decision making in LNG production system design. Section 2.6 presents identified research opportunities. Section 2.7 explains research contributions of this thesis. Section 2.8 summarizes this chapter.

2.2 Real options and flexibility in engineering design

Since last decades, real options and flexibility in engineering design, as a real options analysis evaluation techniques, have been introduced by adapting the concept from financial options analysis (e.g. Black and Scholes (1973); Cox, Ross et al. (1979)) and real options analysis (e.g. (Dixit and Pindyck 1994; Trigeorgis 1996)) in a way to suit the needs of engineering design in such a highly uncertain world. Browning and Honour (2008) proposed a conceptual approach to quantify a systems' life cycle value. They concluded that to provide maximum life cycle value, a system may need to be designed to facilitate adaptability to changing circumstances and stakeholder preferences. Engel and Browning (2008) presented quantitative models to assess the value of architecture adaptability as quantitative means of optimizing a system architecture to maximize its lifetime value.

Given the term "flexibility" may have different definitions in different contexts, some authors conducted research to clarify its definition to facilitate communication among systems engineering practitioners and academics (Ross, Rhodes et al. 2008; Ryan, Jacques et al. 2013). Flexibility in engineering design is an interdisciplinary field for research and practice (de Neufville and Scholtes 2011). It adapts the concept of financial options to real engineering systems, with the goal of increasing the expected economic value by providing the "right, but not the obligation to change a system" to respond to uncertainties most profitably (Trigeorgis 1996). Flexibility exists "on" and "in" engineering systems. Flexibility "on" systems is associated with managerial flexibility like abandoning, deferring until favorable market conditions, expanding/contracting/reducing capacity, deploying capacity over time, switching inputs/outputs, and/or mixing the above (Trigeorgis 1996). Flexibility "in" systems refers to technical engineering and design components enabling the real options – another word for flexibility – in deployment and operations (Wang 2005). Cardin (2014) provides a taxonomy and a design framework to organize design and evaluation activities to enable flexibility in engineering systems design. Table 2.1 summarizes the application of real options/ flexibility in different domain applications.

Table 2.1: Classification of flexibility in engineering design in terms of application domain

Research	Application
(de Weck, de Neufville et al. 2004; Hassan, de Neufville et al. 2005; Wang 2005; McConnell 2007)	Aerospace
(Chambers 2007; de Neufville 2008)	Airport design
(Mangin, de Neufville et al. 1995; Neely III and de Neufville 2001; Kalligeros, de Weck et al. 2006; Yang 2009)	Automotive
(Bartolomei, Hastings et al. 2006)	Defense
(Mittal 2004; Hassan and de Neufville 2006; Kalligeros 2006; Roques, Nuttall et al. 2006; Babajide 2007; Babajide, de Neufville et al. 2009; Lin 2009)	Energy
(Lee 2007; de Neufville, Lee et al. 2008; Maseda 2008)	Healthcare
(de Neufville and Pirnar 1999; de Neufville 2000; Rouse, Howard et al. 2000; Pochard 2003; Quispez-Asin 2007; Rivey 2007; Ohama 2008)	Management
(Kazakidis and Scoble 2003; Cardin, de Neufville et al. 2008)	Mining
(Ramirez 2002; Wang 2003; Wang and de Neufville 2004; Wang 2005; Gupta 2011)	Public infrastructure
(Greden, de Neufville et al. 2005; Greden 2005; Barman 2007; Cardin 2007; Lister 2007; Masunaga 2007; Guma 2008; Pearson and Wittels 2008; Guma, Pearson et al. 2009; Zhang 2010)	Real estate
(Tsui 2005; Petkova 2007; Sussman and McConnell 2007; de Neufville, Hodota et al. 2008; Ohama 2008; Morgado, Nagaralu et al. 2011)	Transportation

2.2.1 Relevant research studies

The literature shows that complex engineering systems that cannot change their configuration when facing uncertainty may result in failure. This uncertainty, particularly in capital-intensive and long-term projects, can create both risk and opportunity. The underlying assumption is that flexibility can improve the expected systems performance by reducing the downside risks and taking advantage of the upside opportunities, as has been shown in many case studies (de Neufville and Scholtes 2011).

Flexibility enables systems to proactively adapt to future uncertainty through managerial decision rules. For instance, to respond to demand uncertainty, an LNG production plant may use capacity expansion as a strategy and expansion in different modular volumes as an enabler in its design. In the evaluation of flexibility in complex engineering systems design, one approach to support the decision-making process is by embedding decision rules. Decision rules can be modeled to assess the value of flexibility. A decision rule is a triggering mechanism that determines when it is appropriate to exercise a particular flexibility, based on some uncertainty observation. For instance, one may decide to expand LNG production capacity after demand reaches a certain threshold.

According to Cardin (2014), the evaluation techniques that are suitable for real options analysis in an engineering context are binomial lattice, decision tree analysis and Monte Carlo simulations. Binomial lattice, a discrete binomial formulation of the Black-Scholes formula (Black and Scholes 1973), is used to value financial options (Cox, Ross et al. 1979). However, the path independence assumptions used in the lattice model may not be appropriate in an engineering context. Because of the lattice's rigid structure embedding Bellman's dynamic programming equations, it is difficult to model more complex managerial decision rules. In addition, the lattice evolution assumes a stationary process, which may not be realistic. Decision tree analysis is a standard system analysis and scenario planning tool used under uncertainty. However, in this technique the number of paths typically increases exponentially even with the minimum possible decision nodes and chance outcomes.

Given using such modeling methods have shortcomings for real-world applications, Monte Carlo simulation is used. It provides a flexible platform so that even complex systems and decision rules can be easily modeled and analyzed. Longstaff and Schwartz (2001) presented a simulation model based on the least squares Monte Carlo simulation method to evaluate options. Research has revealed that the Monte Carlo simulation technique is suitable for systems modeling, especially in the case of existing multi-factor uncertainty and path dependency. In these cases, the objective function is typically a numerical simulation model describing a complex process that is often dynamic. Such simulation models often require uncertainty analysis or optimization for parameter estimation or to identify the best management or design decisions. de Neufville, Scholtes et al. (2006) introduced later a practical four-step procedure to evaluate real options in projects using a spreadsheet model based on Monte Carlo simulation based on decision rules, and a more practical approach for real options analysis.

Building upon the Monte Carlo approach proposed by de Neufville et al. (2006), Cardin (2007) applied the same simulation method in his proposed design catalog screening approach. Lin (2009) relies on the same simulation framework in his proposed evaluation framework to evaluate flexibility in different domains of capital-intensive projects with different types of uncertainty. In his research, both design variables and decision rules were analyzed. However, decision variables and parameters embedded in decision rules need to be discretized and determined by trial and error and engineering practices. Lin's study (2009) did not consider a systematic approach to fine tune the decision rule parameters. Yang (2009) developed an integrated model to evaluate flexibility in automotive manufacturing systems under demand uncertainty. However, only design variables were considered in Yang's research and decisions were made based on realized demand scenarios and different problem settings. No decision rules were used in her proposed simulation model, resulting in the plant's inability to change its capacity over the project lifetime. Fitzgerald, Ross et al. (2012) presented a Valuation Approach for Strategic Changeability (VASC) developed based on Epoch Era Analysis (EEA) (Ross 2006; Ross and Rhodes 2008) to investigate the value of changeability in complex engineering systems in the early stage of the design process. In their five-step VASC model, Fitzgerald, Ross et al. (2012) used transition rules that are defined as a set of change mechanisms. In contrast, in this study, different decision rules and their embedded threshold parameters are used in the proposed simulation framework. Such decision rules aim to explicitly model the kinds of decisions that system operators would make to change and adapt the system in light of uncertainty realizations.

Although using simulation-based models to evaluate flexibility have multiple advantages, exhaustively exploring the flexible design solution space can be computationally intensive. The following section covers the screening models used to efficiently explore the flexible design solutions.

2.3 Screening models

In the conceptual phases of complex systems design, finding the promising flexible designs from the large number of possible design alternatives is not an easy task. One of the motivations for using simulation-based evaluation method is because of the recent advances in computational technology. However, an exhaustive search and evaluation of all design alternatives can still be computationally expensive and intractable if many design variables and parameters, decision rules, and uncertainty scenarios are considered. Thus, screening models as surrogates of the original simulation models are valuable to efficiently explore the flexible design space, aiming to find adequate flexible designs before proceeding to a more detailed design analysis phase.

Screening models in engineering systems design can be classified into three groups: 1) top-down; 2) bottom-up and 3) simulator. The choice between them depends on the details and nature of the problem under consideration. In practice, different types of screening models for a particular problem may be used in combination (de Neufville and Scholtes 2011).

Top-Down Screening Models

In the top-down screening model, only the major relationships between the elements of the systems are considered. For instance, in systems dynamics, higher systems-level views are investigated instead of focusing on detailed relationships.

Bottom-Up Screening Models

Bottom-up screening models simplify the complexity of the systems' high-fidelity model by taking the major factors of the model into account, e.g., by reducing the number of stochastic parameters in the model and considering them as fixed values. Jacoby and Loucks (1972) first proposed a bottom-up screening model based on a combination of optimization and simulation. They developed both static and dynamic optimization models to screen worthy river basin designs. The results derived from the solutions of the screening models were then analyzed in detail in the simulation model. Wang (2005) proposed a bottom-up screening framework using stochastic mixed-integer linear programming followed by simulation to filter out the worthwhile options. To show the efficiency of the proposed method, two case studies in river basin development and satellite communications were investigated. The screening model, however, is limited to a low-fidelity, non-linear programming model with discrete values for uncertain parameters. Moreover, the research does not provide a systematic way to identify parameters in screening models. Despite the promising performance of the proposed screening model, developing a stochastic mixed-integer programming algorithm can be highly complex and difficult, making the applicability of the screening model questionable.

Hassan, de Neufville et al. (2005) then developed a framework that integrates spacecraft engineering design with an economic analysis to maximize the financial value of a fleet to an operator under market uncertainty. Subsequently, Hassan and de Neufville (2006) developed a framework for using real options valuation in the design optimization of complex engineering systems with a genetic algorithm. They relied on a low-fidelity financial and hypothetical model with discrete values for uncertain parameters.

Lin (2009) proposed a mid-fidelity screening model based on the bottom-up approach considering flexible strategies under multi-domain uncertainties to identify and evaluate architecture and develop strategies for capital-intensive projects. Figure 2.1 shows the four-step screening process.

The screening framework was applied to design and develop off-shore petroleum projects, particularly in architecture project design and the development of tieback strategies. Different strategies, comprising design variables and decision rules, were synthesized to explore the solution space aimed at finding promising design alternatives. However, the decision rules used in the procedure were based on engineering practices and a trial and error approach in an iterative procedure. The trial and error nature of the analysis may have resulted in a biased sampling of the flexible design space. A more systematic approach for exploring such design space (especially the decision rules) is needed for flexibility analysis.

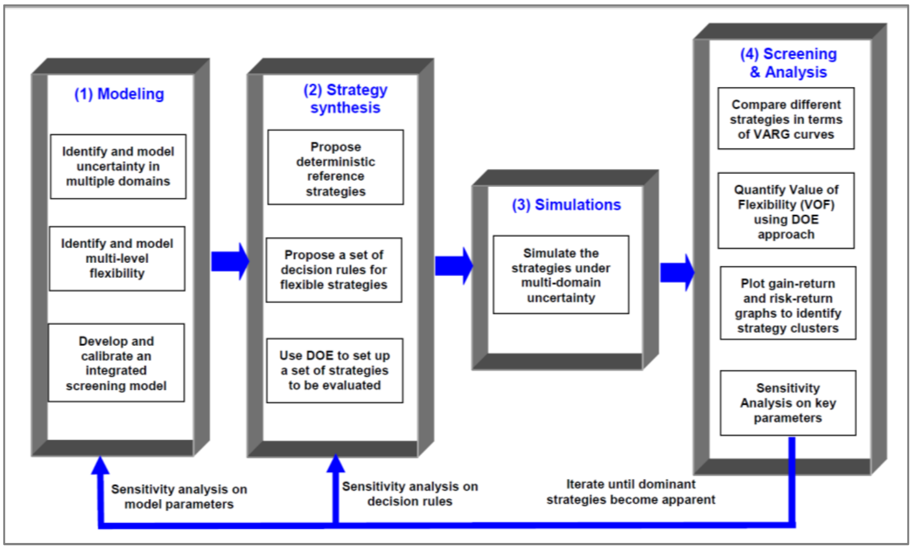


Figure 2.1: A generic four-step process for screening flexible strategies under uncertainty, adapted from Lin (2009)

Viscito, Chattopadhyay et al. (2009) proposed a bottom-up screening model where a metric called the Filtered Out degree was used for identifying valuable flexible systems. This metric calls out designs that are both highly changeable and valuable to the stakeholder. This metric enhances trade-space exploration as the prior trade-space analysis techniques only accounted for the cost of flexibility. Subsequently, Fitzgerald, Ross et al. (2012) expanded the set of screening and valuation metrics compared to the previous Epoch Era Analyses (Ross 2006; Ross and Rhodes 2008).

Zhang and Babovic (2011) proposed an evolutionary real options framework to integrate real options valuation, decision analysis techniques, Monte Carlo simulations and evolutionary algorithms. This approach can be considered as as bottom-up screening model. They applied their evolutionary framework on a test problem and results show that the evolutionary framework delivers considerable improvements over current real options practices. The paper does not account, however, for multi-objective approach in real options analysis.

To lessen the computational burden of the simulation, there is another alternative which is optimizing the simulation directly without using surrogate models but using efficient mechanisms based on computing budget allocation. These approaches can be considered as bottom-up screening models as well. They aim to optimize the simulation model by focusing on exploration of promising area of the solution space. Therefore one possible suggestion is applying Discrete Optimization via Simulation (DOvS) algorithms, which is based on random search. For instance, an algorithm called *convergent optimization via most-promising-area stochastic search* (COMPASS) was developed based on random search (Hong and Nelson 2006), and can be used in the context of flexibility analysis. In this method, solutions are sampled stochastically within the most promising area, in which all solutions have shorter Euclidian distance to the current optima than the distance to any current non optima. The solutions are to be evaluated according to certain simulation allocation rule (SAR) and used to construct the next most promising area. It has been proven that the search typically converges to the local optima. In a multi-objective setting, Multi-objective COMPASS was proposed by Lee, Chew et al. (2011), as well as multi-objective computing budget allocation (MOCBA) (Lee, Chew et al. 2010).

Simulator Screening Model

The simulator screening models create an approximate surrogate of the computationally expensive simulation models (e.g., it might take from minutes to hours for each objective function evaluation). The response of these simulation models is often multimodal and the objective function is a “blackbox”. The simulator screening models are called meta-models in the statistics discipline, meaning a model of the original simulation model. Meta-models are widely used in simulations of real-world complex problems, due to the complexity of the simulation models. There are different types of meta-models, for instance the Kriging model, polynomial regression model, multivariate adaptive regression splines model, radial basis function model and artificial neural network model. More information about the application of these techniques as meta-models in engineering design can be found in the work by (Kleijnen 2009), Van Groenendaal and Kleijnen (1998), Friedman (1991), Meckesheimer, Barton et al. (2001) and Hsu, Cho et al. (1995), among others. Cardin (2007) proposed a combined bottom-up and simulator-based screening model to efficiently search for catalogs of operating plans using the adaptive one-factor-at-a-time (OFAT) model developed by Frey and Wang (2006). Yang (2009) developed a coupled simulator and bottom-up based screening framework to explore planning decisions under demand uncertainty in automotive manufacturing systems. Figure 2.2 shows the screening process.

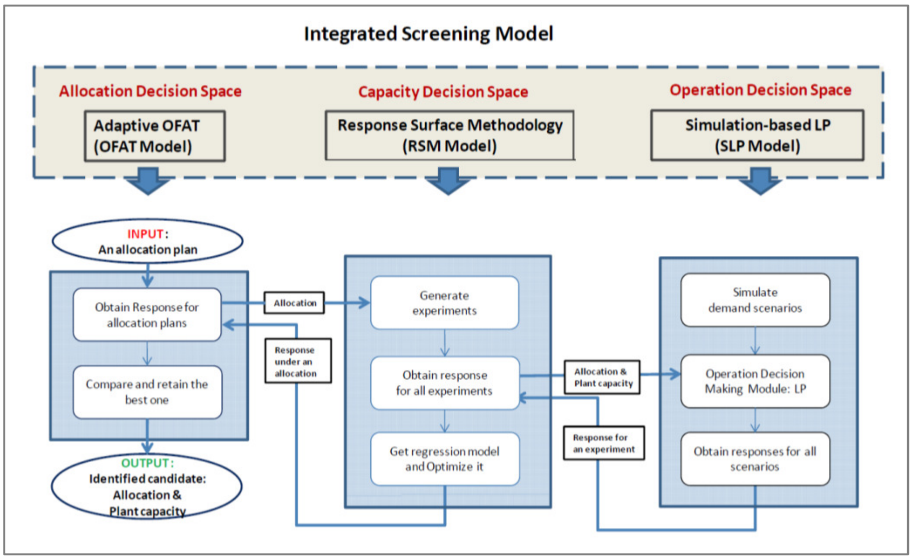


Figure 2.2: General overview of the screening model, adapted from Yang (2009)

In the screening framework, she used adaptive OFAT for strategic plant-product allocation decisions and a simulator-based quadratic regression model for tactical plant capacity decisions. To screen the plant capacity decisions, the regression model was built based on the response of the operational level decisions obtained through a linear programming model. The screening model showed good performance at providing adequate solutions with less computational effort compared to the stochastic mixed integer model, especially when the size of the problem increases.

Güyagüler (2002) introduced a hybrid optimization technique (HGA), based on genetic algorithms (GA) with the help of a Kriging algorithm to determine the best location for new wells in offshore petroleum industries. The rationale behind using a simulator approach was to tackle the computational issue of the expensive numerical simulation through the low-fidelity surrogate response surface. Performance of the proposed technique was investigated by two real-world case studies. The first case was associated with optimizing placement of injection wells in the Gulf of Mexico Pompano field. The second case aimed to optimize the development plan of a reservoir located in the Middle East. The results were verified by comparison to exhaustive simulations. The research focused on a way to reduce the computational burden of making numerous numerical simulations.

Besides the computational issue, finding promising flexible designs that are consistent with decision-makers' preferences is not an easy task. The following section reviews the work on multi-criteria decision-making in engineering systems design.

2.4 Multi-criteria decision-making

In flexibility analysis under uncertainty, each flexible design corresponds to a distribution of outcomes rather than a single-point solution. The different properties of these distributions (i.e., usually in a form of cumulative distribution function) can be interpreted as different objectives and criteria from the decision-makers' perspective. For instance, a risk neutral decision maker aims to maximize ENPV at the lowest standard deviation possible (Markowitz 1991). In other words, s/he aims to maximize the value of the unit return per unit of risk taken based on Capital Asset Pricing Model (CAPM) (Brealey and Myers 2000). On the other hand, considering only one objective, which comprises a linear combination of several objectives within a single measure of goodness, may not be practical (de Neufville and Scholtes 2011). It would thus be of interest to decision-makers that the promising flexible design solutions provide a satisfying tradeoff between several objectives and preferences. To do so, a multi-objective optimization approach is useful. From a multi-objective optimization perspective, the ideal flexible design is one that can change its configuration in order to satisfy the optimum performance level associated with different objectives.

A popular approach to multi-objective optimization is the generation of a Pareto front. A Pareto front, here referred to as a set of dominant flexible designs, consists of a set of solutions that satisfy what is known as the Pareto optimality criterion. Based on the Pareto optimality criterion, a solution based on given objectives that one cannot improve upon in any single objective without giving up performance in some other objectives are characterized as dominant solutions (Deb 2001). Many techniques for generating a Pareto front are found in the literature (Horn 1996). These include multi-objective versions of genetic algorithms (Deb and Tiwari 2005; Grierson 2008), simulated annealing (Czyzżak and Jaszkiewicz 1998; Ulungu, Teghem et al. 1999), weighting methods (Kim and De Weck 2006) and multi-start methods (Jaszkiewicz 2004).

de Weck, de Neufville et al. (2004) investigated the staged deployment of a satellite constellation using trade-space paths instead of optimal design points. The flexible design was found based on trade-offs between lifecycle cost and capacity, resulting in significant economic benefits over the baseline design. Olewnik and Lewis (2006) presented a decision support framework, based on multi-objective optimization, consumer choice theory, and utility theory, for the design of flexible engineering systems. Only design variables were considered, however, in the flexible design vector, and the framework lacked a screening approach to explore the flexible design space for computationally demanding problems. Ross, Diller et al. (2002) introduced a multi-attribute decision-making process based on decision-making preferences and simulation-based analysis. Subsequently, Ross and Hastings (2005) introduced the idea of Multi-Attribute Trade-space Exploration (MATE) for considering a large number of design alternatives in terms of conceptual benefits and lifecycle cost. As opposed to relying on identifying the “optimum” design, their approach sought to evaluate even so-called “bad” designs due to the existing multi-dimensional trade-offs inherent in a complex design problem. Typically, with MATE represented as a utility-cost plot, the trade-space concisely reveals the structure of the high-order benefit-cost information of many design alternatives. Subsequently, Viscito, Chattopadhyay et al. (2009) coupled the idea of high Pareto Traces with high Filtered Out Degree designs to screen for valuable flexible designs. The framework was designed to provide subsets of designs in a trade-space, including those that are highly robust and highly changeable. To make the algorithm efficient, only transitions to designs in the subset were allowed. In their research, the designs of interest were screened first in terms of different attributes and the transition rules were then applied.

When dominant flexible design alternatives are generated, decision-makers must confront several criteria based on their preferences and make the trade-offs appropriately. Unfortunately, the number of dominant flexible designs is often large and the designs can become difficult to comprehend and consider. Some researchers have thus proposed Pareto set post-processing techniques, such as the pseudo-ranking and clustering method (Taboada, Baheranwala et al. 2007; Justesen 2010), weighted-sum approach and the recently developed Pareto filtering method (Raphael 2011). These approaches can help in narrowing down the number of dominant flexible designs to several distinct flexible designs, thereby facilitating trade-off analysis for decision-makers.

2.5 LNG production system design

LNG production system design has become more critical due to the growth of natural gas supply and demand and the great risks in this industry. The design of the LNG production system seeks a solution that offers better expected economic value over system lifetime, and an efficient LNG supply chain, from LNG upstream to the end user. The LNG supply chain can be defined as all processes from extraction of the natural gas until used by end users, which consists of exploration, extraction, liquefaction, transportation, storage and regasification. There are different types of LNG supply chains as there are different types of upstream resources (e.g. gas well at onshore or offshore sites), liquefaction process types (e.g. onshore or offshore liquefaction plants), and end users (e.g. power plant, home use and transportation sector).

Literature has shown a growing research towards designing value LNG production systems focusing on different segments of the LNG supply chain, depending on the problem under consideration and geographical situation. Özelkan, D'Ambrosio et al. (2008) studied the coupled segments of large scale shipping and receiving terminal of an LNG supply chain to minimize cost and storage inventory, while maximizing the output of natural gas to be sold to the market. Grønhaug and Christiansen (2009) presented both an arc-flow and a path-flow model for tactical planning to optimize the LNG inventory routing problem. Andersson, Christiansen et al. (2010) worked on transportation planning and inventory management of a LNG supply chain used in tactical planning during negotiations about deliveries to different regasification terminals and annual delivery plan used in operational level decision making.

As the overview above suggests most of the works focus on operational level problems, therefore more work is needed to evaluate LNG production systems in the early stages of design. In particular, more efforts are needed considering strategic level decisions involving flexibility and uncertainty in the analysis of site production capacity, design, and deployment over time. This thesis investigates the effects of uncertainty and explicit considerations of flexibility on key strategic factors affecting the design of LNG production systems, a downstream portion of LNG supply chain, from onshore natural gas transmission pipeline to end users at candidate geographical demand sites. It does so more specifically by focusing on the computational and multi-criteria issues relevant to the design decision-making process.

2.6 Research opportunities

In the previous section, research studies relevant to this thesis were briefly described and limitations associated with these studies were also investigated. The aim in this section is to illuminate the axes of research opportunities so that this research can fill the identified research gaps.

There is a need to study real-world capacity expansion problems under uncertainty. Julka, Baines et al. (2007) reviewed thoroughly research papers relevant to capacity expansion problem regarding todays' complex global manufacturing system. Findings of the research show that multiple factors need to be considered so that designers can make critical decisions in the early phases of system designs. The paper's extensive literature review and structured assessment of the strengths and weaknesses of the research demonstrate the lack of consideration of real-world capacity expansion problems under uncertainty, with explicit considerations of flexibility. Most of the research conducted implements proposed methods on some predefined test problems in the literature rather than real-world ones. This study therefore directly address capacity expansion problem in the field of LNG systems by focusing on a real problem in the LNG industry, motivated by close discussions with an offshore infrastructure facility provider for oil and gas production.

In this thesis, four main axes of research opportunities are explored: 1) flexibility analysis that accounts for both design variables and decision rules; 2) different types of flexibility, considering operational, tactical, and strategic level decisions; 3) screening model to deal with the computational issues arising from flexibility analysis; and 4) multi-criteria decision-making approach to account for different risk preferences and profiles in design decision-making.

Research gaps identified in this research are shown in Table 2.2.

Table 2.2: Research gaps and anticipated contributions of this research

No.	Author(s) (year)	Flexibility analysis	Different types of flexibility	Screening model	Multi-criteria decision-making
1	Jacoby and Loucks (1972)			✓	
2	Güyagüler (2002)			✓	
3	de Weck, de Neufville et al. (2004)	✓			✓
4	Wang (2005)	✓	✓	✓	
5	Hassan, de Neufville et al. (2005)	✓	✓	✓	
6	de Neufville, Scholtes et al. (2006)	✓			
7	Ross (2006)	✓	✓		✓
8	Hong and Nelson (2006)			✓	✓
9	Olewnik and Lewis (2006)	✓	✓		✓
10	Cardin (2007)	✓	✓	✓	
11	Lin (2009)	✓	✓	✓	
12	Yang (2009)	✓	✓	✓	
13	Viscito, Chattopadhyay et al. (2009)	✓	✓		✓
14	Lee et al. (2010)			✓	✓
15	Zhang and Babovic (2011)	✓	✓	✓	
16	Fitzgerald, Ross et al. (2012)	✓	✓		✓
This research Ranjbar-Bourani (2015)		✓	✓	✓	✓

This research is designed to address the following research questions and to investigate all four axes of research simultaneously, since so far existing studies have only considered one but not all such aspect simultaneously. The thesis is thereby contributing to the existing body of knowledge by investigating:

- How to develop flexibility analysis that accounts for both design variables and decision rules?
- How to take into account different types of flexible strategies, accounting for operational, tactical, and strategic level decisions?
- How to develop a screening model to explore the flexible solution space in a computationally efficient way?
- How to take into account different objectives and preferences in the conceptual phase of design processes?

2.7 **Summary**

In this chapter, a comprehensive literature survey was done from multiple standpoints: real options and flexibility in engineering design, screening models, multi-criteria decision-making in design stage, and domain literature on LNG production and infrastructure systems. Several observations and research gaps have been drawn from the review.

The identified research gaps are: 1) a lack of consideration of different types of flexibility in different domains of capital-intensive complex systems; 2) limitations in applying both design variables and decision rules in simulation-based evaluation models for flexibility and uncertainty; 3) a lack of a systematic approach to quickly explore the flexible design space through efficient tuning procedures for decision rules and design variables; and 4) limitations in exploring flexible design solutions with different objectives and criteria. From a broader perspective, although considerable research has been devoted to evaluating flexibility in engineering systems design, little attention has been paid to considering screening models and multi-criteria decision-making techniques simultaneously. More specifically, although separate research has been done on each aspect, there is currently no integrated framework to fill all of the identified research gaps. Therefore, to address these research opportunities, this thesis develops an integrated multi-criteria screening framework to explore flexible design strategies for complex engineering systems efficiently and effectively.

Chapter 3 Methodology: An Integrated Multi-Criteria Screening Framework for Flexibility Analysis

3.1 Introduction

In the previous chapter, relevant research studies were briefly described and their limitations were identified. The main research gap addressed in this thesis is the lack of an integrated framework enabling: 1) analysis of flexibility in different domains of the systems (e.g. operational, tactical, strategic), and considering different types of flexibility strategies; 2) considerations of both design variables and decision rules simultaneously in simulation models; 3) systematic and computationally efficient analysis for tuning decision rules and design variables (i.e. essentially exploring the design space effectively and efficiently); 4) exploring the flexible design solutions subject to different objectives and criteria. From a broader perspective, although considerable research has been devoted to evaluating flexibility in engineering systems design, in the exploration of flexible designs less attention has been paid to screening methodology and more than one single performance measure simultaneously. Therefore, to address these research opportunities, this thesis develops and proposes an integrated multi-criteria screening framework to explore flexible design space efficiently and effectively.

A structured methodology is developed to address the research questions posed at the end of the previous chapter. To address these questions, this thesis proposes a methodology referred as integrated multi-criteria screening framework to analyze flexibility in engineering systems design. The proposed methodology builds upon and expands a four-step simulation based analysis for uncertainty and flexibility proposed by de Neufville and Scholtes (2011), and adapts existing computational methods to suit the needs of flexibility analysis in an engineering context. The proposed framework, as a practical procedure, aims to facilitate the decision-making process especially when computational resources are limited and more than one objective is important in the design phase. The proposed model can be applied to assess flexibility in engineering systems designs.

The main contribution of this thesis is this integrated and systematic three-phase framework that enables: 1) developing multi-domain flexibility to deliver better value designs through determining decisions when there are different types of flexibility, 2) developing flexibility analysis for engineering system design under uncertainty considering design variables and decision rules at the same time, 3) developing a screening model based on a meta-modeling approach and computing budget allocation approach to alleviate the computationally intensive real-world simulations, through balancing exploration and exploitation in searching the design space, 4) developing a multi-criteria model to provide distinct dominant flexible designs consistent with decision makers' preferences. To this author's knowledge, there is no framework currently enabling the analysis of complex systems considering simultaneously these four important angles.

A secondary and important contribution is an in-depth study and application of the proposed framework to support the design and management of LNG infrastructure systems under explicit consideration of uncertainty and flexibility. Based on existing literature, this thesis is the first to investigate applications of the flexibility paradigm in the design and management of such infrastructures, and to demonstrate significant performance improvements as compared to the outcomes of existing methods and practice.

The proposed multi-criteria screening framework is applied in subsequent chapters to analyze real-world on-shore LNG production systems as case studies. In this thesis, two variations of the same engineering system are investigated: 1: A centralized LNG production system and 2: A decentralized LNG production system. The goal is to quantify the potential value improvements not recognized by standard design and evaluation approaches while benefiting from efficient and effective design space exploration to find promising flexible design and management strategies for the system. The analysis focuses on two variants of an LNG production infrastructure to demonstrate applicability of the framework to different instantiations of an engineering system, and further support validation towards better generalizability of the framework.

3.2 Proposed Framework

This section introduces and describes the proposed three-phase framework, as seen in figure 3.1. The phases are: Phase 1: Design problem modelling, Phase 2: Screening, and Phase 3: Multi-criteria decision-making analysis. The second phase, which is the screening procedure, may rely on two screening approaches, 1) meta-modeling approach and 2) computing budget allocation approach. The transition between the phases is shown with arrows in the figure.

For instance, when computing budget allocation based screening is applied, there is a back and forth procedure between phase 2 and 3 while in case of using meta-model based screening approach, phase 3 starts when phase 2 is already accomplished. The details of each phase are elaborated in following sections.

Finally, the preferred trade-off flexible design, that is the output of the Phase 3, should be further investigated in a high-fidelity model.

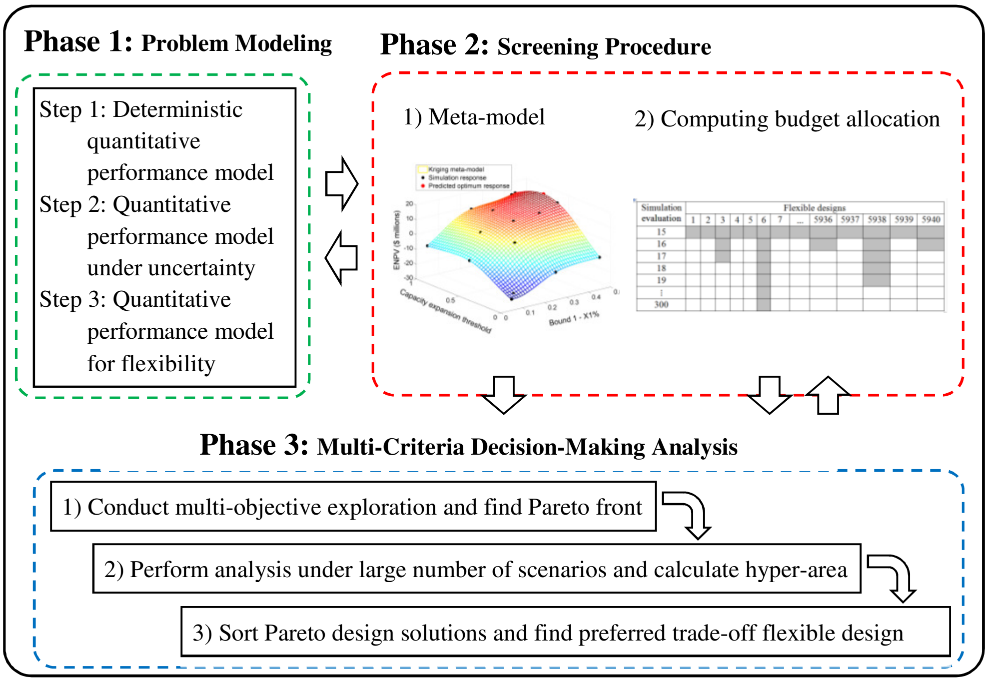


Figure 3.1: Proposed multi-criteria screening framework for flexibility in engineering design

For better understanding of the function of the proposed framework, input and output for each phase of the proposed framework are represented in a flowchart. Figure 3.2 shows the process.

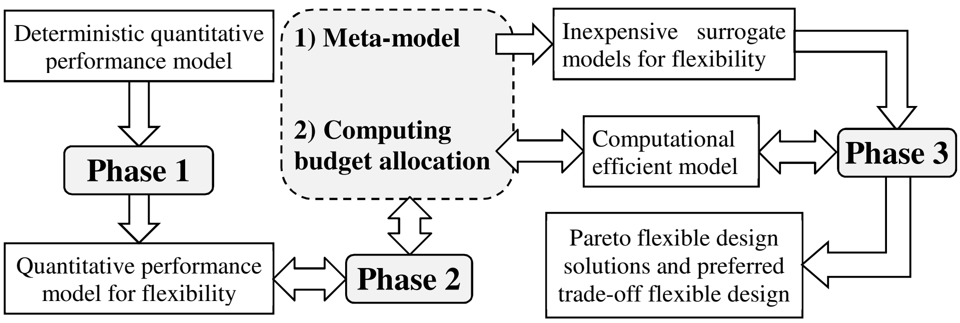


Figure 3.2: Input and output for each phase of the proposed framework

The input to phase 1 is the deterministic quantitative performance model and the output of phase 1 is the quantitative performance model for uncertainty and flexibility analysis. Using the output model from phase 1 that accounts for flexibility and uncertainty, a family of flexible design solutions can be generated, but the best flexible design is not known yet. The enumeration of possible flexible designs can be demanding, hence there is a need for phase 2 to help quickly find preferred flexible solutions. Phase 2 of the proposed model relies on two screening approaches to address the computational issue: 1) meta-model and 2) computing budget allocation. When the meta-model screening approach is used, the outputs of phase 2 are inexpensive surrogate models for flexibility. On the other hand, when computing budget allocation screening approach is used, there is a back and forth procedure to create a computational efficient model for flexibility. Finally, the outputs of phase 3 are Pareto flexible design solutions and the preferred trade-off flexible design based on decision-makers' preference.

3.3 Phase 1: Problem modeling

The starting phase of the proposed screening framework is a simulation-based flexibility and uncertainty analysis that starts with the three following steps, as illustrated in Figure 3.3. Each step is further described below.

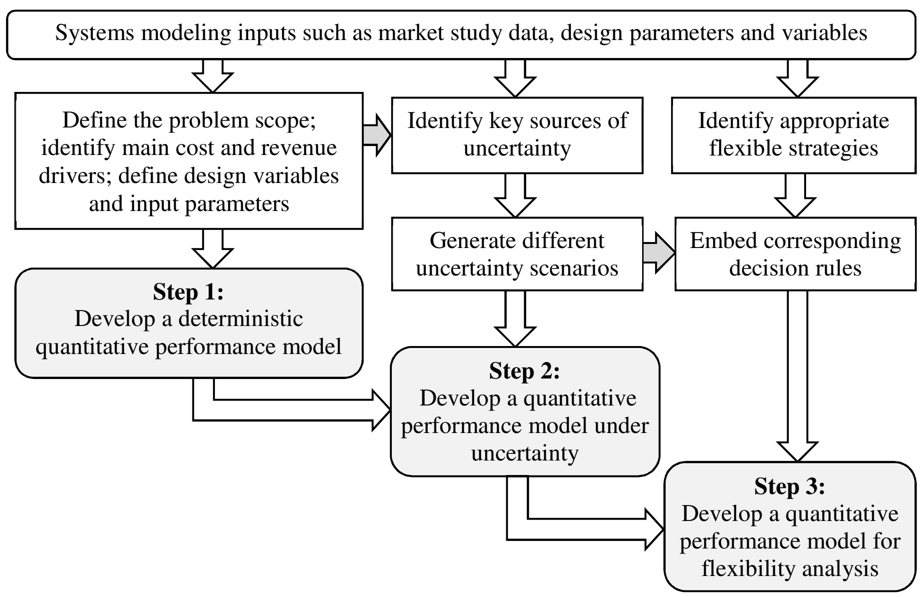


Figure 3.3: Problem modeling phase for flexibility and uncertainty analysis

In these steps, different sensitivity analyses can be conducted to observe the sensitivity of the system responses with respect to input parameters, design variables, and problem assumptions. Different tradeoffs can be studied, for example between economies of scale factor, volatility, discount factor, learning rate, and the value of flexibility.

3.3.1 Step 1: Develop deterministic quantitative performance model

This step builds a baseline quantitative performance model to evaluate the design alternatives. To do so, the scope of the problem and underlying assumptions about problem modeling and parameters need to be determined, such as market parameters, design variables, key costs and revenue drivers of the system. Following this, a deterministic quantitative performance-based model is developed to represent the relations among components of the system and to measure the lifecycle performance of the design alternatives using different metrics, such as Net Present Value. At the end of this step, the model can generate single-point outputs in terms of different values of design variables. This model, however, provides unrealistic solutions as it does not recognize uncertainty.

3.3.2 Step 2: Develop quantitative performance model under uncertainty

In this step, the deterministic quantitative performance model is extended into the model under uncertainty. To do so, the major uncertainty drivers of the system are first identified using a deterministic sensitivity analysis to determine and compare the relative importance of the model parameters. There are tools, such as Tornado diagrams, that can help prioritize a long list of uncertainty drivers and be used as a complement to – not a substitute for – expert judgment (de Neufville and Scholtes 2011). In a Tornado diagram of design alternatives, the top bars represent the parameters that contribute the most to the variability of the outcome, and therefore what the decision-maker should focus on. Once the main sources of uncertainty have been identified, the corresponding historical trends need to be analyzed by understanding the data, developing the overall pattern and assessing the uncertainty in their trends. Stochastic functions, such as Geometric Brownian Motion (GBM), s-curve function and Mean Reverting Process, can be used to model the uncertainty behavior over the evaluation period. By incorporating these stochastic behaviors into the deterministic model using the Monte Carlo simulation, a large number of possible scenarios can be generated. In this step, hence, one deals with distributions of outcomes in terms of different input variables.

Considering a large enough number of sample demand scenarios (i.e. 2,000) as inputs for the quantitative performance model under uncertainty, cumulative distribution functions of the different design alternatives can be generated and compared based on different performance metrics, such as expected net present value (ENPV), value at risk (VaR) like 10^{th} percentile (or P10), value at gain (VaG) like 90^{th} percentile (or P90), and variability (standard deviation) (de Neufville and Scholtes 2011). The input variables of the model in this step are only design variables.

3.3.3 Step 3: Develop quantitative performance model for flexibility

This step introduces the notion of flexibility in the design, deployment and evaluation processes. In the proposed framework, step 1 of phase 1 takes as input a deterministic quantitative performance model, and step 2 of phase 1 augments this model by modeling uncertainty explicitly, as part of the quantitative performance model development under uncertainty. Essentially there is no flexibility in these two steps. Flexibility is considered in step 3 of phase 1. The process here mainly focuses on flexibility valuation, but it is augmented by engineering design tools in systems design concept generation that help identify the valuable flexibility strategies. For instance, flexible strategies such as capacity expansion/reduction, switching inputs/outputs and deferring investment can be considered. In this step, for the "generating the flexibility" that requires expert domain knowledge, systematic processes such prompting, as suggested by Cardin, Kolfschoten et al. (2013), the Integrated Real Options Framework by Mikaelian, Nightingale et al. (2011), or the procedure explained in Hu and Cardin (2015) are all ways to generate the flexible alternatives as part of phase 1. When the effective flexible strategies have been identified, corresponding decision rules need to be explicitly embedded in the quantitative performance model under uncertainty. The concept of defining decision rules with threshold variables, which was first developed by Ranjbar-Bourani, Cardin et al. (2013), is extended to generate different flexible managerial strategies and solutions. Flexible strategies are characterized by a combination of design variables and decision rules, thereby defining the design space. Similar to Step 2, there are different performance metrics to evaluate design alternatives in this step.

To evaluate each flexible design, a Monte Carlo simulation model with large enough number of scenarios needs to be run, which may take a few seconds, minutes or even hours depending on the complexity of the simulation model for the case under consideration. The total number of the flexible solution space combinations is determined by the numbers and step sizes of design variables and decision rule parameters. The larger number of flexibility options and the smaller the step sizes, the larger the number of possible combinations will be and, eventually, the more computationally intensive the exhaustive enumeration will be. In addition, considering different assessment criteria requires further computational effort to explore the solution space in different directions. As a result, the enumeration technique can be further computationally intensive. Therefore, a screening model needs to be developed to quickly explore the flexible design solution space subject to different objectives.

3.4 Phase 2: Screening

There are several methods to screen complex systems design based on computer simulation. In the proposed framework, two approaches are explored: 1) A meta-model based screening approach and 2) A computing budget allocation based screening approach. As opposed to all other approaches, the rationale for investigating these approaches is that these approaches rely on balancing between exploration and exploitation to search the flexible design space efficiently and systematically. Procedures for these screening approaches are explained in detail in the following subsections.

3.4.1 A meta-model based screening approach

This part of the analysis is the crux of the proposed screening framework where the response surfaces in terms of different objective are formed adaptively. Figure 3.4 shows the procedure of the screening phase based on meta-model approach. In this approach, an inexpensive model is used instead of the original simulation model that is created in phase 1 for flexibility analysis. The proposed screening procedure is a simulator-based screening model with an embedded bottom-up screening procedure for operational flexibility. Here, surrogate approximation of the expensive (original) simulation is updated using all of the expensive simulation evaluations done in the previous and current iterations. When the stopping criterion is met, the surrogate model of the original simulation model is accepted (i.e., good-enough). This surrogate is very inexpensive to evaluate in terms of computation time (i.e., it takes a fraction of a second) and very efficient compared to an exhaustive search. The inexpensive surrogate model can then be explored by nonlinear programming methods to help identify points where the original simulation model should be evaluated.

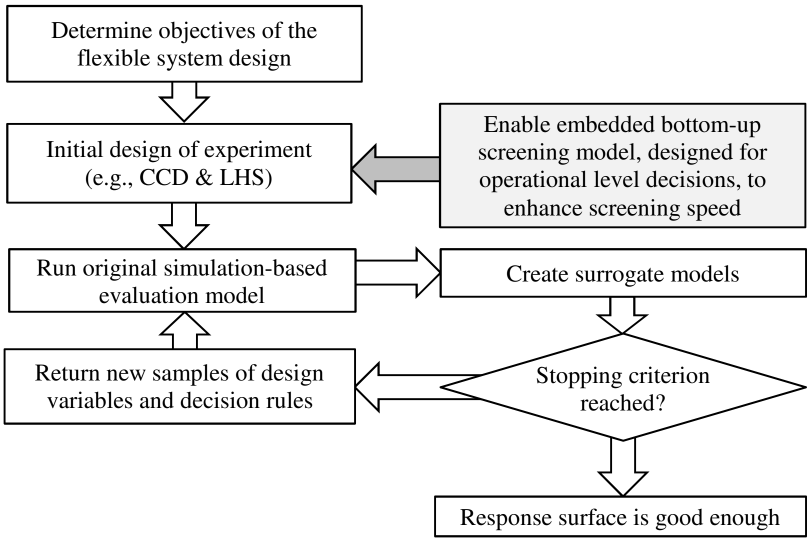


Figure 3.4: Screening phase procedure to create good-enough and inexpensive surrogate models based on meta-model approach, CCD stands for Central Composite Design and LHS stands for Latin Hypercube Sampling

When operational flexibility is enabled (i.e., turned “on”) in the simulation model, the simulator-based screening model captures the value added due to operational flexibility. In operational decision-making, the corresponding sub-problem (e.g., transportation, allocation, scheduling or inventory control problems) needs to be optimized at each operational period (e.g., one month, three months, six months, one year, etc.). Depending on the number of uncertainty scenarios, the optimization procedure must be repeated several times. Hence, finding the optimum decisions for all operational periods can be computationally intensive if a large number of uncertainty scenarios and small operational periods are considered.

To enhance the speed of the screening phase, a bottom-up screening model for the operational flexibility can be enabled, as shown in the grey box in Figure 3.3. A bottom-up screening models can be developed in a form of heuristic algorithms (e.g., heuristic rebalancing schemas) instead of calling optimization procedures (e.g., transportation model) repeatedly. Essentially, heuristic algorithms simplify the procedures used in original detailed operational models.

In this thesis, an Efficient Global Optimization (EGO) algorithm proposed by Jones, Schonlau et al. (1998) will be used for screening the flexible solution space. Unlike conventional Response Surface Method (RSM) techniques, the key to using EGO for finding the best flexible design lies in balancing the need to exploit the approximating surface (by sampling where it is optimized) with the need to improve the approximation (by sampling where prediction error may be high).

EGO is chosen as it explores the solution space efficiently and systematically. More specifically it: 1) Balances the local (also refereed as exploitation) and global (also refereed as exploration) search strategies to explore the solution space, while the conventional RSM methods have some limitations in highly non-linear systems responses (Jones 2001; Kleijnen 2009); 2) Benefits from the adaptive sequential response surface procedure, which is based on a Gaussian process, to lessen the computational time and evaluation number; 3) Takes advantage of a viable stopping criterion which is tied with simulation-optimization procedures to control the adequacy of the response surface.

The EGO procedure finds the global optimum of a surrogate model of an original simulation model. The Kriging meta-model was adapted from the Design and Analysis of Computer Experiments (DACE) model (Nielsen, Lophaven et al.

2002). In this study, the DACE model is used to construct a Kriging approximation model as a surrogate of the Monte Carlo simulation computer model for flexibility and uncertainty. Following Sacks, Welch et al. (1989), the DACE model considers the deterministic response y(x) as a realization of a regression model and a random function or stochastic process, as shown in equation 3.1. An interpretation of the model is that deviations from the regression model, though the response is considered deterministic, may look like a sample path of a stochastic process z.

$$Y(x) = \sum_{j=1}^{k} \beta_j f_j(x) + Z(x) \tag{3.1}$$

In Equation 3.1, Y can be considered as a Bayesian prior in the true response function. One method of analysis for the use of a stochastic process as a prior in true response functions is known as the Kriging method (Matheron 1963). Given a design vector $S = [s_1, \ldots, s_2]$ and system response $y_s = [y_{(s_1)}, \ldots, y_{(s_n)}]'$, consider the linear predictor of $y(x)$ at an untried x. The y_s can be replaced by the corresponding random quantity $Y_s = [Y_{(s_1)}, \ldots, Y_{(s_n)}]'$. Accordingly, $\hat{y}(x) = c'(x)y_{(s)}$ can be treated as random and its mean squared error over the random process can be computed. A Bayesian estimation would predict $y(x)$ by the posterior mean and the Kriging predictor would be $\hat{y}(x) = E[Y(x)|y_s]$. The random process Z is assumed to have a mean of zero and a covariance between Z(w) and Z(x), where σ^2 is the process variance and $R(\theta, w, x)$ is the correlation model with parameters θ, as shown in equation 3.2.

$$\mathrm{Cov}(w, x) = \sigma^2 R(\theta, w, x) \tag{3.2}$$

For interpolation purposes, different types of correlation functions provided by the DACE model can be used. In this study, a Gaussian correlation function is used with parameter θ, as shown in equation 3.3. In the DACE model, this parameter is estimated using maximum likelihood estimation (MLE). In the correlation function, the correlation decreases with the Euclidian distance, $|d_j|$, and a larger value for θ_j leads to a faster decrease.

$$R(\theta, w, x) = \exp\left(-\theta_j d_j^2\right); \quad d_j = w_j - x_j \tag{3.3}$$

Assuming a Gaussian process, the likelihood is a function of β in the regression model, the process variance σ^2 and the correlation parameter θ. The DACE model can then be used to determine the optimum value for the optimal coefficients θ^* of the correlation function. The predictor in the DACE model provides the mean squared error (variance). The mean squared error can be used to build the confidence interval for the Kriging response surface. The EGO approach allows one to obtain an adequate response surface through a sequential procedure using a viable stopping criterion. Equation 3.4 calculates the expected improvement in the current response surface (Jones, Schonlau et al. 1998) where Φ is the cumulative normal distribution and ϕ is the normal distribution; f_{min} shows the minimum value among the tried points, where $f_{min} = \min(y^1, \dots, y^n)$; $\hat{y}$ is the model predictor; and s shows the standard error (mean square error) of the Kriging meta-model. By optimizing the expected improvement function the optimum point X is obtained. The original simulation is then run at this point

$$E[I(X)] = (f_{\min} - \hat{y})\Phi\left(\frac{f_{min} - \hat{y}}{s}\right) + s\phi\left(\frac{f_{min} - \hat{y}}{s}\right) \tag{3.4}$$

The EGO technique creates the first response surface using the initial samples drawn from the design space. To fill the initial design space, a combination of Central Composite Design (CCD) and Latin Hypercube Design (LHD) is used. For the initial design in this study, the “faced” type of central composite design provided in MATLAB is used to cover the corner points and central point of the design space. In addition, the Latin Hypercube sampling design technique is used to efficiently and randomly fill the initial design space. Next, sampling from the design space needs to be continued until the stopping criterion (i.e., expected improvement) is met. In this study, the following EGO procedure is applied to create an adaptive response surface for different system responses (i.e., here ENPV and standard deviation):

Step 1: Conduct the initial design of the experiment (i.e., "space-filling" using Central Composite Design (CCD) and Latin Hypercube Design (LHD)).

Step 2: Run the simulations at the points suggested in the previous step.

Step 3: Fit the Kriging model parameters using the maximum likelihood estimation. Once the initial designs are complete and the response surface has been created, the iterative procedure can start.

Step 4: Build the Expected Improvement (EI) function using equation 3.4 and maximize it.

Step 5: Is the optimum value of EI less than the expected EI threshold?

If yes, the current response surface is adequate. Stop the procedure and go to Step 7.

If no, sample from the design space with the maximum EI and proceed to the next step.

Step 6: Run the simulation with the suggested sample and fit the Kriging model, then go to Step 4.

Step 7: The stopping criterion is met and the current response surface model is adequate.

Subsequently, in phase 3 Pareto flexible design solutions are generated using the generated inexpensive meta-models and further Pareto post-processing analysis are performed in the following phases of the proposed framework.

For better understanding of the meta-model screening procedure, consider a demand site for designing a flexible LNG production system. In this hypothetical example, the system configuration is adapted using modular capacity 25 tpd in the face of LNG demand uncertainty over its lifetime. In the quantitative model for flexibility and uncertainty, for the LNG capacity expansion only one decision rule is considered: IF "*the observed demand reaches certain percentage of the modular capacity 25 tpd*" THEN "*deploy the first capacity or expand the current capacity*" ELSE "*do nothing*". The threshold value can be set from 50% to 95%. The aim is to find an optimum threshold value leads to highest flexible design value in terms of ENPV. To find the best flexible design, the optimum threshold value needs to be found. To do so, an exhaustive enumeration method can be applied. Using this method, however, can be computationally expensive especially if complex simulation models are used. Thus, a screening approach is needed to quickly explore the flexible design solution aiming at finding good enough flexible design solutions. Figure 3.5 shows the meta-model screening procedure for the hypothetical example as shown in iterations "a" to "c".

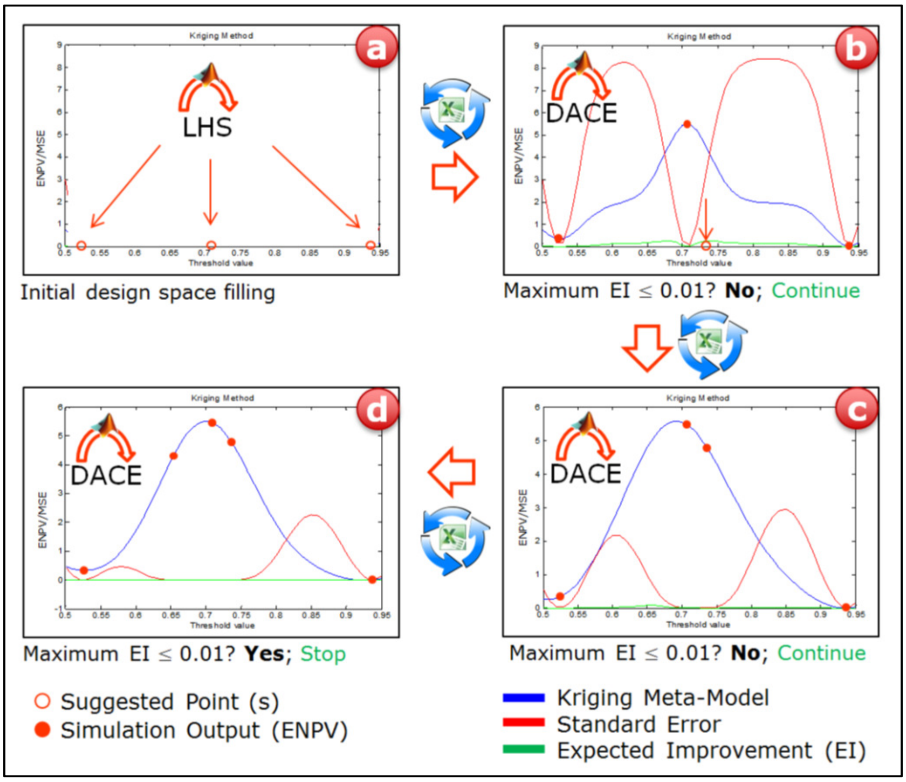


Figure 3.5: The meta-model screening procedure for the hypothetical example

The meta-model screening procedure starts at iteration "a" where the initial design space is filled using the Latin Hypercube Sampling (LHS) design. As can be seen, three threshold points are suggested by LHS and these points are plugged in the simulation model for flexibility and uncertainty. Simulation model developed in the Microsoft Excel® is run for large number of demand scenarios (i.e. 2000 demand scenarios). In next iteration "b", Design and Analysis for Computer Experiment (DACE) model developed in MATLAB® is applied, using the obtained simulation outputs, to create an inexpensive model of the original simulation model (i.e. the output of Phase 1 of the proposed framework). Once the meta-model is built, using the Mean Square Error (MSE) produced as a byproduct of the meta-model and the Efficient Global Optimization (EGO) procedure, Expected Improvement (EI) function is calculated. Subsequently, the EI function is optimized. Given the optimum value of the EI function is not less than or equal to the stopping value (i.e. 0.01), the current meta-model is not good enough and it should be updated accordingly. Thus, the corresponding optimum threshold value obtained by optimizing the EI function is suggested as a new untried threshold value. The new threshold value is plugged in the original simulation model and after running the simulation the simulation output is used in the next iteration "c". In this iteration, the DACE model is applied to update the current meta-model by adding the new sample. Again, the EI function is calculated and its optimum value is obtained. The results show that the meta-model is not good-enough, and the corresponding optimum threshold for EI function should be considered. Following the same procedure performed at iteration "b" and "c", the Kriging meta-model is updated in iteration "d" and its optimum EI function is calculated. The results show that the optimum value of the EI function is less than or equal to the stopping criteria (i.e. 0.01), and thus the algorithm stops at this iteration and the current Kriging meta-model can be used as a good-enough meta-model instead of the original simulation model. The actual programming code for this hypothetical capacity expansion problem is available in Appendix H.

Essentially the meta-model screening method presented in phase 2 of the proposed framework, builds an inexpensive model of the original simulation model for flexibility and uncertainty (i.e. the output model of the phase 1 of the proposed framework). The meta-model is updated adaptively until good-enough meta-models are achieved, when the stopping criterion (i.e. expected improvement) is met.

3.4.2 A computing budget allocation based screening approach

In this section, a multi-objective computing budget allocation is proposed to explore the flexible design solutions efficiently and effectively. This screening approach is considered as a bottom-up screening approach. Given a finite set of design alternatives and limited budget for simulation evaluation, the aim is to appropriately allocate more simulation evaluation budgets to promising flexible designs rather than less important ones. This approach is considerably different from the meta-model based screening approach, and offers an attractive alternative from a computational standpoint.

Figure 3.6 shows the flowchart of the proposed multi-objective computing budget allocation (MOCBA) framework. The proposed heuristic MOCBA framework has been adapted from Lee, Chew et al. (2010) to suit the purpose of flexibility analysis. Before starting the procedure, some parameters of the MOCBA must be set first. Initial Budget Rate (IBR) refers to a portion of the Maximum Budget (MB). The MB determines the maximum budget available for each design alternative. In this study, different computer experiments are conducted by setting different values of MB. Essentially, when the budget allocated to any design alternative reaches MB the algorithm terminates, and final results are returned. Budget Incremental Rate (BIR) refers to the incremental rate of budget for each design alternative at each iteration. Design archive keep rate (DAKR) determines the percentage of designs that are transferred to the next iteration. For instance, if DAKR is set to 40%, it means that only 40% of the top flexible designs, which are sorted according to dominance relation, will be analyzed in the next iteration and the rest of the flexible designs are then discarded. Besides the MB, Minimum design archive size (MDAS) is another stopping criterion to ensure that enough flexible designs are returned at the end of the algorithmic procedure, before proceeding to the analysis with large number of scenarios in phase 3.

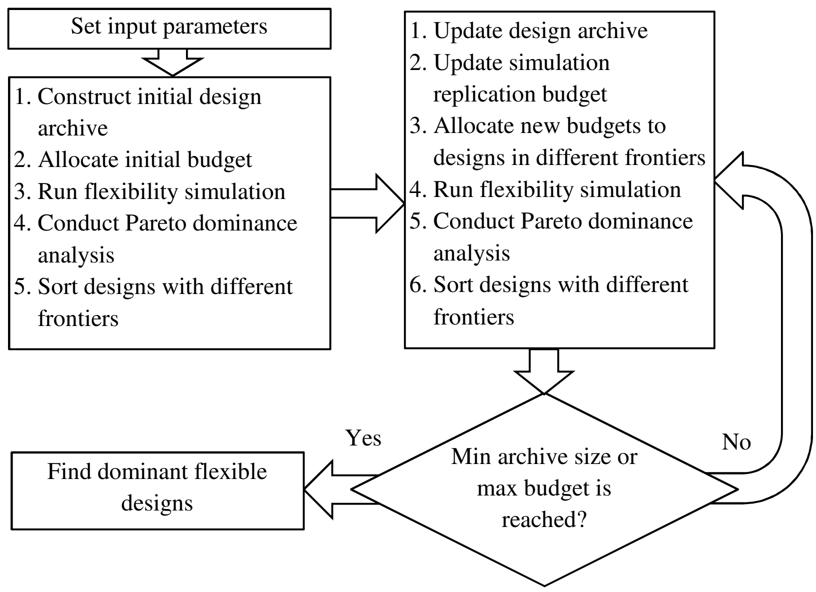


Figure 3.6: A multi-objective computing budget allocation flowchart

The Allocation factor (AF) determines how the total simulation replication budget is allocated to flexible designs in different layers of the Pareto fronts at each iteration. This analysis is a part of the procedure used in Phase 3 of the proposed framework on multi-criteria decision-making analysis. Under the computing budget allocation approach, flexible designs are generated as shown in Figure 3.5, and classified into different Pareto fronts (e.g. here Pareto fronts 1 to 4) using the Pareto dominance relation. The Pareto dominance relation will be explained in detail in the following section, phase 3.

As can be seen, design numbers 1 to 4 are non-dominated designs and are in Pareto front level 1. Subsequently, design number 5 lies in Pareto front level 2, designs 6 and 7 lies in Pareto front level 3 and designs number 8 and 9 lies in Pareto front level 4. For simplicity, in the process of computing budget allocation it was assumed that the same budget is allocated to designs that are in a similar Pareto front level at each iteration. Total budget at each iteration is calculated using equation 3.5.

Total budget= updated budget for each design × size of design archive (3.5)

For instance, let flexible solutions contain 4 levels of Pareto fronts, as Figure 3.7 shows and, AF be the allocation factor as an input parameter.

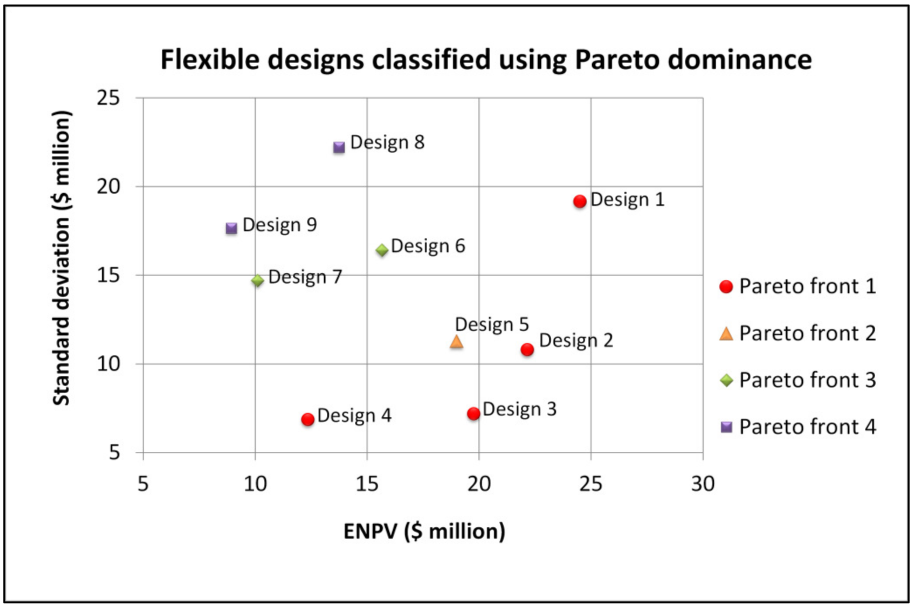


Figure 3.7: Flexible designs classified using Pareto dominance relation

The allocation factor determines how simulation budgets are allocated to different Pareto fronts. Equations 3.6 to 3.9 express the linear allocation problem.

$w_1 = AF\, w_2 \rightarrow w_1 - AF\, w_2 = 0$ (3.6)

$w_2 = AF\, w_3 \rightarrow w_2 - AF\, w_3 = 0$ (3.7)

$w_3 = AF\, w_4 \rightarrow w_3 - AF\, w_4 = 0$ (3.8)

$w_1 + w_2 + w_3 + w_4 = 1 \rightarrow w_1 + w_2 + w_3 + w_4 - 1 = 0$ (3.9)

By solving these equations, the simulation replication budget for designs located at each Pareto front W_i is obtained. Now new budget for flexible designs in Pareto front i can be calculated as Total budget × W_i. According to this procedure, if AF=1 similar simulation budgets are then allocated to different Pareto front levels. On the other hand, if AF>1 budgets allocated to Pareto front 1 are AF times more than budgets allocated to Pareto front 2 and budgets allocated to Pareto front 2 are AF times more than budgets allocated to Pareto 3 and budgets allocated to Pareto front 3 are AF times more than budgets allocated to Pareto 4.

The reason for this type of simulation budget allocation is that how simulation budgets are allocated to different Pareto fronts can be controlled. The bigger value of allocation factor is, the more budgets are allocated to the designs that are close to true Pareto front rather than those that are far away from true Pareto front.

When the meta-modeling screening approach is used, the output of the phase 2 is the meta-models of the intended objective functions (e.g. ENPV and Standard deviation). There is a need to go phase 3 to find dominant flexible designs using the computationally inexpensive meta-models created in phase 2 and based on DMs preferences. It should be emphasized that there is a back and forth procedure between phases 2 and 3 when the computing budget allocation approach is used in phase 2. In contrast, using the meta-model approach in phase 2, the inexpensive meta-models are passed to the phase 3 for further analysis. In phase 3, dominant flexible designs are generated, and the best trade-off flexible solution is found based on decision makers' preferences using the weighted-sum method as a Pareto post processing approach.

3.5 Phase 3: Multi-criteria decision-making analysis

Until recently, most of the relevant screening models developed for analyzing flexibility in engineering systems design (e.g., Cardin (2007); Lin (2009); Yang (2009)) considered only one single criterion for design space exploration. However, researchers are increasingly aware of the importance of collaborative decision-making in the conceptual design phase.

To illustrate the tradeoffs, Figure 3.8 shows dominant flexible designs with move option showing ENPV and standard deviation of the dominant flexible designs. The figure provides a range of flexible design solutions so that decision makers can trade-off between flexible design solutions in terms of different objectives (i.e., ENPV and standard deviation).

Towards a better flexible design with respect to ENPV

ENPV	18.60	19.02	19.23	19.90	20.37	20.38	20.58	20.74	21.37	22.63	23.19	23.35	24.22
Std.	8.78	9.07	9.29	10.60	10.69	10.82	10.93	12.39	13.37	13.61	14.99	15.30	15.51

Towards a better flexible design with respect to Standard deviation

Figure 3.8: Dominant flexible designs, with move option

The choice of a flexible design depends on the risk preferences of the decision makers. While standard approach explores a design space with respect to only one objective to find the best flexible design, exploring the solution space with respect to different objectives provides a range of feasible flexible design solutions. Thus, more options will be given to decision makers.

Given a range of flexible design solutions, a risk seeker decision maker may tend to choose flexible designs with higher value at risk (e.g. P95). On the other hand, a risk averse decision maker tend to choose flexible designs with lower standard deviation (e.g., flexible design with Std. = $8.78M). Both types of decision-makers aim to maximize return for a given level of risk, but the risk-averse decision maker may prefer less risk, and be willing to sacrifice additional returns in exchange. The risk neutral decision-maker is indifferent between upsides and downsides, and therefore will aim to choose a design maximizing the expected value ENPV (e.g., flexible design with ENPV=$24.22M).

Let us assume that there are m objective functions and x is an n dimensional flexibility vector having n design variables and/or decision rules. Solutions to a multi-objective optimization problem are mathematically expressed in terms of non-dominated points.

It is useful to express non-dominance in terms of vector comparison; let x and y be two design vectors of n components. Thus, x = (x_1, x_2,.., x_n) and y = (y_1, y_2,.., y_n). For a maximization problem, we say that x dominates y if and only if (Deb 2014), see equation 3.10:

$$f_j\,(\mathrm{x}) \geq f_j\,(\mathrm{y}) \text{ and } f_j\,(\mathrm{x}) > f_j\,(\mathrm{y}) \text{ for at least one } j \quad j \in \{1,2,\dots,m\} \tag{3.10}$$

Similarly, for a minimization problem, that x dominates y if and only if, see equation 3.11:

$$f_j(\mathrm{x}) \leq f_j(\mathrm{y}) \text{ and } f_j(\mathrm{x}) < f_j(\mathrm{y}) \text{ for at least one } j \quad j \in \{1,2,\dots,m\} \tag{3.11}$$

There are three possibilities that can be the outcome of the dominance check between two solutions x and y. That is (i) solution x dominates solution y, (ii) solution x gets dominated by solution y, or (iii) solutions x and y do not dominate each other.

Let us assume a two-objective optimization problem, maximizing ENPV and minimizing the standard deviation as exemplified above, and with nine different design solutions shown in the objective space, as illustrated in Figure 3.7.

Given both objective functions are of importance to us, it is usually difficult to find one solution that is best with respect to both objectives. However, one can use the above definition of domination to decide which solution is better among any two given solutions in terms of both objectives. For example, if solutions 2 and 5 are to be compared, we observe that solution 2 is better than solution 5 in terms of both objectives. Thus, both the above conditions for domination are also satisfied and we may write that solution 2 dominates solution 5. The solutions in each Pareto level do not dominate each other. The set of all non-dominated solutions are usually known as the Pareto-optimal (e.g. here design 1, 2, 3 and 4 are in level 1).

Figure 3.9 shows the proposed multi-criteria decision-making procedure to explore flexible design space with respect to more than one objective function. Under the meta-modeling approach, Pareto fronts are generated using inexpensive surrogate models obtained from phase 2.

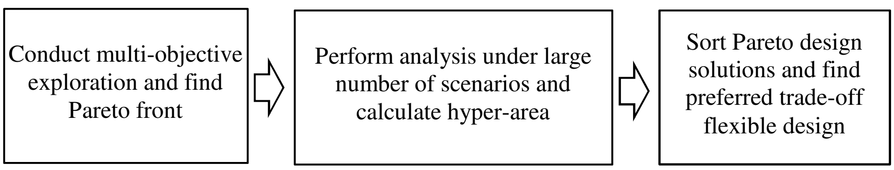


Figure 3.9: Procedure of the Multi-criteria decision-making analysis (Phase 3)

3.5.1 Hypervolume

Pareto front obtained from the screening phase is further analyzed using large enough number of scenarios. In this study 2000 scenarios are considered as system response converges to the same value with negligible variation. Then using Pareto dominance relation, true Pareto front are obtained. To measure the quality of each Pareto front, Hyper-volume (also hyper-area for two objectives) is used. This criterion accounts for dominance, spread and density of Pareto designs simultaneously (Zitzler, Thiele et al. 2003; Bradstreet, While et al. 2008; Nebro, Durillo et al. 2008). The hyper-volume is dominated by the solutions in each Pareto set and closed by an arbitrary worst-case point. For illustration purposes, Figure 3.10 depicts the area dominated by a Pareto front using an arbitrarily chosen worst case scenario as a reference point with ENPV=$5M and Standard deviation=$25M.

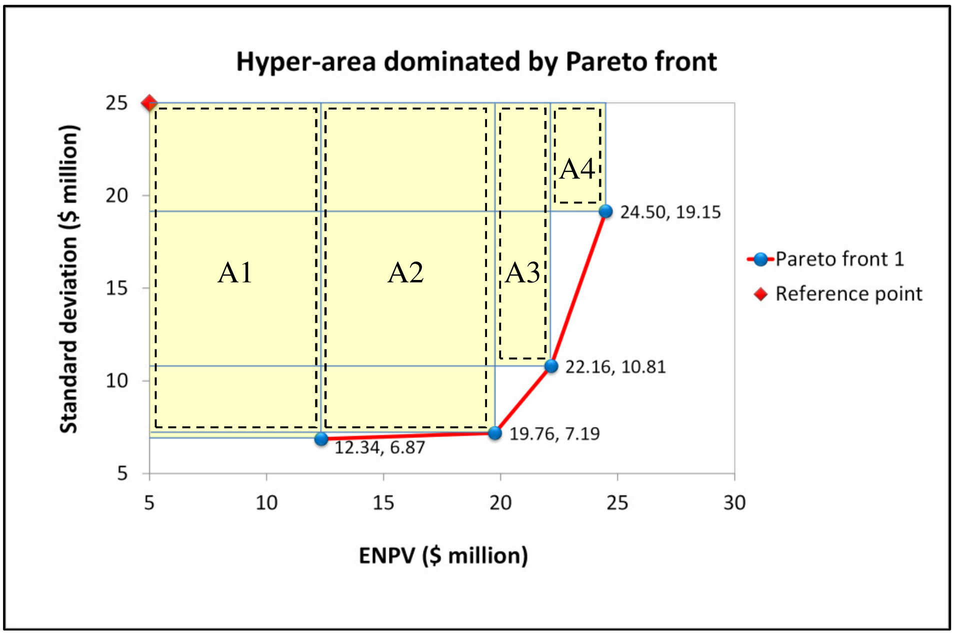


Figure 3.10: Hyper-area dominated by Pareto front and an arbitrary worst case with ENPV=$5M and Standard deviation = $25M was used

The higher value of the hyper-volume, the better the quality of the Pareto front. In this example, the hyper-area is the sum of the areas of the vertical rectangles surrounded by the reference point and Pareto front points from left to right. Alternatively, the area can be numerically integrated in a horizontal way. The hyper-area is calculated as follows:

A1= (12.34-5) × (25-6.87) = 133.14; A2= (19.76-12.34) × (25-7.19) = 132.01; A3= (22.16-19.76) × (25-10.81) = 34.03; A4= (24.50-22.16) × (25-19.15)= 13.69

Hyper-area= A1+A2+A3+A4=133.14+132.01+34.03+13.69= 312.87

3.5.2 Pareto post processing: weighted-sum method

Flexible solutions in the Pareto front are often large and can become difficult to comprehend and consider. The following section describes a procedure for evaluating the tradeoffs between the different objectives captured in the Pareto front analysis, and select recommended design alternatives. One approach is to find the best trade-off between flexible design solutions consistent with the preferences of the decision-makers. A common approach to evaluate the trade-offs between flexible solutions lying on the true Pareto front is the weighted-sum method. In this method, decision makers provide weight for each objective function so that weighted-sum can be calculated. All the flexible design solutions can then be sorted accordingly. For illustration purposes, Figure 3.11 shows how dominant flexible designs are sorted using a weighted-sum method.

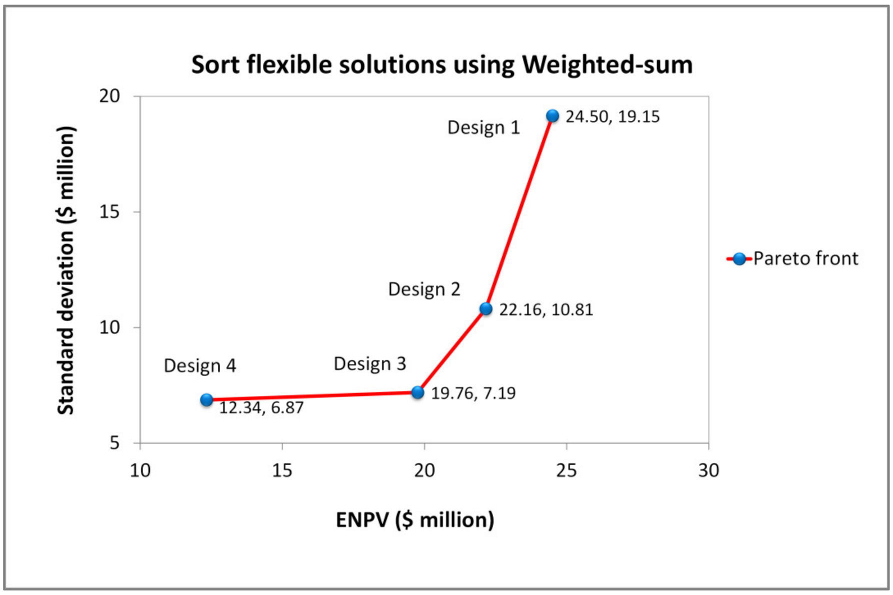


Figure 3.11: Sorting dominant flexible designs using weighted-sum method

This method is different from the additive multiple attribute utility method. While the additive multiple attribute utility deals with attribute functions, the weighted-sum method in this thesis aims to find the best trade-off dominant flexible design according to the decision makers' preferences.

In the two case studies, a demonstration of how to identify the recommended design(s) will be done. Of course, such recommendation depends on the decision-maker's preference, and is only for illustration purposes. Table 3.1 shows an example of weighted-sum calculation to minimize (-W1×Normalized (ENPV)) + (W2 × Normalized (Std.)) considering W1+W2=1. As can be seen, Pareto designs can be sorted in terms of different decision makers' preferences.

Table 3.1: Sorting flexible designs with respect to different DM preferences, Weighted-sum values are in millions dollars

Decision maker preference		**weighted-sum (sorted design number)**			
W1	50%	0.21 (3)	0.26 (2)	0.5 (4)	0.5 (1)
W2	50%				
W1	60%	0.24 (3)	0.24 (2)	0.4 (1)	0.6 (4)
W2	40%				
W1	40%	0.17 (3)	0.27 (2)	0.4 (4)	0.6 (1)
W2	60%				

The following procedure is proposed to find the preferred flexible design and sort flexible designs based on their weighted sum values.

1. Convert the problem to a minimization problem for all objective functions, if needed.

2. Find the utopia point for objective function i which is minimum, shown as O_i^U.

3. Find the nadir point for objective function i which is maximum, shown as O_i^N.

4. Normalized the objective function i in objective space, using equation 3.12

$$\bar{O}_i = \frac{O_i - O_i^U}{O_i^N - O_i^U} \tag{3.12}$$

5. Calculate the weighted sum value for flexible design k using equation 3.13 where k=1 …K and K is the total number of dominant flexible designs. Then sort flexible designs increasingly based on weighted-sum value; if two flexible designs have the same weighted-sum value, give the priority to the design with a bigger design number.

$$WS_k = \sum_{i=1}^{2} w_i \times \bar{O}_i \tag{3.13}$$

The same abovementioned procedure was followed to evaluate the recommended designs in chapter 4 and chapter 5.

For example, given w1=50% and w2=50%, design number 3 has the least weighted-sum value 0.21. Following design number 3, design numbers 2, 4 and 1 with values 0.26, 0.5 and 0.5 respectively have the least weighted-sum value. In the Table, weighted-sum value with sorted design numbers in terms of (w1=60%, w2=40%) and (w1=40%, w2=60%) are also provided.

A preferred trade-off dominant flexible design is obtained in this phase. The solution representation corresponding to the preferred flexible design represents the best trade-off values of the decision rule parameters and design variables. The example of possible solutions from the process are provided and described at the end of each case study.

The proposed framework is able to optimize both design variables and decision rules using meta-model and computing budget allocation approaches subject to multiple performance assessment criteria. Essentially, the procedures presented in phase 2 and phase 3 of the proposed multi-criteria screening framework can be considered as “decision-rule and design-variable optimizer" considering multiple performance assessment criteria.

3.6 Exhaustive enumeration

A full exhaustive enumeration is done with each case study application to validate the solutions found by the screening approaches, using the simulation model developed in Phase 1 of the proposed framework. The simulation model is used to generate different flexible design solutions by altering feasible values of the design variables and decision rule variables. Considering possible values for design variables and decision rules, a large number of flexible designs is generated and can make the exploration of flexible designs challenging. The proposed simulation model for flexibility and uncertainty described in this phase can be treated as an input-output model.

By following the dominance relation procedure, the dominant flexible designs can be obtained with different simulation evaluation number in different computer experiments. For instance, in experiment with 50 simulation replications, all possible 5,940 designs in the first case study are analyzed with 50 simulation evaluation which resulting in 5,940×50=297,000 simulation evaluations. Once the Pareto fronts of the experiment with 50 simulation evaluations are found, for the fair basis analysis 2000 simulation evaluations are used as the system responses converge to a value with negligible variations. Figure 3.12 summarizes the exhaustive enumeration technique.

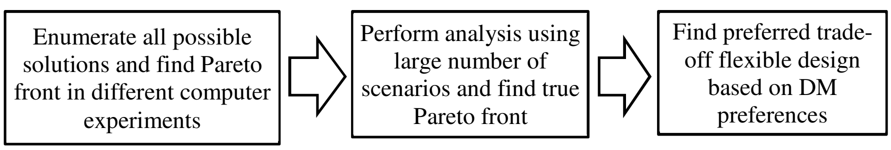


Figure 3.12: Exhaustive enumeration analysis

Essentially, the Pareto front of a given experiment (e.g., 50 scenarios) is found first. Then the Pareto front solutions are further investigated using large enough number of scenarios. Finally, the true Pareto front for each computer experiment is found and the hyper-area is calculated. Once true Pareto front is obtained, Pareto post processing can be applied to find a preferred trade-off flexible design.

3.7 Summary

In this section, a screening methodology has been proposed to explore the space of flexible design solutions efficiently and effectively. Essentially the proposed screening approach is an extension of an existing four-step simulation-based approach for flexibility analysis. Two screening approaches have been proposed 1) A meta-model based screening model; 2) A computing budget allocation based screening model. To validate the results found using these two screening approaches, an exhaustive enumeration method is conducted. Then the results of the three approaches are compared subject to Pareto quality and simulation runtime in terms of different computer experiments. To investigate the generalizability of the proposed multi-criteria screening framework, the proposed screening approaches are applied to two case studies: 1) A centralized LNG production system design that will be described in Chapter 4; and 2) A decentralized LNG production system design that will be explained in Chapter 5.

Chapter 4 Case Study I: Centralized LNG Production System

4.1 Introduction

This chapter focuses on the design and development of a centralized LNG production system to provide fuel for trucks used in on-road product transportation in southeast Australia. The scope of the problem lies in the LNG supply chain where natural gas from on-shore pipeline is converted into LNG through liquefaction process, and then delivered to the transportation sector for the end users, heavy transportation sector. The goal is to meet the LNG demand at different geographical sites. Figure 4.1 schematically represents the LNG production system, from a fixed towards more flexible designs. This example has five candidate demand points equipped with filling station facilities and a main production site dedicated to a centralized LNG plant. All sites have access to the on-shore pipeline distributing the natural gas. In the main production site, LNG produced through the liquefaction process is transferred to the candidate demand sites. In this study, two main LNG system designs are investigated, 1) fixed centralized design (also referred as the fixed design), Figure 4.1 (a); and 2) flexible modular designs, Figure 4.1 (b and c).

In the fixed centralized design, the optimal capacity significantly depends on the strength of the economies of scale. A big LNG plant is built in the main production site and LNG produced is carried to the market sites using fuel trucks. The flexible modular designs includes: 1) flexible modular design– no move, see

Figure 4.1 (b), which considers a phasing approach using a modular LNG plant with the flexibility to expand capacity at the main production site, and transport LNG to demand sites; 2) flexible modular design with move, see Figure 4.1 (c), which is the same design as the no-move flexible modular design but with the ability to move the modular LNG plants to demand sites.

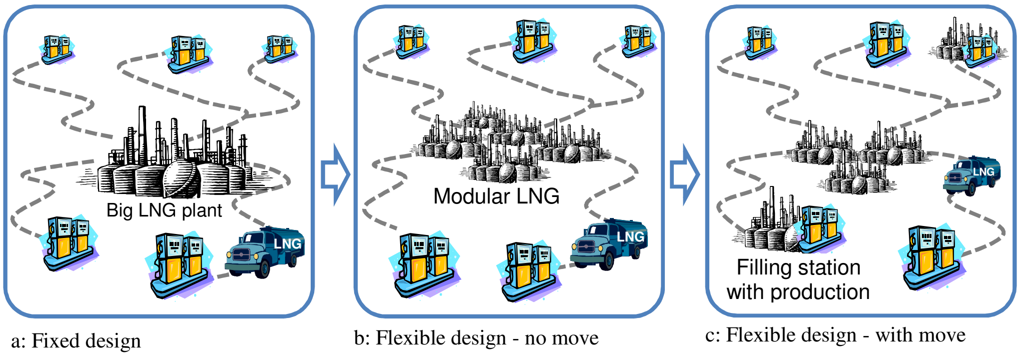


Figure 4.1: Shift from a fixed LNG system design towards a more flexible LNG system design

The proposed integrated multi-criteria screening framework in three phases, explained in section 3.2, is applied to this case study to efficiently and effectively explore the solution space of flexible designs.

4.2 Phase 1: Problem modeling

This section proposes a practical approach to quantify flexibility under uncertainty. The process focuses mainly on flexibility valuation, but should be augmented by engineering design tools that help identifying the main uncertainty drivers, and valuable flexibility strategies. This approach improves the lifecycle performance of a project dependent on a range of potential uncertainties. To compare the design alternatives under uncertainty, the thesis provides and applies a structured three-step methodology based on several economic lifecycle performance indicators (e.g. Net Present Value, Initial Capex, etc.) in order to illustrate the “Value of Flexibility”. Figure 3.2 in chapter 3 illustrates the generic process. In this case study, the three-step process is followed to analyze the system for flexibility, under market uncertainty related to LNG demand growth. More specifically, first, the deterministic DCF model is presented and second by taking uncertainty into account the DCF model under uncertainty is evaluated. Third, by incorporating decision rules into the DCF model under uncertainty the flexible DCF model is analyzed. A sensitivity analysis is performed to observe how the system responds to different parameters and input data. It is aimed to recognize that some of the modeling assumptions and parameters may be imprecise, and seek to determine where decision reversal might occur.

Example procedures like prompting suggested by Cardin, Kolfschoten et al. (2013) or the Integrated Real Options Framework by Mikaelian, Nightingale et al. (2011) can help generate flexibility strategies. While this thesis focuses on on-shore LNG systems, the proposed frame work could be adapted to measuring the value of flexibility in many other engineering systems as well.

4.2.1 Modeling assumptions

The free cash flows are modeled directly from cost and revenue assumptions, based on discussions with the collaborators at a practising company, and incorporating the best practices in the industry. The following assumptions are made for model development. Demand is assumed to be evenly distributed in the region over five distinct demand sites. There is no market at the main production site. All sites have access to on-shore natural gas pipeline in the region. At the main production site, time to build for the first plant is 3 years while at each demand site, the first plant takes 2 years to be built. Also, if one decides to expand capacity in year t, extra capacity will be available for production in year t+1. Regarding financial parameters, the project lifetime is assumed to be 20 years.

Each year is considered to be 350 working days. A 10-year straight-line depreciation method is used for all LNG production facilities with zero salvage value. The discount rate as an after-tax Minimum Attractive Rate of Return (MARR) is assumed to be 10% and the corporate tax rate is 15%. Essentially, the quantitative performance of the design is evaluated based on an After Tax Cash Flow (ATCF) analysis.

With regards to design parameters, the fixed design analysis examined economies of scale: α=1, 0.95, 0.9 and 0.85. The modular design analysis investigated different learning rates: LR = 0, 5, 10, 15 and 20%. The capacity of modular LNG plant was set to 25 tpd with initial Capex $25 million. The Opex of the plant is assumed 5% of the plant's Capex. Flexibility cost is 10% of the Capex of the first capacity deployment at each site because of gas tie-in to the existing natural gas pipeline and extra land cost. Transportation cost for carrying LNG is set to $0.4 per ton-kilometer, while travel distances from the main production site to demand sites 1, 2, 3, 4, and 5 are 118, 121, 281, 318, and 446 Km respectively.

4.2.2 Step 1: *Develop deterministic quantitative performance model*

The proposed methodology starts with the deterministic analysis, considering first a rigid design as benchmark. The aim is to understand the key components of the system that influence its lifecycle performance. The performance metric used in this problem is NPV, calculated as the sum of discounted cash flows throughout the project lifecycle T = 20 years – see equation 4.1. Variables TR_t and TC_t are the total revenues and costs incurred in years t = 1, 2, ... T, r is the discount rate, Tax is the effective income tax on ordinary income and d_t is the sum of all noncash, or book, costs during year t, such as depreciation. A mathematical representation of the case study I is provided in Appendix F.

$$NPV = \sum_{t=1}^{T} \frac{(1 - Tax)(TR_t - TC_t) + Tax\ d_t}{(1 + r)^t} \tag{4.1}$$

LNG demand is a key driver of system performance. A deterministic s-curve function is assumed to simulate LNG demand over the study period, as shown in equation 4.2. The rationale is that LNG demand initially grows slowly; it then increases exponentially, and finally tapers as it approaches a saturation limit. Variable M_T^D is the maximum expected demand for LNG, b^D is the sharpness parameter that determines how fast demand grows over time to reach the upper bound for demand. The parameter a^Dtranslates the curve horizontally.

$$D_t^D = \frac{M_T^D}{1 + a^D e^{-b^D t}} \tag{4.2}$$

where $a^D$is calculated using equation 4.3.

$$a^D = \frac{M_T^D}{D_0^D} - 1 \tag{4.3}$$

In general, the conventional DCF model is built to assess the performance of the system under deterministic conditions. This step captures standard industry practice in terms of design and project evaluation (Cardin, Ranjbar-Bourani et al. 2013). Parameters associated with deterministic LNG demand modeling obtained through a combination of personal communications and market research at the collaborating firm are summarized in Table 4.1.

Table 4.1: Parameters used in deterministic demand modeling for each site

Deterministic demand model	
Parameter	Value
D_0^D	5 tpd
b^D	0.35
M_T^D	50 tpd

Figure 4.2 shows the results of the fixed design analysis assuming a deterministic LNG demand forecast. It shows the NPV for different sizes of plants that have various economies of scale factors. It shows, as might be anticipated intuitively, that: a) for any set of plant size and economies of scale, there is a "sweet spot": build too small, and there is no profit from higher demands; build too large, and there is risk of overcapacity and attendant losses (stars on the curves indicate the best design for each set of parameters), and b) the greater the economies of scale (smaller α), the larger the fixed design should be.

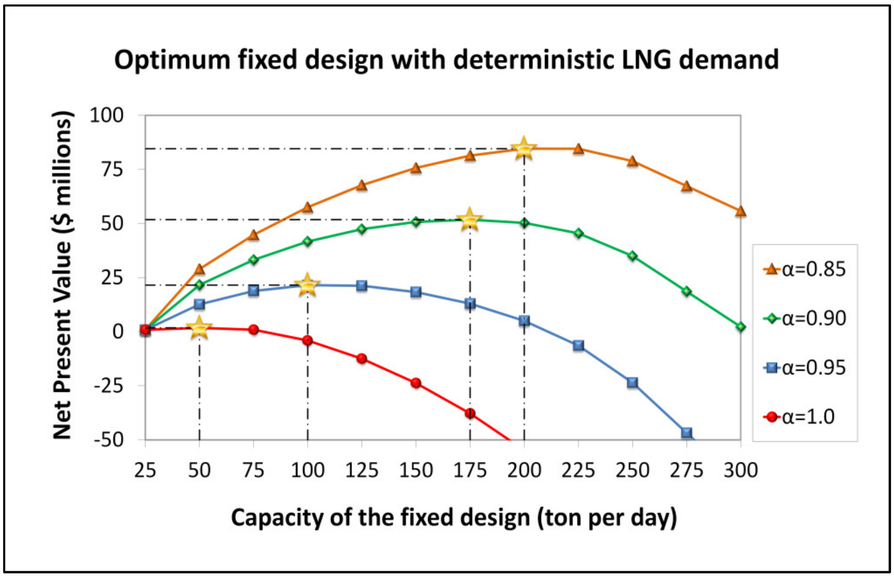


Figure 4.2: NPV of fixed designs under deterministic LNG demand. A star shows the optimum design for a given economies of scale factor

The advantages of these economies compensate for the overcapacity of the greater size over initial demand, and counterbalance the economic advantages of deferring costs (due to the discount rate). The discount rate is a key factor in the valuation process. It captures the time value of money and provides incentives to delay initial capital expenditures to later in the future, especially when the opportunity cost of capital is high. Note however, that deterministic analysis based on expected LNG demand gives misleading results, compared to realistic analysis that recognizes uncertainty, as shown in step 2.

4.2.2.1 Economies of scale

Economies of scale mean that the average cost per unit of production capacity decreases as one builds larger plants. Economies of scale are crucial factors because they drive designers to create the largest economically reasonable facilities, thereby counteracting a modular approach to capacity deployment (de Neufville and Scholtes 2011). This phenomenon is typically represented by the so-called cost function in equation 4.4. The parameter α is the economies of scale factor: the lower α is, the greater the economies of scale. Here it is assumed that the Operating Costs (Opex) of an LNG plant is proportional to its Capex as in equation 4.5.

$$\text{Capex of a fixed LNG plant} = \text{capacity}^{\alpha} \tag{4.4}$$

$$\text{Opex of a fixed LNG plant} = \text{k} \times \text{Capex} \tag{4.5}$$

The case study analyzed designs with different capacities for the fixed LNG plant ranging from 25 to 300 tpd, with 25 tpd capacity increments. The sensitivity analysis investigated different economies of scale factors to see their influence on optimum capacity for fixed LNG designs, and thus on the value of flexibility.

4.2.2.2 Key demand parameter

The most effective sensitivity analyses consider the joint effect of the variability of a parameter and their effects. This contrasts with the approach often encountered in practice of varying each parameter by a fixed percentage (such as +/– 10%). The reality is that some parameters are more uncertain than others. Also, some parameters may not vary considerably, yet have great effect – while others can vary considerably but have little effect. The cost-effective approach to sensitivity analysis then first estimates the plausible range of the spread of these parameters (such as their standard deviation if available) and then calculates the possible effect on the outcomes. The sensitivity analysis then focuses on the parameters with the greatest impact.

Figure 4.3 illustrates the first result of this approach. It shows the calculated effect of probable ranges of values for the parameters of the assumed demand projection, specifically of its initial and final levels and of the rate of growth. It presents the results in the form of a "Tornado" diagram, which stacks the parameters with the most effect at the top, thus presenting an image reminiscent of the cone of a tornado. For the example case, this first stage of sensitivity analysis indicates that the most sensitive assumption concerns the sharpness factor.

Based upon the first stage of the sensitivity analysis that highlighted the importance of the sharpness factor on the evaluation, its effect on the design evaluations for combinations of economies of scale and learning rate will be examined.

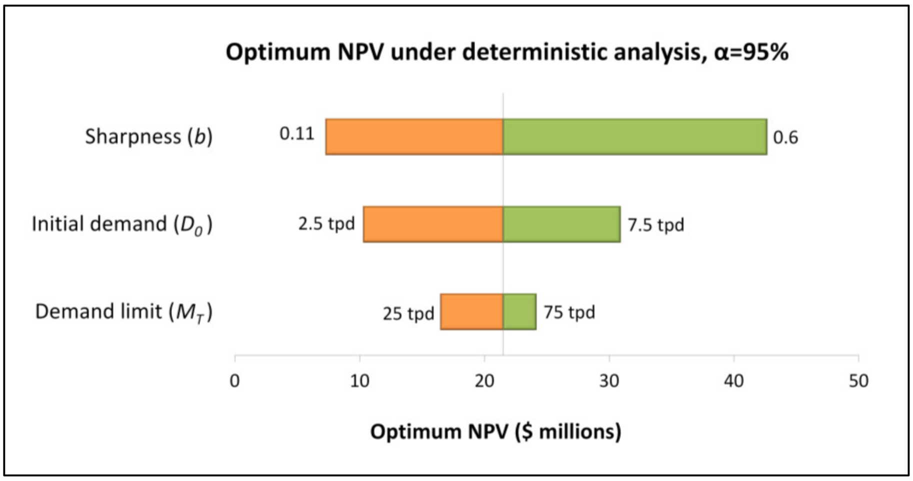


Figure 4.3: Tornado diagram showing effects of demand parameters on the optimum NPV (fixed design, deterministic analysis, α = 95%)

4.2.3 Step 2: *Develop the quantitative performance model under uncertainty*

This step models the major uncertainty drivers and analyzes their effect on lifetime system performance. The analysis uses the distribution of input parameters over time to calculate the distribution of the performance metric. Each demand scenario s leads to a performance outcome, $\mathrm{NPV_S}$. Simulation is the conventional way to do this, but analysts can use different techniques (e.g., decision trees, binomial lattice).

A stochastic version of demand using uncertainty factors is created. The case study used the s-shaped model of demand. As in equation 4.6, M_T^U is stochastic demand limit and b^U is stochastic sharpness parameter in demand models with uncertainty. Equation 4.7 defines a^U as the stochastic translation factor that varies due to volatilities in initial demand, D_0^U, and demand limit, M_T^U. Realized demand at time *t+1* equals realized demand at time *t* plus annual volatility multiplied by growth rate G_t at time *t*, as shown in equation 4.8. While other assumptions are possible, it is convenient to assume that G_t follows a standard normal distribution and Av is a fixed parameter calibrated using historical data.

$$D_t^U = \frac{M_T^U}{1 + a^U e^{-(b^U)t}} \tag{4.6}$$

$$a^U = \frac{M_T^U}{D_0^U} - 1 \tag{4.7}$$

$$D_{t+1}^U = D_t^U + (Av \times G_t) \tag{4.8}$$

Realistically, future demand over the 20-year life of the project is highly uncertain due to currently unknown prices, competition, government regulations, and other factors. Market research at the collaborating firm provided the stochastic LNG demand modeling parameters summarized in Table 4.2.

Table 4.2: Parameters used in stochastic demand modeling for each site

Stochastic demand model		
Parameters ~ Uniform distribution	Volatility	Value
D_0^U ~ Uniform ($D_0^D(1-\Delta_{D_0}), D_0^D(1+\Delta_{D_0})$)	Δ_{D_0}	50%
b^U ~ Uniform ($b^D(1-\ \Delta_b), b^D(1+\Delta_b)$)	Δ_b	70%
M_T^U ~ Uniform ($M_T^D(1-\Delta_{M_T}), M_T^D(1+\Delta_{M_T}\ )$)	Δ_{M_T}	50%

While other types of distributions such as Normal and Lognormal are possible, it is convenient to assume that D_0^U , b^U and M_T^U follows a uniform distribution; where Δ_{D_0} is the limit on volatility of the realized demand in year 0 as it differs from its projected value; Δ_b defines the volatility of the sharpness parameter as it differs from its forecasted value; Δ_{M_T} defines the volatility of the demand limit parameter as it differs from its forecasted value.

The uncertainty analysis results in a distribution of possible performance outcomes. The obvious way to compare this result to that of the deterministic model is to focus on the expected value of the distribution of NPV, or ENPV, calculated according to equation 4.9. The overall result is that the ENPV does not equal the deterministic NPV, which makes the point that the deterministic analysis that ignores uncertainties may lead to an erroneous result.

$$\mathrm{ENPV} = \frac{1}{N} \times \sum_{s=1}^{N} NPV_s \tag{4.9}$$

Note that the ENPV metric implies risk neutral preferences, which may not always be appropriate. Indeed, decision-makers often take downside risk into account and weight it heavily. It is thus often useful to supplement the ENPV metric with others that represent the extreme distributions of the outcomes, such as the Value at Risk (VaR) for a given level of probability and, complementarily, the potential for upside gain, the Value at Gain (VaG) (de Neufville and Scholtes 2011).

The deterministic analysis gives a false impression of lower value due to the Flaw of Averages (Savage 2009). Engineering systems typically respond non-linearly to inputs, and any decision based on average value of these factors is almost certain to provide a false reading on the actual average value of an alternative. To get the right answer, one needs to analyze the system under uncertainty.

The case study recognized LNG demand as a key source of uncertainty. Using Monte Carlo simulation it explored how design alternatives behave under different LNG demand scenarios. These simulations used different LNG plant capacities and economies of scale factors. The aim was to find the stochastically optimum design for plant capacity. The results show when using 2000 demand scenarios the system performance converged to a steady state value with a negligible variation. Figure 4.4 compares the projected LNG demand (i.e. dashed line) with 25 representative LNG demand scenarios (i.e. grey lines).

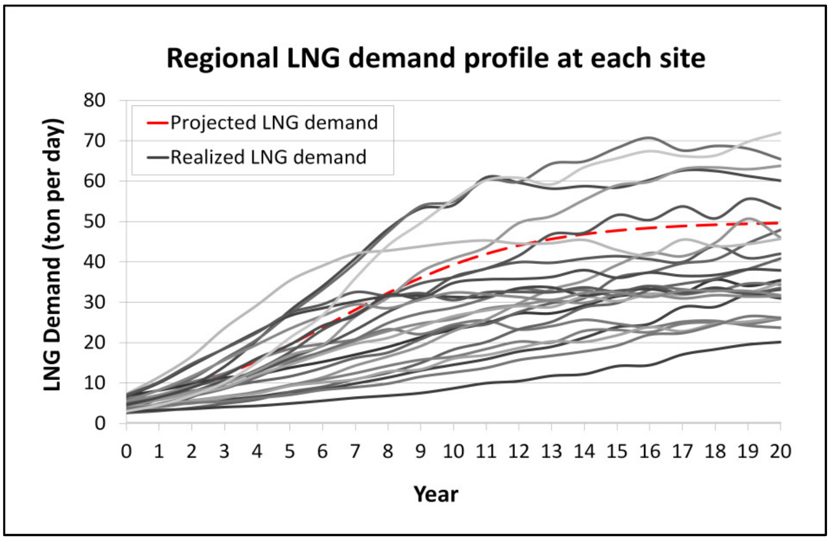


Figure 4.4: Projected and realized regional LNG demand at each geographical site

Table 4.3 compares the results of the deterministic and uncertainty analyses. The result is that optimum capacities and values generated by the uncertainty analysis are systematically different (in this case, smaller) than those obtained from the deterministic analysis. The intuition is that an asymmetric response of the system occurs because of variations in demand: lower demands lead to losses, which higher demands can only partially compensate, because of limitations in installed capacity. Given that the system's response is not linear (which is also the case for most engineering systems), designs selected based on optimizing the left hand side (i.e. deterministic analysis) will not be the same as designs selected based on optimizing the right hand side (i.e. uncertainty analysis).

Table 4.3: Optimum fixed designs under deterministic and uncertain LNG demand with different economies of scale factors α

α	**Optimum capacity (ton per day)**		**Optimum value ($ millions)**	
	Deterministic	Uncertainty	Deterministic (NPV)	Uncertainty (ENPV)
1	50	25	1.75	0.87
0.95	100	75	21.51	14.27
0.90	175	125	51.75	37.18
0.85	200	175	84.56	61.18

Here, the Flaw of Averages favors smaller capacity designs that are cheaper because less capacity is needed upfront. In return, such designs minimize unused capacity when demand grows slower than planned, and therefore reduce exposure to potential losses.

4.2.4 Step 3: *Develop quantitative performance model for flexibility*

This step recognizes system operators' ability to change, adapt, and reconfigure the system in light of uncertainty realizations. To account for system flexibility, decision rules are embedded into the DCF model under uncertainty. For example, to embed the capacity expansion policy in flexible modular designs, a set of simple decision rules is programmed in the Excel® spreadsheet DCF model under uncertainty. For instance a capacity expansion policy can be: IF "*observed* *aggregate demand in the current year is higher than a certain threshold value at the main production site*" THEN "*build extra modular plant*" ELSE "*do nothing*". The threshold value determines when extra capacity should be built, either at the main production site or other demand sites. For example, decision-makers may decide to add another modular plant as soon as the difference between the realized and current capacity (i.e. unmet demand) reaches 60% of the capacity of a modular plant for the site.

In this thesis, decision rules with feasible ranges for their threshold values were designed using the prompting procedure proposed by Cardin, Kolfschoten et al. (2013) based on discussion with collaborators at a local company. To find the optimum or near-optimum value for the threshold values, three methods are proposed in this thesis: 1) enumeration method; 2) meta-model based screening method; 3) computing budget allocation based screening method. Given a set of defined decision rules for each case study, optimum values for the thresholds can be found using the enumeration method while near-optimal threshold values are obtained using the meta-model and computing budget allocation based screening methods.

The value of flexibility is calculated as shown in equation 4.10. Whether ENPV of flexible design is less than the ENPV of optimum fixed design depends whether the cost premium for flexibility (i.e. cost of enabling flexibility) is considered. If not considered, then ENPV of flexible design cannot be less than ENPV of optimum fixed design because flexibility would not be embedded in the first place. In this case, the analysis focuses on finding the value of flexibility, which determines the maximum a decision-maker should be willing to pay to enable it in the system. In other words, the correct formulation should be Value of flexibility = max [0, ENPV of flexible design – ENPV of optimum fixed design]. If the premium cost for flexibility is included and it costs more than the value of flexibility, then yes the ENPV of the flexible design could be less than the ENPV of the optimum fixed design. Indeed, flexibility could add little to no value if there is a bad decision rule.

$$\text{Flexibility Value} = \max(0, \text{ENPV}_{\text{Flexible design}} - \text{ENPV}_{\text{Optimum fixed design}}) \quad (4.10)$$

4.2.4.1 Multi-criteria decision-making

In evaluating flexible designs, the analyst needs to factor in a distribution of outcomes instead of one single point to support design decision-making. These distributions can be interpreted using the shape of different criteria. For instance, one may seek to maximize ENPV or to minimize downside risk or to choose some balance between these criteria. Given the several possible criteria that are not directly compatible, it is useful to create a multi-criteria table, providing decision makers with the information needed to trade-off criteria among flexible design alternatives. In the field of decision-making under uncertainty, the expected value is widely used as an objective function, for instance using expected NPV. The ENPV is calculated using equation 4.11.

$$\text{ENPV} = \frac{1}{N} \times \sum_{s=1}^{N} NPV_s \quad (4.11)$$

This value, however, is based on risk neutral preference, which may not match with different risk preferences in reality. In practice indeed, downside risk is an important factor that decision makers often need to take into account. For instance, typical decision makers prefer lower risks given the same value of expected value. So other criteria for selection of projects include the Value at Risk

(VaR) for a given level of probability and, equally, the potential for upside gain, the Value at Gain (VaG). While this analysis relies here on a multi-criteria decision making table to trade-off quantitative life cycle performance metrics, more sophisticated multi-criteria decision-making approach can be applied when both quantitative and qualitative criteria are considered (Georgiadis, Mazzuchi et al. 2013).

4.2.4.2 Learning rate

The case study considered modular designs for LNG plants in the proven size of 25 tpd. Because of the learning phenomenon, the unit cost of these modules can decrease as more are installed. The more one builds, the more efficient one becomes. The learning curve in equation 4.12 represents this situation (de Neufville and Scholtes 2011):

$$\mathrm{U_i} = U_1 \times i^B \tag{4.12}$$

where U_i is the Capex of the ith modular LNG plant, U_1 the Capex of the first modular LNG plant, and B is the slope of the learning curve. The slope is calculated with different empirical values for LR, from 0%, 5%, 10%, 15% and 20%, using equation 4.13.

$$\mathrm{B} = \log\left(100\ \mathrm{percent} - \mathrm{LR\ percent}\right) / \log\left(2\right) \tag{4.13}$$

Thus if the cost of the first modular LNG plant is \$25 million, the cost of the 5th module (given a 10% learning rate) is: B = log (100 percent – 10 percent) / log (2) = –0.1520 so that U_5 = \$25M (5)–0.1520= \$19.57M. The learning phenomenon provides great incentives to install capacity consisting of many smaller units instead of a few large units. Together with high discount rates, learning counteracts the effects of economies of scale.

4.2.4.3 Flexible design strategies

Using concept generation techniques inspired from Cardin, Kolfschoten et al. (2013), flexibility to expand capacity is recognized as a strategy to deal with uncertain demand growth. The idea is to build less capacity at the start – to avoid over commitment and over capacity, and to add capacity based upon demonstrated demand. Key to this strategy, of course, is that the original design should be designed to facilitate capacity expansion easily. The analysis considered two kinds of capacity expansion. First, it looked at the benefits of building up capacity incrementally at the main site. Second, it considered the further advantage of moving additional modules in the field, close to the demand sites, as way of lowering transportation costs, and further exploiting the benefits from a modular approach to design and management. The average aggregate demand in the main production site and the average observed demand at demand sites are sensed annually by the relevant decision rules. For the first capacity deployment, besides its capex, there is a cost of flexibility while for the capacity expansion only modular capex is considered. At the main production site, time to build for the first plant is 3 years while at each demand site, the first plant takes 2 years to be built. At any location, however, capacity expansion takes only 1 year.

4.2.4.3.1 Flexible modular design - no move

Figure 4.5 illustrates the results of the flexibility analysis. This result is typical of what is observed in flexibility studies in the sense that it shows that flexibility can reduce the down side risks while allowing to capture upside opportunities, and improving the economic performance metrics such as VaR, VaG and ENPV (de Neufville and Scholtes 2011). It compares the performance under uncertainty of an optimal fixed design and a flexible design that expands capacity at the main production site [‘no move’ option]. Specifically, Figure 4.5 displays the cumulative distribution of the performance of each design (that is, the target curve). The lower left side of each curve indicates the lowest level of performance of each design as observed in the simulation, which is at 0% on the vertical scale of the cumulative distribution. The curve extends to the upper right, where it indicates the maximum performance observed, at the 100% level of the cumulative distribution.

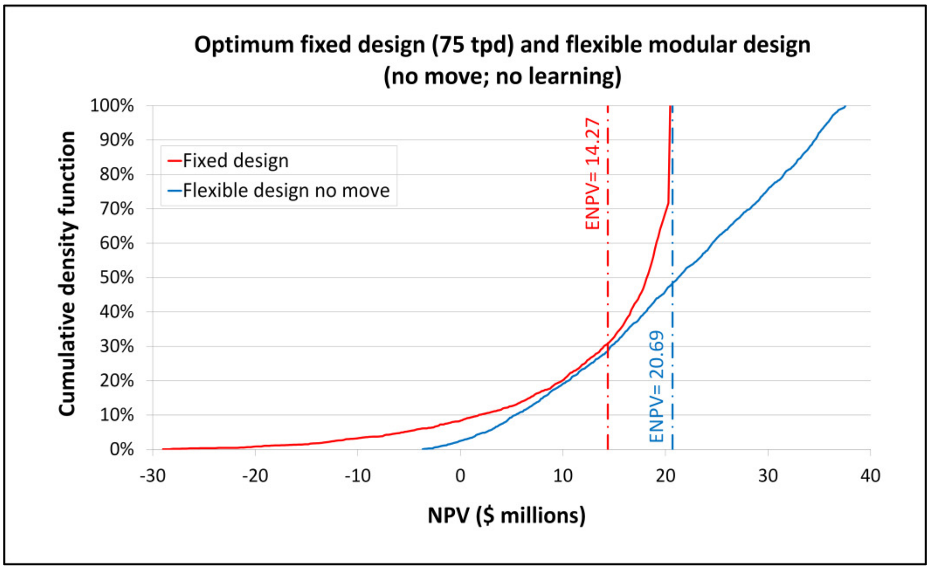


Figure 4.5: Optimum fixed design (α=0.95 → 75 tpd) and flexible modular design no move

As an example, the case study embedded the following decision rule in the simulation spreadsheet model:

- IF “*the difference between the observed aggregate demand and current capacity at this site is higher than a certain percentage of the modular design capacity being used in the design*”
- THEN “*the current capacity using the modular design capacity is expanded*”

- ELSE "*do nothing*".

Using an exhaustive enumeration technique, the threshold value 80% offered a better system performance among other threshold values.

The curve for the fixed design has an ENPV of $14.27M if the system exhibits modest economies of scale (α = 0.95), as indicated in Table 4.3. Notice that this fixed design, that takes advantage of economies of scale to build a large facility at the central site, has two unattractive features:

- It can lead to large losses (ENPV < – $25M), this is because the big plant can lose a lot if sufficient demand does not materialize; and
- Has limited upside potential (ENPV < $21M), since its fixed capacity cannot serve highest LNG demands.

The flexible design does significantly better than the fixed design, with the same assumed range of uncertainties:

- Its ENPV = $20.69M (see Table 4.4), that is nearly 44% better than that of the fixed design [$20.69M vs. $14.27 M]!
- Moreover, the performance of the flexible design in this case dominates stochastically that of the fixed design (i.e., its cumulative or target curve is absolutely to the right of that of the fixed design).
- The flexible design reduces exposure to downside risks: the strategy of building small at first puts less investment at risk and lowers maximum losses if demand is low. In this particular example the flexible design strategy reduces the maximum loss from about – $25M to less than – $5M.
- Similarly, the flexible design provides the ability to take advantage of upside opportunities: it enables the easy addition of capacity when demand soars and increases the maximum gain, in this case from about $21M to nearly $38M.

4.2.4.3.2 Flexible modular design - with move

The flexibility analysis for the 'move' strategy, which allows flexibility both as to when and where to add capacity, is similar to the previous example. However, this analysis had to implement additional decision rules to explore this flexibility, to address three questions: when should we build the modular plant for the first time at distance, where should we build it, and when should we expand it?

The decision rule regarding the capacity expansion at a distance was**:**

- IF "*demand at each demand site reaches Y% of the modular design capacity in the previous period*",
- THEN "*build a modular production plant at the demand site*",
- ELSE "*do nothing*".

Comprehensive enumeration determined that in this case the optimal economical threshold value was Y =100%.

The decision rule regarding the geographical location for capacity expansion was**:**

- IF "*the demand sites qualified for the first capacity deployment in terms of timing are located beyond the maximum coverage distance D*",
- THEN "*consider building the first modular production facility at those sites*",
- ELSE "*do nothing*".

Again, enumeration determined the best threshold distance D = 400Km.

The decision rule to build extra modular plants at any demand site was:

- IF "*unmet demand (i.e., the difference between the observed demand and the current capacity at the site) reaches Z% of the modular capacity*",
- THEN "*deploy extra modular capacity*",
- ELSE "*do nothing*".

Further enumeration found the optimal Z = 50%.

Figure 4.6 and Table 4.4 show the additional advantages of the flexibility to locate capacity away from the main site. As must be expected, looser constraints on system design increase maximum potential value. In this case, the ability to distribute capacity across the region (and thus to reduce logistical costs) further increases system ENPV, in this case from 20.69 to 23.29$M

This flexibility and added value, however, complicates the evaluation! In this case, the design with the flexibility to move capacity away from the main site does not dominate stochastically the design that fixes capacity there. Visually, the target curve for the design with the move option crosses the target curves for other designs. In this case, as often happens, designers may not want to choose the solution based upon a single metric such as ENPV. Indeed, no one metric is sufficient to characterize a general distribution. In this context we need to consider multiple criteria of evaluation.

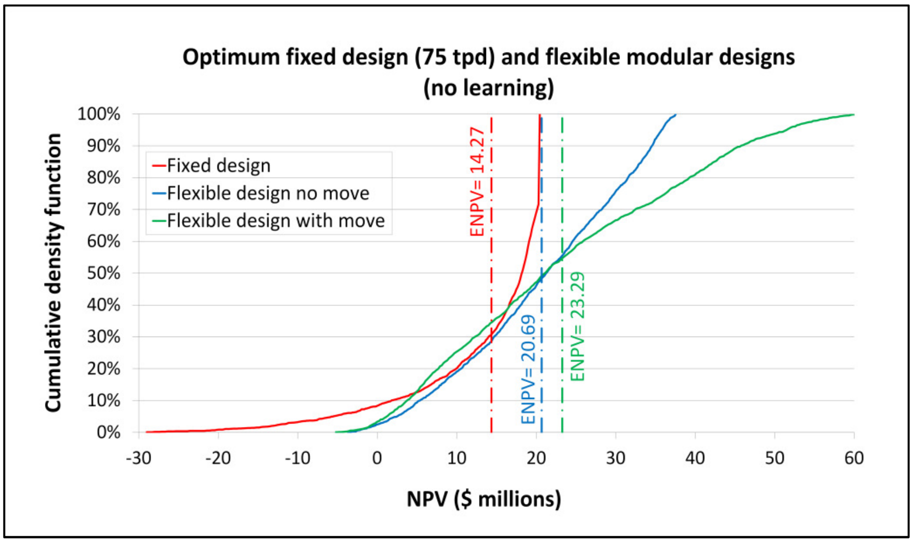


Figure 4.6: Optimum fixed design (α=0.95 → 75 tpd) and flexible modular designs

Table 4.4 provides a multi-criteria display of the performance of the fixed and flexible designs. It displays the average ENPV value and two measures of the extreme values. In terms of extremes, better practice generally focuses on some threshold level of cumulative performance rather than on the absolute maxima and minima values from the Monte Carlo simulation. This is because those highest and lowest values, being very rare, can vary considerably between simulations. The threshold values are quite stable, however. Standard thresholds of value are $VaR_{10\%}$, the 10% Value at Risk, the performance at the 10% cumulative probability or percentile, and $VaR_{10\%}$, the 90% Value at Gain. Table 4.4 compares the performance of the fixed and two flexible designs in these terms.

Table 4.4: Improvement of multi-criteria performance metrics due to flexibility with no learning

Criteria	Value ($ millions)			Improvement (%)	
	Optimum fixed design	Flexible no move	Flexible with move	Flexible no move	Flexible with move
ENPV	14.27	20.69	23.29	43.90%	61.97%
$VaR_{10\%}$	1.82	5.40	3.74	196.40%	105.59%
$VaG_{90\%}$	20.46	34.54	45.78	68.82%	123.79%

4.2.4.4 Effect of learning

Learning affects the value of flexibility. Because learning reduces the cost of modules as they get implemented, it favors their use and thus the usefulness and value of flexibility. Figure 4.7 shows how this occurs.

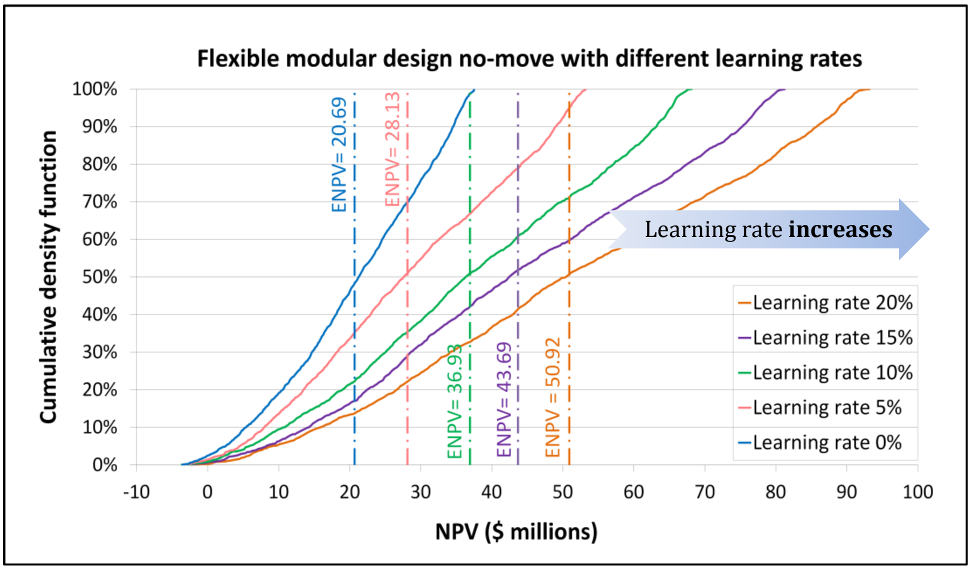


Figure 4.7: Flexible modular design with move in terms of different learning rates

It compares the target curves for the flexible design with move with no learning to those that have various levels of learning. The message is clear: the greater the potential for learning, the better the flexibility through the use of modules.

4.2.4.5 Multi-criteria decision-making

The best design alternative can be chosen based on many criteria. Some common economic metrics in project evaluation under uncertainty are shown in Table 4.5. The results correspond to the optimum fixed design with the economies of scale 0.95 and the flexible designs (with and without move) in terms of different learning rates. The aim is to choose a design based on the highest value for ENPV (or mean NPV), P10VaR and P90VaG, and smaller values for standard deviation of NPV distribution and initial Capex. Corresponding results in terms of other economies of scale factors are shown in the relevant tables in Appendix A.

Table 4.5: Multi-criteria decision-making table considering α=0.95, figures are in million dollars

α=0.95	on-shore LNG production system design												
	Fixed design	Flexible 1: no move			Flexible 2: with move			Best design			Value of flexibility		
		Learning rate			Learning rate			Learning rate			Learning rate		
Criteria	(75 tpd)	0%	10%	20%	0%	10%	20%	0%	10%	20%	0%	10%	20%
ENPV	14.27	20.69	36.93	50.92	**23.29**	**43.17**	**59.00**	Flexible 2	Flexible 2	Flexible 2	9.02	28.90	44.73
VaR	1.82	**5.40**	10.82	15.71	3.74	**11.06**	**16.47**	Flexible 1	Flexible 2	Flexible 2	3.58	9.24	14.65
VaG	20.46	34.54	63.17	85.65	**45.78**	**80.09**	**108.29**	Flexible 2	Flexible 2	Flexible 2	25.33	59.63	87.84
STD	**8.78**	10.57	18.91	25.30	15.79	25.31	33.35	Fixed	Fixed	Fixed	0.00	0.00	0.00
Capex	60.44	**27.50**	**27.50**	**27.50**	**27.5**	**27.5**	**27.5**	Flexible	Flexible	Flexible	N/A	N/A	N/A

4.2.4.1 Effect of economies of scale and learning rate on choice of flexible design

The proper role of sensitivity analysis for a design under uncertainty is to explore the robustness of the choice of design. Once we recognize that we cannot accurately predict future demands on a system, we have also acknowledged that we cannot define future performance precisely. The key question is: is the recommended design robust to variability in parameter estimation? This is the focus of the sensitivity analysis section. Since this section of the thesis proposes an approach to improved design, rather than a specific solution to a particular issue, the following paragraphs focus on illustrating the approach to sensitivity analysis for flexibility in design. They do not try to justify the details of the particular design that emerged from the case study analysis, which depended on the specific assumptions deemed appropriate by a company at a given moment. The case study is used to illustrate the effects of important parameters and tradeoffs.

As the analysis stresses, the discount rate and intensities of economies of scale and learning rate have an important effect on the desirability of flexible designs. In the practical context of this demonstration case, we could reasonably assume that the proposed contractor knew its acceptable discount rate, so the effect of this parameter was not investigated. Thus one focus of the sensitivity analysis is on the joint effect of the economies of scale and learning rate factors. Although experienced designers in a particular field can reasonably estimate these factors, they cannot know them unambiguously.

The sensitivity analysis explored the joint effect of various economies of scale and learning rate by repeating the analysis for combinations of these parameters. Figure 4.8 displays the results. It brings out two important results:

- As expected, lower economies of scale and greater learning rates increase the value of flexibility. Expressed another way, high economies of scale favor larger fixed designs.
- In this example case, the flexible design strategy is valuable for all but the most extreme cases, that is, where the economies of scale are particularly high and there is no learning. For even modest learning rates and economies of scale, the flexible modular design is valuable overall. One

may thus conclude that, in the demonstration case, the modular flexible design is robust over a wide range against variations in these parameters.

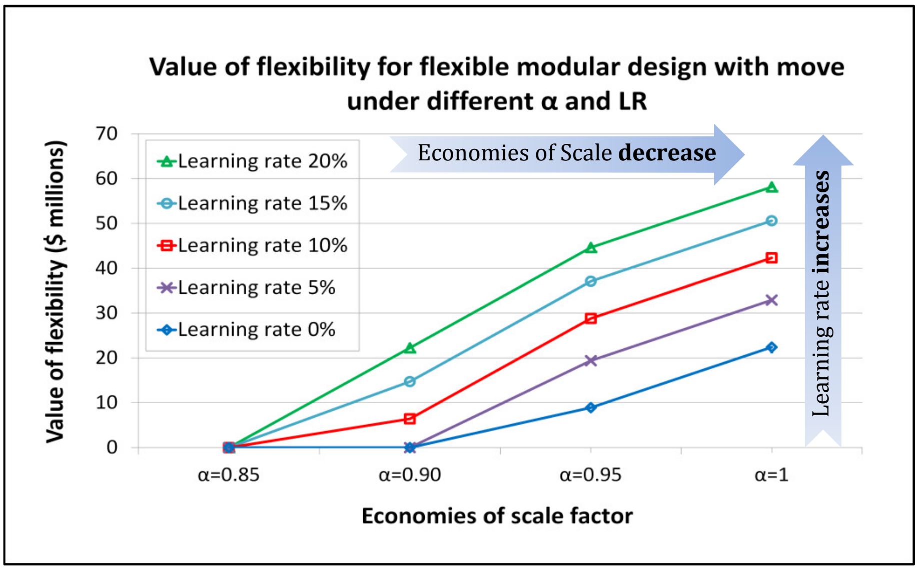


Figure 4.8: Value of flexibility with different economies of scale and learning rates

4.3 Phase 2: Screening

In this section, the screening phase of the proposed framework is applied to the first case study. In this phase, two screening approaches are considered: 1) A meta-model based screening approach and 2) A computing budget allocation based screening approach. It should be noted that there is a back and forth procedure between phase 2 and phase 3 of the proposed framework when the multi-objective computing budget allocation is applied. The procedures of the screening approaches are described in detail in the following subsections.

4.3.1 A meta-model based screening approach

In this section, a meta-model based screening approach is applied to the first case study, the centralized LNG production system. Table 4.6 shows the parameters used in the meta-model screening approach. The parameters were set based on trial and error and engineering practice. As can be seen, a Gaussian process was used in the correlation model and parameter theta was set between 0 and 2. This parameter is a correlation parameter and the DACE model is used to determine the optimum value for its optimal coefficient θ^* of the correlation function. In the correlation function, the correlation decreases with the Euclidian distance, $|d_j|$, and a larger value for θ_j leads to a faster decrease, see equation 3.2 in chapter 3.

Table 4.6: Parameters used in the meta-model based screening approach

Meta-model based screening parameters	Value
Expected improvement	4
Samples drawn from Latin Hypercube Design	15
Samples drawn from Central Composite Design	45
Correlation model	Gaussian
Theta band	[0 - 2]

Unlike the exhaustive enumeration where only Excel is used to explore the solution space, this meta-model approach builds upon the computational power of both MATLAB and Excel. Figure 4.9 shows the Microsoft Excel and MATLAB interfaces connected via spreadsheet link EX® in the meta-model screening approach. Essentially, in the MATLAB workspace, a DACE model was used to create a Kriging response surface, and the optimization Toolbox was used to optimize the meta-model surface.

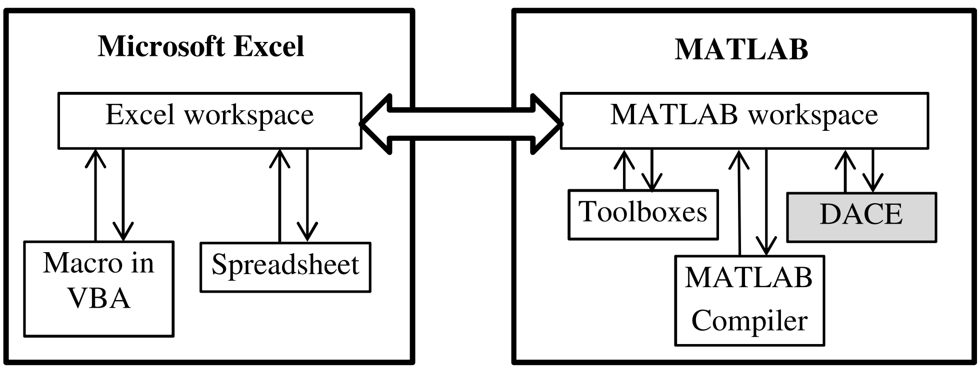


Figure 4.9: Microsoft Excel and MATLAB interaction via spreadsheet link EX® in the meta-model screening approach

Obtaining the final response surface of each objective requires an iterative procedure. Table 4.7 shows the procedure. The sample programming code for the one-site capacity expansion problem demonstrated in section 3.4.1 is provided in Appendix H.

Table 4.7: Procedure of meta-model screening approach

Set input parameters
Response surface for each objective function, ENPV or Standard deviation
– Step 1 Conduct initial design of experiment (i.e. "space-filling" using Latin Hypercube Sampling and Central Composite Design) in MATLAB
– Step 2 Conduct initial simulation using Monte Carlo Simulation in Excel at the points suggested in the previous step.
– Step 3 Fit the parameters of a DACE model using maximum likelihood estimation and build Kriging meta-model.
Once the initial DACE surface is fit and any transformation made, the iterative procedure starts.
– Step 4): The expected improvement function is maximized using MATLAB optimization toolbox
– Step 5): Is the maximum value of the expected improvement (EI) function is less than the EI threshold value?
If Yes): Global optimum is expected we stop. Otherwise
If No): Sampling of the design space including design variables and decision rules is conducted where expected improvement is maximized, run simulation in Excel and re-estimate the DACE parameters in MATLAB
– Step 6) Iterate until stopping criteria at step 4 is met.
Return Kriging surface, ENPV or standard deviation
Enumerate all flexible designs in objective function space

Using this approach, first a few samples are drawn, using a Central Composite Design (CCD) and Latin Hypercube sampling (LHS), from the solution space of feasible flexible designs. Essentially, initial samples are generated in MATLAB and simulations of corresponding flexible designs are performed in Excel. Then using the Gaussian model, a simulation surface is created for each objective (i.e., ENPV and Standard deviation). The surface is adaptively evolved until a stopping criterion is met.

4.3.2 A computing budget allocation based screening approach

In this section, a multi-objective computing budget allocation (MOCBA) screening model is applied to the analysis of case study 1, a centralized LNG production system design; indeed a bi-objective computing budget allocation (BOCBA) approach is used in this case study but let us use the general term "MOCBA" as represented in the proposed framework for consistency. Table 4.8 shows the parameters used in this approach. It should be noted that there is a back and forth procedure between phase 2 and 3. Using this approach, more budgets are allocated to designs that are close to the true Pareto fronts. The process is terminated when the maximum budget is exhausted or the design archive size reaches its minimum size. Eventually a preliminary true Pareto front is found and further analysis using large number of scenarios (i.e. with 2,000 demand scenarios) is conducted to find true Pareto fronts in phase 3.

Table 4.8: Parameters used in computing budget allocation screening model

MOCBA parameters	**Value**
Initial Budget Rate	5%
Incremental Budget Rate	1.4
Archive keep rate	50%
Minimum archive size	100
Allocation factor	1.2

Like the meta-model based screening approach, this approach also benefits from the computational power of both Excel and MATLAB. Figure 4.10 shows the interface between Microsoft Excel and MATLAB via spreadsheet link EX® in the computing budget allocation approach. Using the MATLAB workspace, Pareto dominance rule and allocation schema were applied in the MOCBA procedure.

To give an example how the procedure works, let us assume the maximum simulation budget is equal to 300 simulation evaluations. Given initial budget rate is 5%, see Table 4.8, initial simulation budget is 300×0.05=15. Thus all 5,940 flexible designs are first evaluated using 15 simulation evaluations. Subsequently, more budget allocations are performed systematically by following the pseudocode shown in Table 4.9.

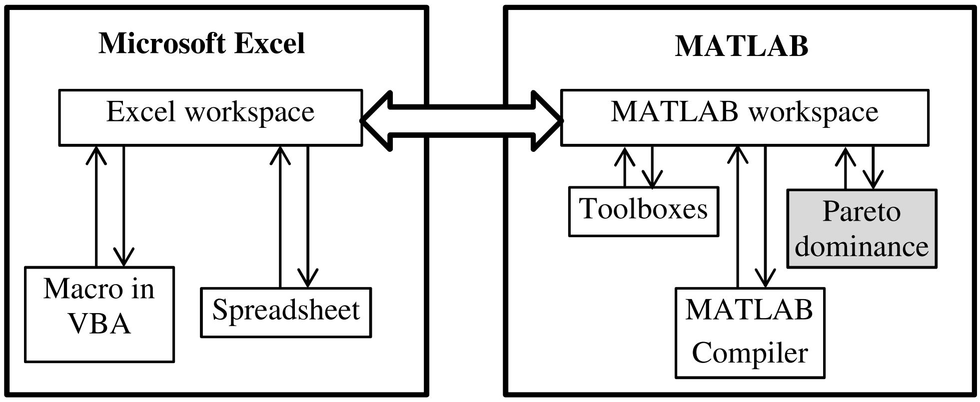


Figure 4.10: Microsoft Excel and MATLAB interface via spreadsheet link EX® in the computing budget allocation screening approach

Table 4.9: Pseudocode of a multi-objective computing budget allocation

```
Construct initial design archive
Allocate initial budget→MATLAB
Run flexibility simulation→Excel
Conduct Pareto dominance analysis→MATLAB
Sort designs with different frontiers→MATLAB
    Do while (Min_archive size ≤ archive size) or (each design budget ≤ Max_budget)
            Update design archive→MATLAB
            Update simulation replication budget → MATLAB
            Allocate new budgets to designs in different frontiers
            Run flexibility simulation→Excel
            Conduct Pareto dominance analysis→MATLAB
            Sort designs with different frontiers→MATLAB
    End while
Return Pareto front
Conduct analysis with 2000 demand scenarios
Return true Pareto front
```

Table 4.10 shows a schematic example of computing budget allocation. As can be seen, in this example 300 simulation evaluations was allocated to design number 6, and the algorithm was terminated. Following the computing budget allocation approach, more budgets are allocated to promising designs (i.e., near the true Pareto front) rather than less important flexible designs.

Table 4.10: A schematic example of computing budget allocation

Simulation evaluation	Flexible designs											
	1	2	3	4	5	6	7	...	5936	5937	5938	5939	5940
15													
16													
17													
18													
19													
⋮													
300													

Figure 4.11 shows the evolution of a design archive in MOCBA in an experiment with maximum budget 300 demand scenarios. In Figure 4.11 (a) all 5,940 flexible designs are first evaluated with 15 simulation evaluations in Excel.

As mentioned earlier, this number is the result of the initial budget rate times the maximum budget, 5%×300=15. Then all the 5,940 flexible designs are ranked in terms of Pareto dominance aiming at allocating more simulation budgets to designs near the Pareto front. The algorithm iteratively continues until the stopping criteria are met, $Min_{archive\ size}$ ≤ archive size or each design budget ≤ Max_{budget}. The design archive is updated by keeping only 50% of the top flexible designs sorted according to Pareto dominance. Subsequently, using the procedure explained in the methodology section, new simulation budgets are allocated to different layers of Pareto fronts. In the updated flexible design archive, new allocated simulations are conducted in Excel and simulation responses in terms of ENPV and Standard deviation are updated accordingly. Then the current design archive with updated objective function values is transferred to MATLAB to be sorted according to Pareto dominance. Again the size of the design archive is updated based on the design archive keep rate and new simulation budgets are allocated to the updated flexible designs. This procedure continues until the stopping criteria are satisfied. Figure 4.11 (f) is the last design archive and its Pareto front is further analyzed under large number of scenarios in the next phase.

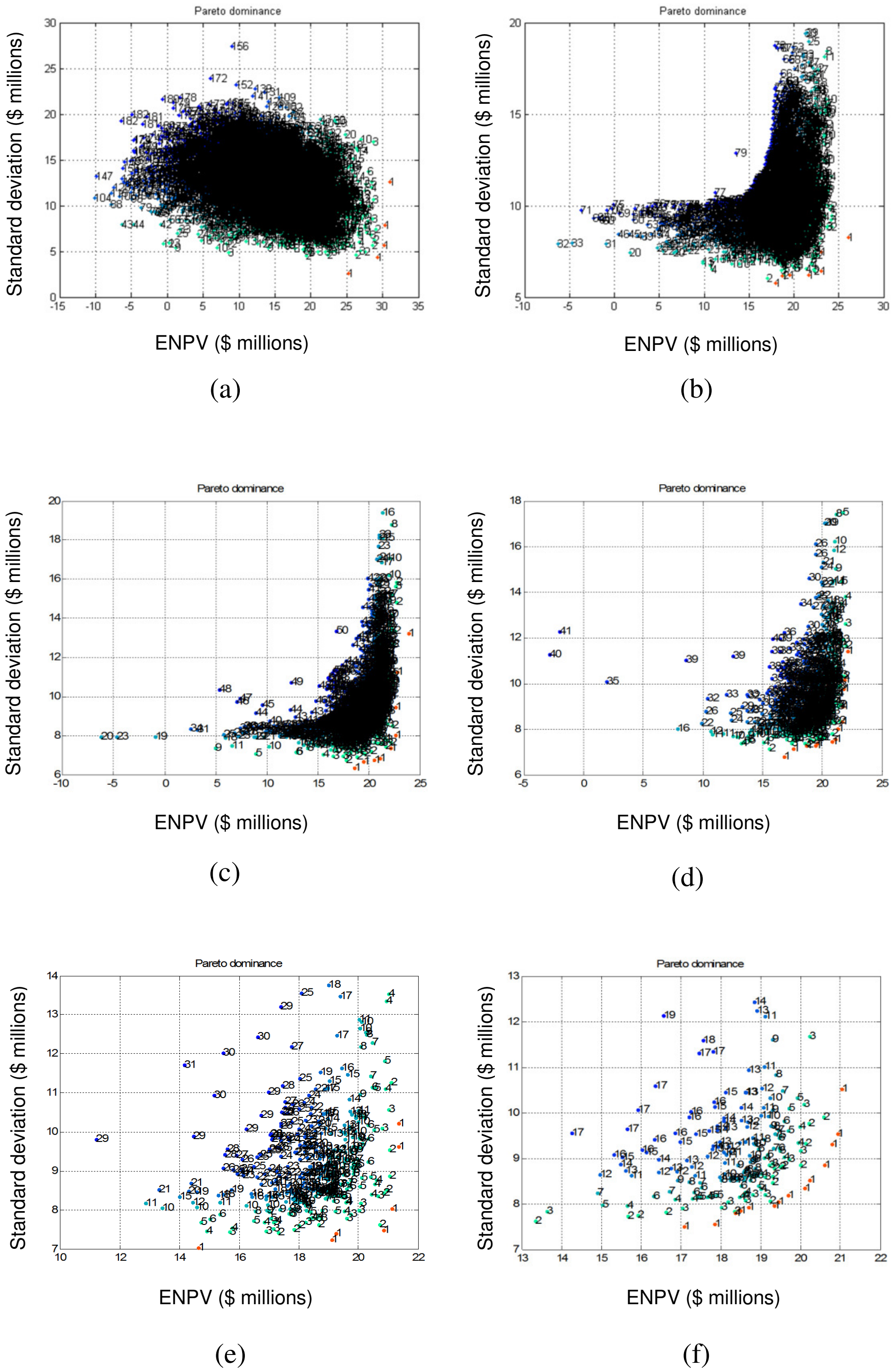


Figure 4.11: Evolution of a design archive in the MOCBA, in an experiment with 300 demand scenarios, from (a) to (f)

4.4 Phase 3: Multi-criteria decision-making analysis

In this section, dominant flexible designs from the screening phase conducted in different computer experiments are further analyzed under a large number of scenarios. Subsequently, true Pareto flexible design solutions are obtained and the hyper-area is calculated. Once the true Pareto fronts are obtained using a large number of demand scenarios, an example preferred trade-off flexible design solution is chosen based on decision makers' preferences. In this section, a weighted-sum approach is applied to choose the preferred dominant flexible design among other flexible designs in the true Pareto set, as a demonstration of how to use the framework. The recommended design solution(s) would then be used as input for a higher-fidelity modeling analysis – if needed.

4.4.1 A meta-model based screening approach

Given there are more than two variables and decision rules in the design vector, response surfaces cannot be demonstrated in the figures. Once the response surfaces are created given the intended objectives, an enumeration is done using these inexpensive meta-models. Figure 4.12 displays dominant flexible designs obtained using the multi-objective function space through inexpensive meta-models, here using objectives ENPV and standard deviation.

Then, a preliminary Pareto front is found and further analysis using large number of scenarios (i.e., with 2000 demand scenarios) is conducted to find the true Pareto fronts. For hyper-volume, an arbitrary reference point ENPV=\$0M and Standard deviation=\$20M are assumed.

To illustrate how a decision-maker would use the above analysis to identify preferred flexible design alternative(s), let's assume that the decision-maker's preference is to put 60% of the weight on maximizing the ENPV, and 40% on minimizing the standard deviation (as a proxy for the risk level). The preferred trade-off flexible design with ENPV=$20.06M and standard deviation=$11.53M is then selected. The preferred trade-off flexible design is shown in a circle in Figure 4.12.

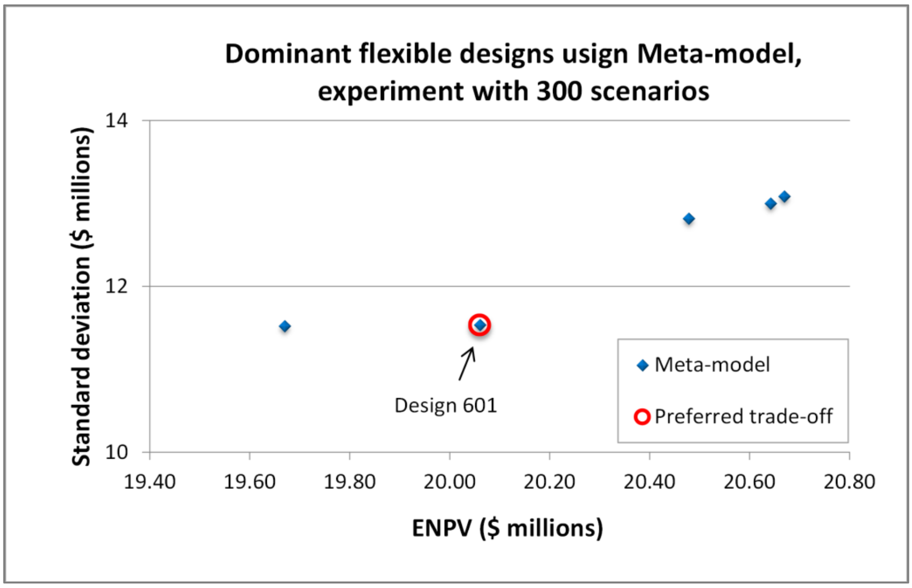


Figure 4.12: Dominant flexible designs obtained using meta-model with an experiment with 300 scenarios

The corresponding design vector of the preferred trade-off flexible design is detailed in Table 4.11. The extension form for all acronyms used in this table is shown in Table 4.13. This design vector would then be selected from the screening process, and further used for a higher fidelity design analysis.

Table 4.11: Design vector of the preferred flexible design using MM

Design number	InCap	MDC	MsiteTV	MoveTV	Cover	DsiteTV
601	0	25	60%	300%	300	60%

The solution suggests that the system operator should not deploy initial capacity and should delay the capacity deployment until the aggregate demand observed at the main production site reaches 60% of 25 tpd modular design capacity. The 25 tpd modular design capacity should be used for capacity expansion. The system operator should expand the capacity at the main production site every time aggregate demand reaches 60% of the 25 tpd modular capacity. The demand sites that are located 300KM far away from the main production site should be considered for the first LNG production facility deployment when the observed demand in these sites reaches 300% of 25 tpd modular capacity. The system operator should also expand the capacity of production facilities at demand sites every time demand reaches 60% of the 25 tpd modular capacity.

Post-optimality sensitivity analysis

A post-optimality sensitivity analysis is performed on the flexible solution found at the end of phase 3 using the meta-model screening approach. The optimum flexible solution is analyzed to see how the performance changes by varying the discount rate, volatility factor and other parameters. The parameters to vary are: 1) discount rate, 2) learning rate and 3) volatility of the sharpness parameter. The effects of changes in these parameters on the value of flexibility are shown in a Tornado diagram in Figure 4.13.

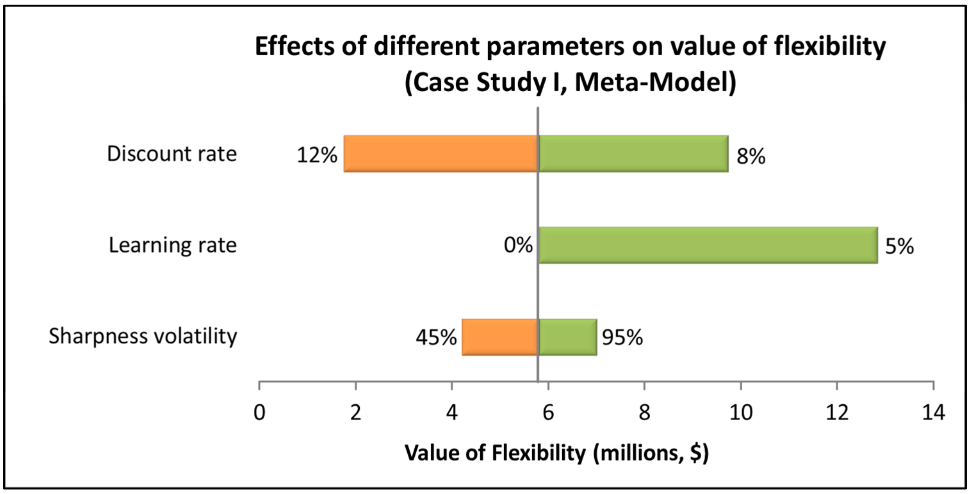


Figure 4.13: Post-optimality sensitivity analysis for the flexible design solution obtained using the meta-model screening approach, Case study I.

The details of the post-optimality sensitivity analysis are provided in Appendix D. Results show that the discount rate, learning rate and sharpness volatility have the most to the least influences on the value of flexibility respectively. The effects of changes in these parameters are analyzed here.

The Tornado diagram shows that the discount rate has the most influence on the value of flexibility. In capital-intensive and long-term project evaluations, when the discount rate increases (i.e. 12%) the present value of the project design decreases because cash flows of future revenues are discounted back at a higher rate to the present time leading to a lower design value. On the other hand, when discount rate decreases (i.e. 8%) cash flows of future revenues are discounted back at a lower rate to the present time leading to a higher design value. The results show that when the discount rate increases the value of both flexible and fixed designs decreases leading to a lower value of flexibility compared to the analysis under the base discount rate (i.e. 10%). On the other hand, when the discount rate decreases the value of both flexible and fixed designs improves, leading to a higher value of flexibility. In this case study, the flexible design is initially built at the main production site to meet the LNG demand at all the demand points. To fulfill the aggregate demand by LNG produced at the main production site, there is a high chance, depending on a given possible scenario, that a considerable number of modular capacity is required in the early years of the project lifetime. For instance, we may need to deploy modular capacity in each year for 6 consecutive years to fulfil the aggregate demand ramping up at the early years. As a result, we may not be able to defer the capacity deployment as much as we can in the case of a decentralized flexible design. In other words, the flexible centralized design, case study I, can be considered less modular than the flexible decentralized design, case study II.

The Tornado diagram shows the sensitivity of the value of flexibility subject to changes in learning rate. The changes in learning rate influences the flexible design value and consequently have effects on the value of flexibility. The results suggest that when learning rate increases (i.e. 5% instead of 0%), the cost of deploying extra modular capacity decreases leading to a higher flexible design value and consequently higher value of flexibility. On the other hand, when there is a low learning rate in the flexible system design that uses modular production facility, the design does not take advantage of cheaper extra modular capacity and thus it leads to a lower flexible design value and consequently lower value of flexibility.

As the sharpness parameter has been recognized as the key demand parameter, it is worthwhile to investigate the effect of different volatilities of this parameter on the designs value and, subsequently, on the value of flexibility. To do so, different values of the sharpness volatility at each geographical site are considered. The values 45%, 70% and 95% correspond to the low, the base and the high for the volatility of the sharpness parameter. When the volatility of the sharpness parameter decreases, the optimum fixed design and the flexible design provide better ENPV while more improvement is observed especially in the fixed design than the flexible one and consequently the value of flexibility is less than one under base sharpness volatility assumption. On the other hand, when the volatility of the sharpness parameter increases, the optimum fixed design and the flexible design provide less ENPV while more decrease is observed especially in the fixed design than the flexible one and consequently the value of flexibility is more than under the base assumption for sharpness volatility.

The results suggest that when sharpness volatility increases, so does the value of flexibility. In other words, the more uncertainty there is, the more valuable flexibility is. The reason for this improvement is that the flexible design provides a better value than the fixed design under highly volatile market. When demand is strong, while the fixed design cannot accommodate extra capacity due to its rigid capacity, the flexible design can acquire more capacity as needed, to meet the stronger-than-expected demand, leading to relatively more improvement in ENPV. On the other hand, when demand is weak, flexible design is less affected because of the smaller capital investment in unfavorable markets whereas the fixed design incurs huge loss due to the relatively higher upfront investment and higher unused capacity over its lifetime. This improvement in the value of flexibility indicate the ability of flexible design to better capture the upside opportunity of strong demand and more adequately prevent the potential loss of weak demand compared to fixed design.

4.4.2 A computing budget allocation based screening approach

Once the computing budget allocation procedure is terminated, a set of Pareto front is returned. Once these flexible designs are obtained, further analysis under a large sample of demand scenarios and Pareto dominance relation are performed to find the true Pareto front in different runs of the computer experiments. Figure 4.14 shows dominant flexible designs obtained using MOCBA with an experiment with 300 scenarios.

Based on the decision makers' preferences, it is assumed again that the weight for ENPV is 60% and 40% for Standard deviation. As a result, the preferred trade-off flexible design with ENPV=$18.93M and Standard deviation=$10.83M is chosen. The preferred trade-off flexible design is shown in a circle in Figure 4.14.

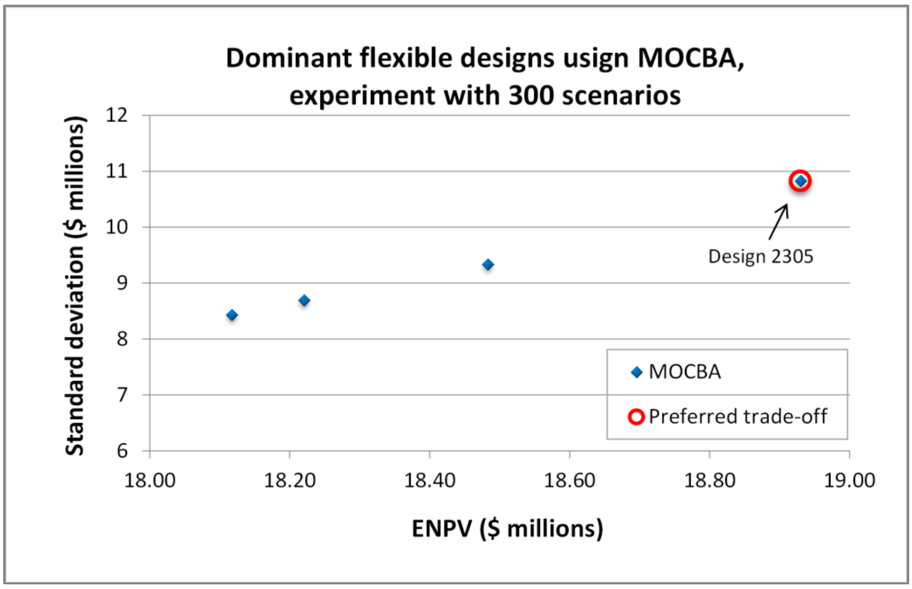


Figure 4.14: Dominant flexible designs obtained using MOCBA with an experiment with 300 scenarios

The corresponding design vector of the preferred trade-off flexible design is shown in Table 4.12. The extension form for all acronyms used in this table is shown in Table 4.13

Table 4.12: Design vector of the preferred trade-off flexible design using MOCBA

Design number	InCap	MDC	MsiteTV	MoveTV	Cover	DsiteTV
2305	25	25	20%	300%	400	50%

The solution suggests that the system operator should consider modular design 25 tpd for capacity expansion and should deploy the initial capacity 25 tpd at the main production site. The system operator should expand the capacity at the main production site every time the aggregate demand reaches 20% of the 25 tpd modular capacity. The demand sites that are located 400KM far away from the main production site should be considered for the first LNG production facility deployment when the observed demand in these sites reaches 300% of the 25 tpd modular capacity. The system operator should expand the capacity of production facilities at demand sites every time demand reaches 50% of the installed 25 tpd modular capacity.

Post-optimality sensitivity analysis

The post-optimality results for the solution obtained from MOCBA are shown in Figure 4.15. The details of the post-optimality sensitivity analysis are provided in Appendix D. Results show that the discount rate, learning rate and sharpness volatility have the most to the least influences on the value of flexibility respectively. Due to similar explanations as provided in Section 4.4.1, the results show that as the discount rate increases (decreases), the value of flexibility decreases (increases). Furthermore, flexibility becomes more valuable when the learning rate increases due to further exploitation of the modularity. Also, when more (less) uncertainty is considered in the simulation process via variations in the sharpness parameter, the value of flexibility increases (decreases).

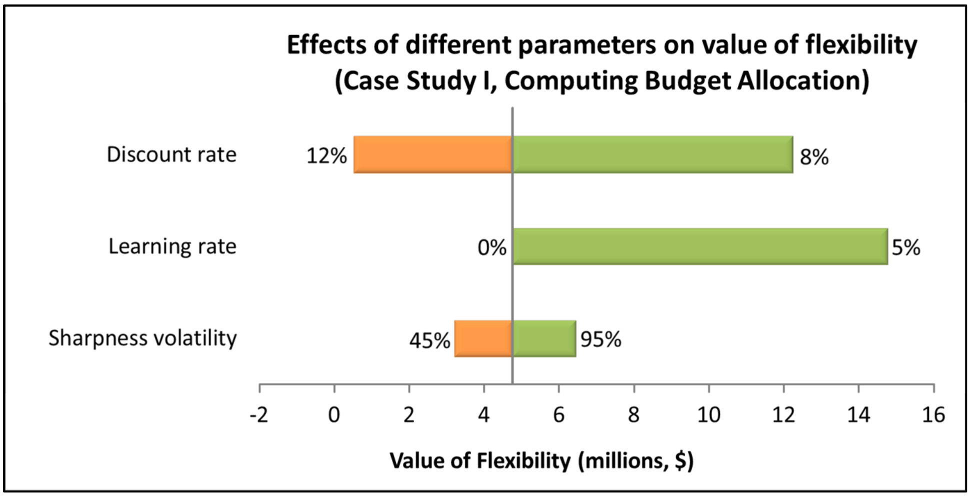


Figure 4.15: Post-optimality sensitivity analysis for the flexible design solution obtained using the computing budget allocation screening approach, Case study I.

4.5 Exhaustive enumeration

In this section, a comprehensive enumeration technique was used to explore the flexible design space aiming at finding promising flexible design solutions. Table 4.13 shows the characterization of the design space for flexibility analysis.

Table 4.13: Characterization of the design space for flexibility analysis

Option	Design variables	Units	Step Size	Values	Steps
No Move only	Initial capacity (InCap)	Tpd	25	0, 25, 50	3
	Modular design capacity (MDC)	Tpd	25	25, 50	2
	Capacity expansion threshold, at main production site (MsiteTV)	% of modular design	20	0 to 100	6
Additions with Move	Moving value threshold (MoveTV)	% of modular design	50	100 to 300	5
	Coverage distance threshold (Cover)	Km	100	200, 300, 400	3
	Capacity expansion threshold, at demand site (DsiteTV)	% of modular design	10	0 to 100	11

The second column of the Table describes the elements of the flexible design vectors comprised of both design variables and decision rules. Design variables describe the system architecture, while decision rules describe managerial flexible design solutions. The third and fourth columns show the values investigated for each vector element and the incremental step size, which determines the precision level of the simulation model in the enumeration process. Looking at the number of possible values in column five, the total number of possible flexible design configuration with move option is 5,940, while the design space for the no-move flexible design is much smaller at 36. Thus, it is mainly aimed to explore the design space of the flexible design with move option as it can be computationally expensive if a high-fidelity simulation model is used.

Table 4.14 shows design vector of flexible designs with move option in a horizontal way. The extension form for all acronyms used in this table is shown in Table 4.13. In this case study n = 5,940 flexible designs are analyzed.

Figure 4.16 illustrates the interface between Microsoft Excel spreadsheets and macros developed in VBA in an exhaustive enumeration approach. Essentially, macros control simulation models and set up different flexible design vectors in an organized way.

Table 4.14: Different design vectors of flexible designs with move options

Flexible design	Elements of flexible design vectors					
1	$InCap_1$	MDC_1	$MsiteTV_1$	$MoveTV_1$	$Cover_1$	$DsiteTV_1$
2	$InCap_2$	MDC_2	$MsiteTV_2$	$MoveTV_2$	$Cover_2$	$DsiteTV_2$
3	$InCap_3$	MDC_3	$MsiteTV_3$	$MoveTV_3$	$Cover_3$	$DsiteTV_3$
⋮	⋮	⋮	⋮	⋮	⋮	⋮
n=5,940	$InCap_n$	MDC_n	$MsiteTV_n$	$MoveTV_n$	$Cover_n$	$DsiteTV_n$

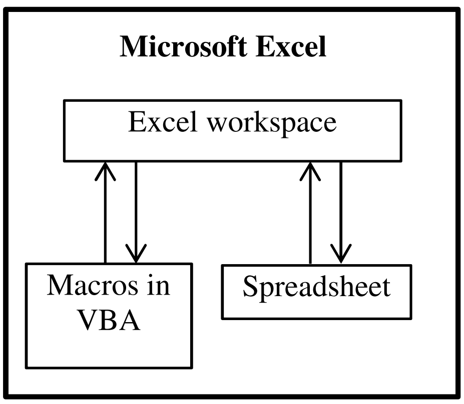


Figure 4.16: Interface between Microsoft Excel spreadsheet and macros developed using VBA in an exhaustive enumeration approach

To better understand how the exhaustive enumeration is conducted, the pseudocode is provided in Table 4.15.

Table 4.15: Pseudocode for Exhaustive Enumeration (EE) approach

```
Set input parameters
For InCap = LB_InCap to UB_InCap Step_InCap
  For MDC = LB_MDC to UB_MDC Step_MDC
    For MsiteTV = LB_MsiteTV to UB_MsiteTV Step_MsiteTV
      For MoveTV = LB_MoveTV to UB_MoveTV Step_MoveTV
        For Cover = LB_Cover to UB_Cover Step_Cover
          For DsiteTV = LB_DsiteTV to UB_DsiteTV Step_DsiteTV
                   Synthesize a flexible design vector
                         For i=1 to number of simulation
                             Application.calculate ← Generate a new scenario
                             Calculate NPV
                         Next
                   Calculate ENPV and Standard deviation of the design
          Next
        Next
      Next
    Next
  Next
Next
Return all design vectors with ENPV and standard deviation
Enumerate all flexible designs in objective function space
```

Exploring exhaustively the solution space of flexible designs with move, which includes 5,940 designs, can be computationally expensive. Different experiments are conducted to show the performance of exhaustive enumeration in terms of different simulation evaluation numbers. The results of different experiments will be discussed in the following results and discussion section 4.6.

Figure 4.17 shows the true Pareto fronts (i.e., with 2,000 demand scenarios) of flexible designs with move and with no move, as well as the optimum fixed design.

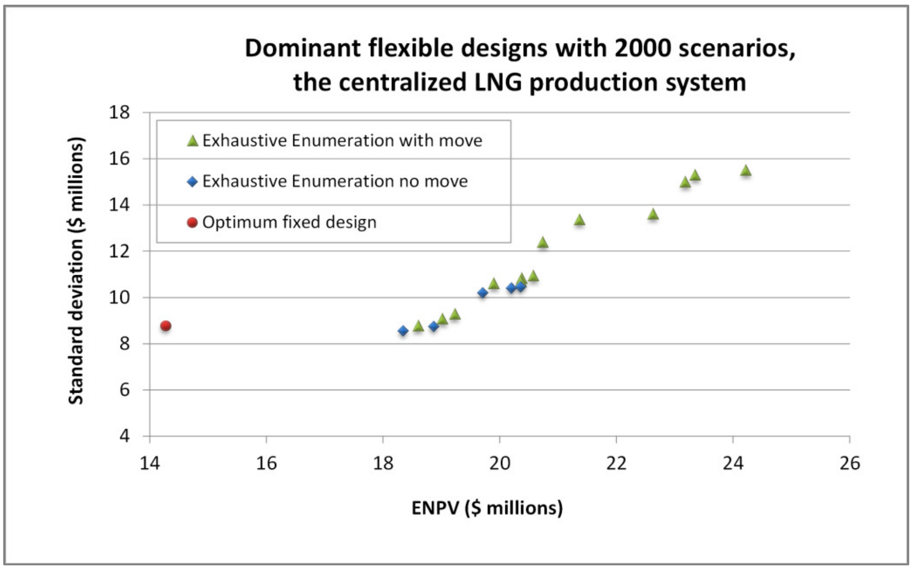


Figure 4.17: Dominant flexible designs with large number of scenarios (i.e., 2,000 scenarios)

Like screening approaches, exhaustive enumeration is conducted in different computer experiments. Once the enumeration in terms of each experiment is conducted, candidate flexible designs in the Pareto front are obtained. The Pareto front will be further analyzed using a large number of sample demand scenarios (i.e., 2,000) and the Pareto dominance rule will be used to obtain the true Pareto front. The true Pareto front flexible solutions will be further analyzed in the Pareto post processing phase.

To evaluate the quality of the Pareto front, the hyper-area criterion is considered. Assuming for illustration purposes again weights for ENPV of 60% and weight for Standard deviation of 40%, a trade-off flexible solution is selected with ENPV=$24.22M and standard deviation=$15.51M as shown in Figure 4.18. The corresponding design vector is shown in Table 4.16.

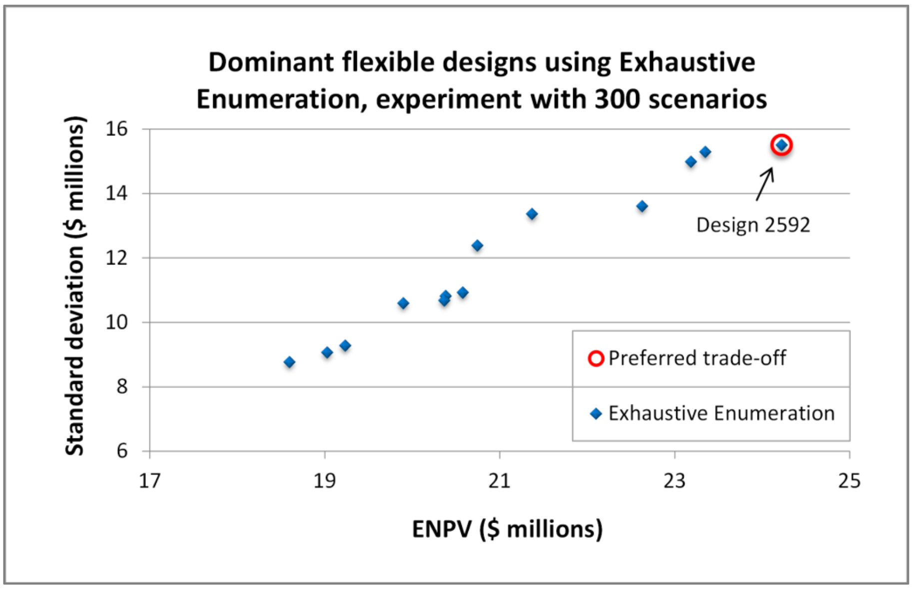


Figure 4.18: Preferred trade-off flexible design with move using exhaustive enumeration

Table 4.16: Design vector of the preferred trade-off flexible design using exhaustive enumeration

Design number	InCap	MDC	MsiteTV	MoveTV	Cover	DsiteTV
2592	25	25	60%	100%	400	60%

The solution suggests that the system operator should consider modular design 25 tpd for capacity expansion in the system and should deploy the initial capacity 25 tpd at the main production site. The system operator should expand the capacity at the main production site every time the aggregate demand reaches 60% of the 25 tpd modular capacity. The demand sites that are located 400KM far away from the main production site should be considered for the first LNG production facility deployment when the observed demand in these reaches 100% of the 25 tpd modular capacity. The system operator also should expand the capacity of production facilities at demand sites every time demand reaches 60% of the installed 25 tpd modular capacity.

Post-optimality sensitivity analysis

The post-optimality results for the solution obtained from Exhaustive Enumeration are shown in Figure 4.19. The details of the post-optimality sensitivity analysis are provided in Appendix D. Results show that the discount rate, learning rate and sharpness volatility have the most to the least influences on the value of flexibility respectively. Due to similar explanations as provided in Section 4.4.1, the results show that as the discount rate increases (decreases), the value of flexibility decreases (increases). Furthermore, flexibility becomes more valuable when the learning rate increases due to further exploitation of the modularity. Also, when more (less) uncertainty is considered in the simulation process via variations in the sharpness parameter, the value of flexibility increases (decreases).

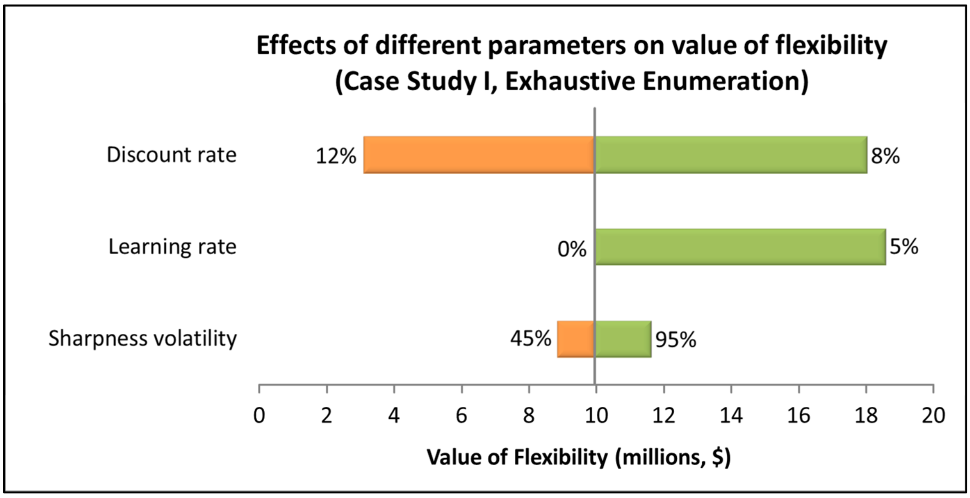


Figure 4.19: Post-optimality sensitivity analysis for the flexible design solution obtained using the exhaustive enumeration approach, Case study I.

4.6 Results and discussion

In this section, results obtained from the proposed screening framework are validated by comparing them with the results from the exhaustive enumeration in different computer experiments. In each computer experiment, Pareto quality and the number of simulation evaluation for all approaches are investigated.

Figure 4.20 shows dominant flexible designs of case study 1 using different screening approaches and exhaustive enumeration in an experiment with 300 scenarios. Results obtained from other experiments are provided in Appendix B. As can be seen, Pareto designs using exhaustive enumeration have more spread as compared to the meta-model and computing budget allocation based methods, because they explore the design space fully. As a result, it provides more dominant flexible solutions so that decision makers have more alternatives to choose from. It, however, requires more simulation evaluation numbers and consequently more computational resources. On the other hand, the meta-model (MM) and MOCBA approaches provide good-enough solutions with reasonable Pareto quality gap and simulation replication number.

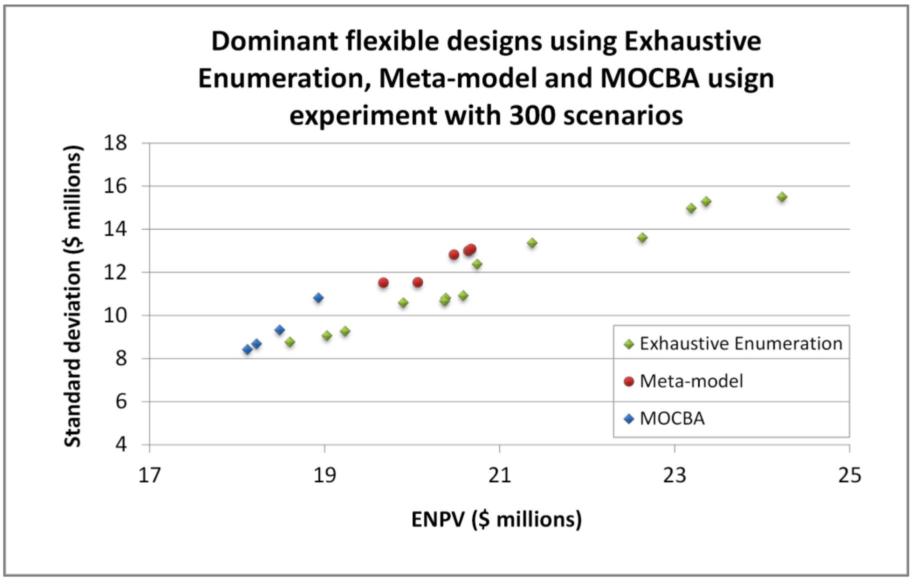


Figure 4.20: Dominant flexible designs using different approaches Meta-model based screening model (MM), Multi- Objective Computing Budget Allocation (MOCBA); Exhaustive Enumeration (EE)

Table 4.17 shows the comparison between meta-model (MM), multi-objective computing budget allocation (MOCBA), and exhaustive enumeration (EE) in terms of different performance metrics, the Pareto quality and the number of simulation evaluations, and computer experiments. The larger the hyper-area the better the Pareto quality and the smaller number of simulation evaluation the more efficient the screening approach.

Table 4.17: Comparison between MM, MOCBA, and EE in terms of different performance metrics, Pareto quality and number of simulation evaluation

Experiments	**Pareto quality (hyper-area)**			**Number of simulation evaluation**		
	MM	MOCBA	EE	MM	MOCBA	EE
50	182	226	237	3,000	27,450	297,000
100	182	209	237	6,000	62,264	594,000
150	184	227	246	9,000	79,396	891,000
200	187	233	239	12,000	104,881	1,188,000
250	183	218	244	15,000	130,162	1,485,000
300	174	218	249	18,000	162,019	1,782,000

The hyper-volume is dominated by the solutions in the true Pareto set (i.e., the Pareto set obtained under analysis using large number of scenarios, here 2000 demand scenarios) and closed by an arbitrary worst case point. This criterion accounts for dominance, spread and density of the Pareto designs simultaneously (Zitzler, Thiele et al. 2003; Bradstreet, While et al. 2008; Nebro, Durillo et al. 2008). For consistency, an arbitrarily worst case scenario is chosen with ENPV=\$0M and Standard deviation=\$20M for calculation of hyper-area in all the experiments.

Let us compare the results in terms of different computer experiments. It should be emphasized that although different number of scenarios are considered in different experiments (i.e., 50 to 300 simulation evaluations), final Pareto fronts in Phase 3 are constructed under large number of sample scenarios (i.e., 2000 demand scenarios).

As the number of simulations in different experiments increases, the number of simulation evaluations increases proportionally. By increasing the number of simulations in different experiments, however, the hyper-area does not strictly increase. This is because of the fact that after running each experiment (i.e., from 50 to 300 scenarios), analysis using a large number of sample scenarios (i.e., with 2000 demand scenarios) is conducted in phase 3. As a result, Pareto solutions in terms of different computer experiments tend to converge to the true Pareto front. Consequently, the hyper-areas calculated in terms of different computer experiments tend to converge to the hyper-area of the true Pareto front. Moreover, the stochastic nature of the developed simulation models can be a part of the reasons.

Now let us compare the results in terms of different screening approaches as well as the exhaustive enumeration method. For Pareto quality, multi-objective computing budget allocation (MOCBA) systematically offers better hyper-areas as compared to meta-model based screening approach (MM). This is because of the lack of appropriate sampling of flexible designs in the latter case with respect to different objectives. As can be seen, the quality of the Pareto front is not so good because only a few dominant flexible designs are found. As a result it leads to a lower hyper-area value. This is also due to the fact that response surfaces for ENPV and standard deviation are built separately. As a result, more samples were drawn in the proximity of the optimum (i.e., minimum of standard deviation and maximum of ENPV) area of the corresponding meta-model surfaces.

One way to overcome this issue is to use a multi-objective version of the meta-modelling approach. On the other hand, the quality of the Pareto front resulting from the MOCBA approach is not much better than for the MM approach, as a trial and error approach was used to set the input parameters. The quality of the

Pareto front resulting from MOCBA can be improved if optimal simulation budget allocation schema is used in its procedure.

As expected, exhaustive enumeration offers the best Pareto quality among the three approaches. On the other hand, in terms of the number of simulation evaluation, the meta-model approach requires the least number of simulation evaluations. According to computer experiments, simulation runtime is roughly proportional to the number of simulation evaluations.

For clarification purpose, let us compare the results in terms of different screening approaches and the exhaustive enumeration with respect to a particular computer experiment. Considering the experiment with 50 sample scenarios, see the first row in Table 4.17, MM with hyper-are 182 and MOCBA with hyper-area 226 approaches provide dominant flexible design solutions with 23% (i.e., (237-182)/237×100) and 5% (i.e., (237-226)/237×100) Pareto quality gap (hyper-area) respectively as compared to exhaustive enumeration. Furthermore, MM and MOCBA approaches require only 1% (3,000/297,000) and 9% (27,450/297,000) of the number of simulation evaluations, respectively, required in the exhaustive enumeration approach. In sum, there is indeed a trade-off between these two screening approaches in terms of Pareto quality and the number of simulation evaluations.

Table 4.18 shows the comparison between MM, MOCBA, and EE in terms of computational runtime. All screening analyses were performed on a Windows 7 platform with 8 GB RAM and 3.3 GHz processing speed.

Assuming each simulation evaluation takes one second, computational runtime for all screening methods are calculated. As can be seen, by increasing the number of scenarios in the computer experiments the computational runtime proportionally increases. Exhaustive enumeration requires the most computational effort while the meta-model based screening method needs the least computational burden. In sum, decision makers based upon observations in Table 4.17 and Table 4.18 can choose which screening approach should be used subject to expected Pareto quality and available computational time and resources.

Table 4.18: Comparison between MM, MOCBA, and EE in terms of computational runtime

Experiments	**Computational runtime (hours)**		
	MM	MOCBA	EE
50	0.83	7.63	82.50
100	1.67	17.30	165.00
150	2.50	22.05	247.50
200	3.33	29.13	330.00
250	4.17	36.16	412.50
300	5.00	45.01	495.00

Table 4.19 summarizes the results for case study 1 when flexible design with move is investigated considering weights 60% for ENPV and 40% for standard deviation in an experiment with 300 scenarios. The value of flexibility for different screening approaches as well as the exhaustive enumeration is provided in Table 4.19.

Table 4.19: Summary of results for case study one, flexible design with move considering W1=60% and W2=40% in a computer experiment with 300 scenarios.

Criteria	**Exploration of flexible design space**		
	MM	MOCBA	EE
Design vector number	601	2305	2592
Value of flexibility ($M)	5.79	4.66	**9.95**
Runtime (hours)	**5.00**	45.01	495.00

The value of flexibility using MM is calculated as $ENPV_{MM} - ENPV_{Fixed}$ = \$20.06M − \$14.27M = \$5.79M, where $ENPV_{Fixed}$ is the ENPV of the benchmark fixed design in Phase 1. The value of flexibility using MOCBA approach is calculated as $ENPV_{MOCBA} - ENPV_{Fixed}$ = \$18.93M– \$14.27M = \$4.66M and the value of flexibility using EE approach is calculated as $ENPV_{EE} - ENPV_{Fixed}$ = \$24.22M– \$14.27M = \$9.95M.

As expected, EE recognizes the most value of flexibility, and is shown as a bold figure in the Table. It requires, however, 495 hours (~ 20 days) to fully enumerate the flexible design space with 300 scenarios. On the other hand, MM and MOCBA approaches provide good-enough flexible solutions within a more reasonable amount of time.

Figure 4.21 shows the cumulative density function of the preferred flexible designs resulted from the proposed screening framework, exhaustive enumeration and the fixed benchmark design. As can be seen, all flexible designs can reduce the downside risk and capture the upsides opportunities. Decision-makers can feed the design(s) to a higher-fidelity model to further investigate these flexible designs in a greater detail.

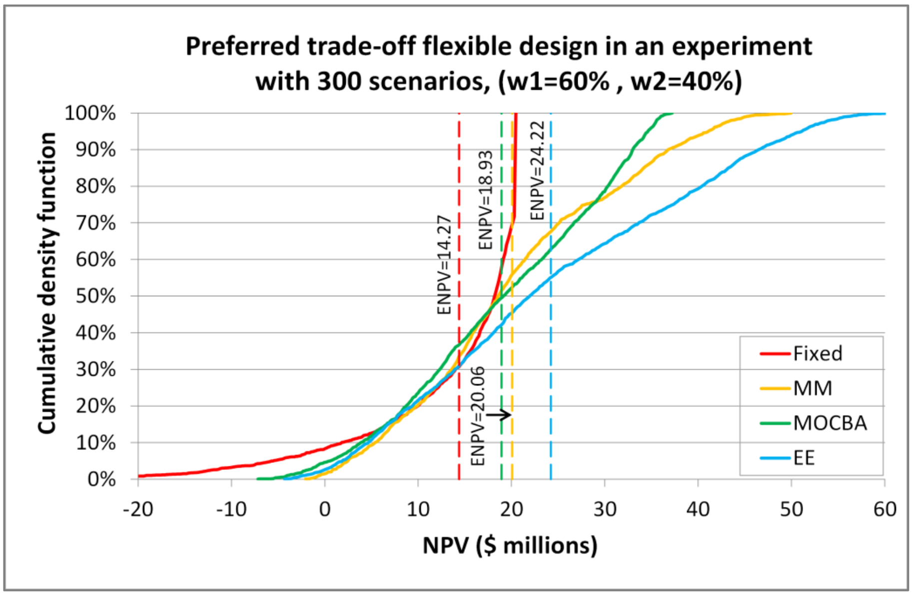


Figure 4.21: CDFs for preferred flexible designs for case study one in a computer experiment with 300 scenarios, (w1=60%, w2=40%)

4.7 Summary

In this chapter, case study one focusing on a centralized on-shore LNG production system design was analyzed. Using the three-step problem modeling methodology, the case study was modeled using Monte-Carlo simulation analysis for uncertainty and flexibility in Excel. Subsequently, to investigate the effect of problem modeling assumptions and input parameter settings, different sensitivity analyses were conducted. Then, meta-model based screening and computing budget allocation based screening model were used to analyze the flexible centralized LNG infrastructure system.

The results of the case study obtained using the proposed methodology can be explained to management laymen, and policy-making audiences. In this case study, the flexible design solution includes these decision variables: InCap, MDC, MsiteTV MoveTV, Cover and DsiteTV. Once the optimum values for these elements are obtained, the solution can be explained to laymen and a team of experts with diverse backgrounds in operations. The solution suggests that the system operator should consider modular design capacity MDC for capacity expansion and should deploy the initial capacity InCap at the main production site at time zero. The system operator should expand the capacity at the main production site every time the aggregate demand reaches the amount MsiteTV of the MDC modular capacity. The demand sites that are located at a distance Cover away from the main production site should be considered for the first LNG production facility deployment when the observed demand in these sites reaches MoveTV of the MDC modular capacity. The system operator should expand the capacity of the production facilities at demand sites every time demand reaches DsiteTV of the MDC modular capacity.

Results show both meta-model and multi-objective computing budget allocation provides good-enough Pareto quality within a reasonable amount of time. Exhaustive enumeration used as validation metric provides the best Pareto quality while requiring the largest number of simulation evaluation as compared to the screening approaches. In sum, both screening models based on meta-modeling and computing budget allocation approaches can be applied to provide good-enough solutions with respect to different objectives while computational resources are limited. While MM and MOCBA requiring respectively 1% and 9% of the computational runtime, the MM and MOCBA find flexible design solutions that recognize 58% and 47% of the value of flexibility identified under the full exhaustive search. This may represent a good tradeoff for decision-makers, depending on the amount of time and computational resources available for the analysis. Even if the value of flexibility is only recognized at about half the value from the exhaustive, it still represents 41% and 33% performance improvements as compared to the benchmark design, which is significant given the multi-million dollar investment required.

Chapter 5 Case Study II: Decentralized LNG production system

5.1 Introduction

Unlike the case study 1, which was primarily about a centralized LNG production system, this chapter investigates a decentralized LNG production system. Although both systems are instantiations of LNG infrastructure systems, from a design problem stand point, they have different forms of flexible design vectors and flexible solution spaces. These differences motivate the application of the proposed multi-criteria screening framework to this second case study, and also to investigate the generalizability of the proposed screening framework as a way to further support its validation in conceptual design analysis.

The case study that will be explained in this chapter focuses on the development of a decentralized on-shore LNG production system to provide fuel for on-road transportation in southeast Australia. Figure 5.1 shows the schematic representation of the LNG production system from a fixed design towards a more flexible design. The scope of the problem lies in the part of the LNG supply chain where natural gas from on-shore pipelines is converted to LNG through a liquefaction process and the fuel is then delivered to the end users. All five sites have access to the existing on-shore natural gas pipeline. Figure 5.1 (a) depicts a fixed design where optimum capacity is deployed at each demand point. Figure 5.1 (b) shows a flexible modular design where the initial capacity is built at each demand point depending on the market situation. Using this design, extra capacity will be deployed based on the managerial capacity expansion policy. Figure 5.1 (c) shows a flexible modular design similar to the design in Figure 5.1 (b), but with extra operational flexibility. This flexibility enables the production system to rebalance its capacity among the demand points using a fuel truck fleet transportation system.

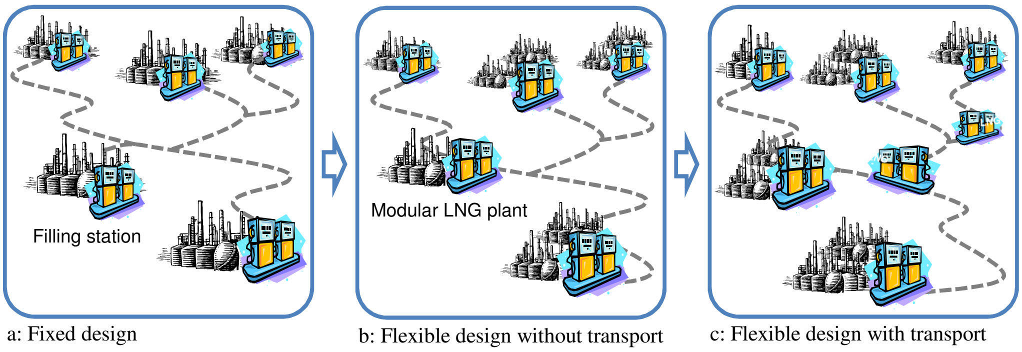


Figure 5.1: A fixed LNG system design towards a more flexible decentralized LNG system design

The proposed integrated multi-criteria screening framework represented in three phases, that was explained in chapter 3, is applied to this case study to efficiently and effectively explore the solution space of flexible designs.

5.2 Phase 1: Problem modeling

In this phase, the three-step process for problem modeling is applied to the second case study. Figure 3.2 in chapter three shows the generic process.

5.2.1 Modeling assumptions

The following assumptions are made for problem modeling. Demand is assumed to be unevenly distributed in the region over five distinct demand sites. Essentially the distributions of the demand at different sites are independent and identical where the same distribution parameters are assumed.

All sites have access to an on-shore natural gas pipeline in the region, but this access has a cost due to gas tie-in operations and acquiring extra land. For all demand sites, the time needed to build the first plant is two years and the capacity expansion takes only one year. In other words, if one decides to expand the current capacity in year t, the extra capacity will be available for production in year t+1. Regarding the financial parameters, the project lifetime is assumed to be 20 years and each year is considered to be 350 working days. A ten-year straight-line depreciation method is used for all LNG production facilities with a zero salvage value. The discount rate as an after-tax MARR is assumed to be 10% and the corporate tax rate is 30%. Essentially, the quantitative performance of the design is evaluated based on an After Tax Cash Flow (ATCF) analysis.

Similar assumptions are used for developing the performance model. According to the data provided by the company, the natural gas purchase price was assumed \$250 per ton and the LNG selling price was assumed as \$800 per ton. It is assumed that the gas purchase and LNG selling prices increase by 3% annually. The LNG margin at time t is calculated based on the LNG selling price minus the gas purchase price at time t. The fixed design analysis examines economies of scale where the economies of scale factor α=95%. The modular design analysis assumes a learning rate under 10%. The Opex of the plant is assumed at 5% of the plant's Capex. The flexibility cost is 10% of the Capex of the first capacity deployment at each site because of gas tie-in operations to the existing natural gas pipeline and extra land costs. Transportation is outsourced through a contract with a transportation company to transfer fuel among the different geographical sites.

The transportation cost for carrying LNG is set at \$0.80 per ton-kilometer. Parameters associated with deterministic and stochastic LNG demand modeling obtained through a combination of personal communications and market research at the collaborating firm are summarized in Table 4.1 and Table 4.2 in chapter 4. The travel distances among the district sites are shown in Table 5.1.

Table 5.1: Distance among the distinct demand sites, figures are in kilometer (Km)

From / to	**Site1**	**Site2**	**Site3**	**Site4**	**Site5**
Site1	N/A	153	164	441	540
Site2	153	N/A	318	413	401
Site3	164	318	N/A	602	706
Site4	441	413	602	N/A	529
Site5	540	401	706	529	N/A

5.2.2 Step 1: Develop deterministic quantitative performance model

The problem modeling starts with the deterministic analysis, as done in case study 1. The aim is to understand the key components of the system that influence its lifecycle performance. The performance metric used in this problem is NPV, calculated as the sum of discounted cash flows throughout the project lifecycle T = 20 years – see equation 5.1. Variables TR_t and TC_t are the total revenues and costs incurred in years t = 1, 2, ..., T, and r is the discount rate, Tax is the effective income tax on ordinary income and d_t is the sum of all noncash, or book, costs during year t, such as depreciation. The detailed mathematical representations of the case study II are provided in Appendix G.

$$NPV = \sum_{t=1}^{T} \frac{(1 - Tax)(TR_t - TC_t) + Tax\, d_t}{(1 + r)^t} \tag{5.1}$$

LNG demand is identified as the key driver of system performance. A deterministic s-curve function is assumed to simulate LNG demand over the study period, as shown in equation 5.2. The values of these deterministic parameters are shown in Table 4.1 in the previous chapter.

$$D_t^D = \frac{M_T^D}{1 + a^D e^{-b^D t}} \tag{5.2}$$

where a^D is calculated using equation 5.3.

$$a^D = \frac{M_T^D}{D_0^D} - 1 \tag{5.3}$$

The parameters of these equations have been explained in section 4.2.2 in chapter 4. In general, the conventional DCF model is built to assess the performance of a system under deterministic conditions. This step captures the standard industry practice in terms of design and project evaluation.

5.2.3 Step 2: Develop the quantitative performance model under uncertainty

This step enables the analyst to explicitly recognize, characterize and model the major uncertainty drivers affecting the future lifecycle performance. The analysis under uncertainty considers a distribution of outcomes instead of a single performance output, which can be modeled using different techniques (e.g., Monte Carlo simulation, decision trees or binomial lattice). Here, NPV_S, which refers to NPV under demand scenario s, is calculated in terms of different realized and uncertain demand scenarios via simulation. A stochastic s-curve function is used to simulate LNG demand over the system's lifecycle using additional uncertainty factors, as shown in equation 5.4.

$$D_t^U = \frac{M_T^U}{1 + a^U e^{-(b^U)t}} \tag{5.4}$$

Equation 5.5 shows how a^U is calculated.

$$a^U = \frac{M_T^U}{D_0^U} - 1 \tag{5.5}$$

The parameters of these equations have been explained in section 4.2.3 in chapter 4. The values of the stochastic demand parameters are shown in Table 4.2. Realized demand at time t + 1 equals realized demand at time t plus annual volatility multiplied by the growth rate at time t, as equation 5.6 shows.

$$D_{t+1}^U = D_t^U + (Av \times G_t) \tag{5.6}$$

In this equation, G_t is the annual growth rate assuming adherence to a standard normal distribution, (G_t ~ Normal (0, 1)), and Av is assumed as a fixed parameter throughout the project lifetime calibrated using historical data. Monte Carlo simulation is used to simulate a wide range of LNG demand scenarios. This analysis recognizing uncertainty provides designers with a more realistic overview of system performance as compared to the deterministic analysis in Step 1. In order to extend the deterministic model into the model under uncertainty, the uncertainty drivers that significantly affect the economic performance of the project must first be identified. Through a sensitivity analysis, LNG demand is again treated as the main source of uncertainty. Next, the Monte Carlo simulation technique can be used to simulate a wide range of LNG demand scenarios.

Figure 5.2 shows regional LNG demand scenarios generated using an uncertain s-curve demand at each geographical site. The analysis under uncertainty provides designers with a more realistic overview of system performance as compared to the deterministic analysis in Step 1. Recognizing the uncertainty in this step, the optimum capacity for the fixed LNG production system is determined as a benchmark design. According to Savage's "Flaw of Averages" (2009), relying on the most likely or average scenario may lead to incorrect design selection and investment decisions. The results show that the optimum system capacity and value under uncertainty are less than those obtained relying on demand forecast, $NPV(D^D) \geq ENPV(D^U)$ and $Capacity^{*D} \geq Capacity^{*U}$.

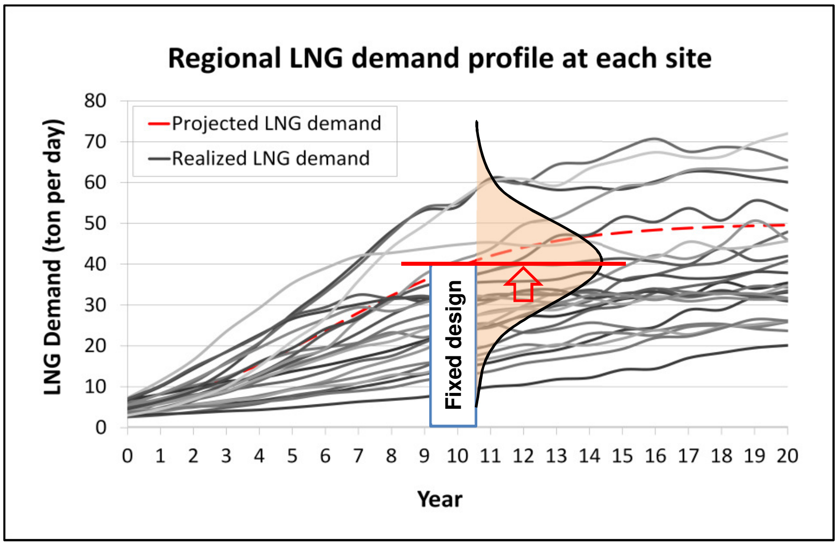


Figure 5.2: Projected and realized regional LNG demand at each geographical site

5.2.4 Step 3: Develop quantitative performance model for flexibility

To deal with uncertain LNG demand, three different flexible strategies are proposed: 1) strategic; 2) tactical and 3) operational flexibility. In the strategic level, flexible decision rules for determining initial capacities are applied. In the tactical level, capacity expansion flexibility is identified as the most relevant strategy to cope with demand uncertainty. Both strategic and tactical flexibility are embedded in the flexible modular design – with no transport – as shown in Figure 5.1(b). To embed these flexible strategies, a set of managerial decision rules is embedded in the programming of the Excel® spreadsheet DCF model under uncertainty. To further extract value from uncertainty, operational flexibility is proposed, as shown in 5.1(c). These three flexible strategies are described in greater detail in the following subsections.

5.2.4.1 Strategic level flexibility

In this case study, determining the initial plant capacity is considered as a strategic level decision. This decision is made by relying on a short-term, forward-looking forecast.

Given the practical modular capacities available to the company, the three decision rules used in the simulation model are as follows: 1) IF "realized demand in year of forecast t <= bound 1" THEN "Initial capacity = 0"; 2) IF "realized demand in year of forecast t > bound 1" AND "realized demand in year of forecast t <= bound 2" THEN "Initial capacity = 25"; and 3) IF "realized demand in year of forecast t > bound 2" THEN "Initial capacity = 50", where bound 1, bound 2 and year of forecast t are parameters of the decision rules.

Figure 5.3 demonstrates a case where Band 1, Band 2 and Band 3 are evenly distributed between the lower and upper bounds of LNG demand and the short-term, forward-looking year of forecast is set to year 6.

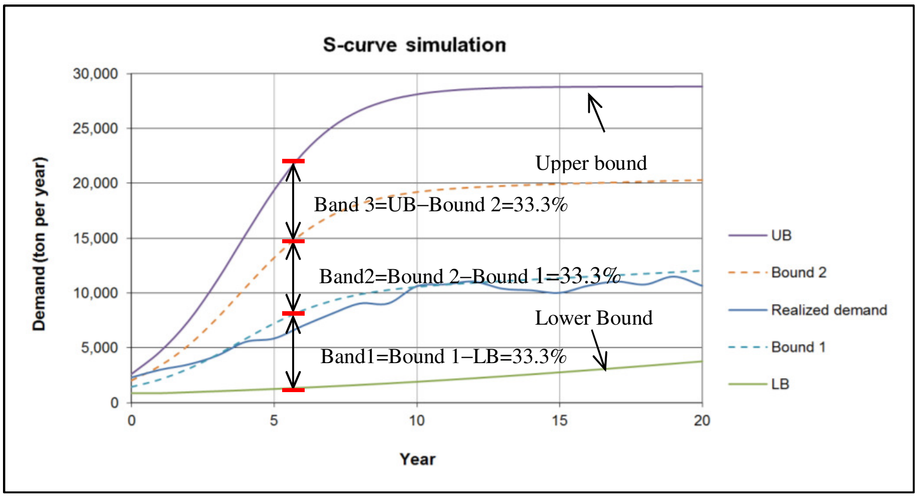


Figure 5.3: Parameters of strategic flexibility for initial demand deployment

5.2.4.2 Tactical level flexibility

In this case study, tactical level capacity expansion policy was considered the most appropriate flexibility for responding to demand uncertainty. For capacity expansion, it is important to know when capacity should be expanded given the available modular designs (i.e., 25 tpd and 50 tpd). Hence, an appropriate managerial decision rule was embedded at each production site.

The decision rule is defined in a logical form as:

- IF "*observed demand is higher than current capacity*" AND *"the difference between the observed demand and current capacity reaches a threshold value that is a certain percentage of the modular design used at each production site in year t*"

- THEN "*build extra modular plant that will be available for production in year t+1"*

- ELSE *"do nothing*".

The threshold value determines when the extra capacity should be built. For example, decision-makers may decide to add another modular plant as soon as the difference between the realized and current capacity reaches 60% of the modular plant capacity for the site.

5.2.4.3 Operational level flexibility

In order to further improve the lifecycle performance of the flexible LNG production system, an operational flexible strategy can be applied to better meet unmet demand with unused capacity in the system. The LNG production at each site is planned to be absorbed by the demand at the same location. However, if the capacity at any operational period (i.e., one year, in this case) is not matched with the realized demand, this will lead to either an unused capacity or unmet demand situation at any given location. The proposed operational flexibility (also referred to as the rebalancing problem) is concerned with the situation in which LNG is transported from sites with unused capacity to locations with unmet demand. The rebalancing transportation problem can be formulated as a linear programming, transportation problem. By embedding this flexibility for each set of demand scenarios for each operational time period, the optimum amount of LNG that should be transported from the supply sites (i.e., those with unused LNG capacity) to the demand sites (i.e., those with unmet LNG demand) can be determined.

The objective of operational planning is to minimize the total transportation cost that leads to maximizing the added value of the system design, which is termed the added value of flexibility. Let m-plant equal the locations with unused capacity (supply) and the n-plant with unmet demand (demand). Let $USC_{i,t,s} \geq 0$, $i= 1, 2,\ldots, m$ be the amount of capacity idle at the i^{th} plant in year t under scenario s from a set of plants with unused capacity. Similarly, let $UMD_{j,t,s} \geq 0$, $j= 1, 2,\ldots,n$ be the amount of demand required at the j^{th} plant from a set of plants with unmet demand in year t under scenario s. Assume the cost of transporting one unit of LNG (i.e., one ton) from i^{th} supply to j^{th} demand site be $C_{i,j}$, in terms of i=1,2, …,m and j=1,2,….n. If $x_{i,j,t,s}$ is the amount of LNG to be transported from i^{th} supply to j^{th} demand point in year t under scenario s, then the problem is to determine $x_{i,j,t,s}$ so as to minimize the following function considering $x_{i,j,t,s} \geq 0$ for all values of i and j.

Equation 5.7 determines the total transportation cost incurred by enabling operational flexibility at time t under demand scenario s. Equation 5.8 ensures that the amount of LNG carried from site i at time t under demand scenario s is equal to the available unused capacity. In a similar fashion, equation 5.9 guarantees that the amount of LNG carried to site i at time t under demand scenario s is equal to the amount of unmet demand.

$$TRSC_{t,s} = \sum_{i=1}^{m}\sum_{j=1}^{n} x_{i,j,t,s} C_{i,j} \qquad \forall\, t = 1 \dots T,\;\; s = 1 \dots S \tag{5.7}$$

$$\sum_{j=1}^{n} x_{ij} = USC_{i,t,s} \qquad \forall\, i = 1 \dots m, t = 1 \dots T,\;\; s = 1 \dots S \tag{5.8}$$

$$\sum_{i=1}^{m} x_{ij} = UMD_{j,t,s} \qquad \forall\, j = 1 \dots n, t = 1 \dots T,\;\; s = 1 \dots S \tag{5.9}$$

The value of flexibility added because of operational flexibility under each set of demand scenarios in each year is calculated using equation 5.10.

$$\begin{aligned}\text{Value added}_t = \;& \max\big(0, \big((\text{ LNG Production added}_t \times \text{ LNG margin}_t) \\ & - \text{Transportation cost}_t\big)\big)\end{aligned} \tag{5.10}$$

For illustration purposes, Table 5.2 shows the optimal solution for transportation planning under demand scenario in year 9.

Table 5.2: Transportation planning in year 9, ton per day

Transportation planning in year 9		*Unmet demand site*					*LNG shipped from*
		D1	D2	D3	D4	D5	
Unused capacity Site	S1	0	0	**9.05**	0	0	9.05
	S2	0	0	**0.23**	0	**3.57**	3.80
	S3	0	0	0	0	0	0
	S4	0	0	0	0	**3.24**	5.63
	S5	0	0	0	0	0	0
LNG shipped to		0	0	9.28	0	6.82	
Transportation Cost=		**$ 2,634,556**					

It is assumed that all sites have flexibility for sending and receiving LNG fuel – full operational flexibility. As can be seen, this flexibility results in $1.41M value added in year 9. Value added in year 9 = max[0, (LNG production added$_t$ × LNG margin$_t$) – Transportation cost] = max [0, ((9.05+0.23+3.57+3.24) × 350) × 717.63) − 2,634,556] = \$1406751/10^6 = \$1.41M.

In the model explained above, it was assumed that all locations have the capability to send and receive fuel under different demand scenarios. However, some locations may not be capable of sending or receiving LNG fuel. Under such circumstances, partial operational flexibility can be considered instead of no operational flexibility or full operational flexibility.

Let O_i be the state of operational flexibility at location i, where 0 means no operational flexibility and 1 means with operational flexibility. It is important to note that operational flexibility can lead to value added to the system design if the operational flexibility of at least two locations is switched "on". In other words, if only one location is operationally flexible, this will not lead to any value added. The number of operational flexibility statuses depends on the number of demand locations and can be calculated using equation 5.11. Hence, for five locations, the total number of combinations – including designs with operational flexibility levels ranging from partial to full – that can lead to value added is 26.

$$\sum_{i=0}^{n-2} \binom{n}{2+i} = \binom{5}{2} + \binom{5}{3} + \binom{5}{4} + \binom{5}{5} = 10 + 10 + 5 + 1 = 26 \tag{5.11}$$

Figure 5.3 illustrates the range of partial operational flexibility towards a full operational flexibility. As can be seen, under full operational flexibility (i.e., state 26 for flexibility of the demand sites) when bound 1 is equal to 45%, bound 2 is equal to 33%, threshold value is equal to 65% of modular design 25 tons per day, value added due to operational flexibility under 2000 demand scenarios is more than 3.5 million dollars. The value of flexibility is calculated as the value of a flexible design minus its corresponding fixed design value, as equation 5.12 shows.

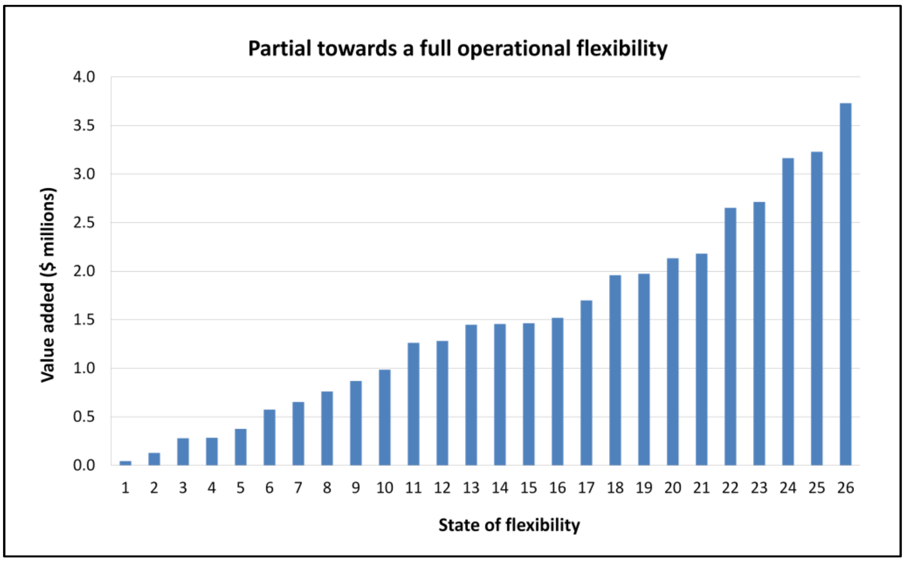


Figure 5.3: Partial operational flexibility towards a full operational flexibility under 2000 demand scenarios

$$\text{Flexibility Value} = \max(0, \text{ENPV}_{\text{Flexible design}} - \text{ENPV}_{\text{Optimum fixed design}}) \quad (5.12)$$

5.2.4.4 Different flexible strategies

In this study, design vectors are used to represent the physical design configuration of complex systems as well as flexible managerial strategy and policy. These vectors are classified into two types: 1) design vectors that represent major flexible design strategies, so-called "flexible design strategy vectors" and 2) design vectors that represent flexible design solutions, so-called "flexible design solution vectors". The major flexible design strategies determine the general approach towards the system design. For instance, in the case under consideration, three types of flexible strategy are investigated and each type has two possible values, either "on" or "off". Hence, 2^3 major flexible strategies can be synthesized. Each major flexible design strategy may correspond to a flexible design vector. Unlike major flexible design strategies, flexible design solutions may require more domain-specific knowledge. Hence, decision-making at this level is delegated to domain-specific designers and experts who can determine and judge about the value of design variables, decision rules and their corresponding threshold variables. In this thesis, screening models are used to assist decision makers to determine these values.

Table 5.3 demonstrates a full factorial experimental design matrix of the two-dimension problem (i.e., Bound 1 and threshold value). The three levels of flexibility correspond to three factors of the experimental design. Each factor has two potential values: Y - with flexibility, or N - no flexibility. Thus, there are 2^3 flexible strategies in total. Last column of the table shows the design vectors. Each design vector has three elements: 1) initial capacity for the fixed design or the value of Bound 1 in case of flexibility shown as InCap/ B1%; 2) no capacity expansion or threshold value of modular design capacity shown as 0%(0) /TV%(tpd); 3) state of operational flexibility shown as No/Full.

Table 5.3: Design of experiment for strategies 1 to 8 under 2000 demand scenarios

Flexible strategy	**Strategic flexibility**	**Tactical flexibility**	**Operational flexibility**	**Design vector**
	Initial capacity (Y/N)	Capacity expansion (Y/N)	transportation flexibility (Y/N)	[InCap/B1% - 0%(0) /TV%(tpd) - No/Full]
1	N	N	N	Initial Cap. 5×30=150 - 0%(0) - No
2	N	N	Y	Initial Cap. 5×30=150 - 0%(0) - Full
3	N	Y	N	Initial Cap. 5×30=150 - 65%(25) - No
4	N	Y	Y	Initial Cap. 5×30=150 - 65%(25) - Full
5	Y	N	N	B1=20% - 0%(0) - No
6	Y	N	Y	B1=20% - 0%(0) - Full
7	Y	Y	N	B1=45% - 65%(25) - No
8	Y	Y	Y	B1=45% - 65%(25) - Full

Each strategy is simulated using 2000 sets of demand scenarios for different locations. The first strategy represents the optimum fixed design with initial capacity 5×30=150 tons per day. An exhaustive enumeration was conducted to find the optimum design variables and decision rule parameters of all flexible strategies. To analyze the contribution of each type of flexibility to the value of flexibility, the NPVs of all strategies are compared to the ENPV of strategy 1. Strategy 1, which represents the optimum fixed design, is considered the baseline design. Figure 5.4 shows the cumulative density function of strategies one to eight.

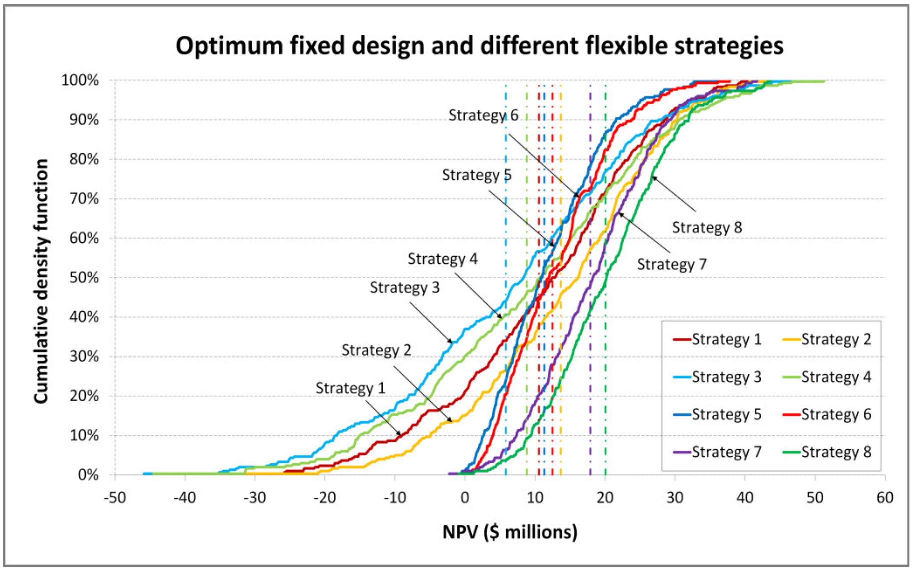


Figure 5.4: Cumulative density function curves for strategy 1 to 8

A pairwise t-test is applied to see whether the ENPVs of any two strategies are statistically different from each other. Given a large number of scenarios, pairwise t-tests show that the differences among strategies are statistically significant. As can be seen, strategy 8 with operational, tactical, and strategic flexibility is the best of the eight flexible strategies in terms of ENPV that is shown in bold figure.

5.2.4.5 Multi-criteria decision-making

Table 5.4 shows a multi-criteria decision-making table to compare and contrasts the different solutions above. Best flexible strategies in terms of different criteria are shown in bold figures in the table. It compares results for the optimum fixed design (i.e., strategy number one) and flexible designs (i.e., strategies two to eight). Strategy number 8 outperforms among the others in terms of ENPV (\$20M) and Value at Risk 10%, by protecting the downside risk by more than \$8M. In terms of value at gain 90%, flexible strategy 3 gains the most value, more than \$33M, from the upside opportunities among the rest. Strategy number 5 provides the least standard deviation, with less than \$7.7M.

Table 5.4: Multi-criteria decision-making table, numbers in million dollar

Criteria	**Flexible strategy**								Value of	Best
	1	2	3	4	5	6	7	8	flexibility	strategy
ENPV	10.56	13.67	5.83	8.82	11.32	12.48	17.90	**20.05**	9.49	8
$VaR_{10\%}$	-8.87	-4.99	3.71	-14.79	2.41	3.55	6.66	**8.53**	17.40	8
$VaG_{90\%}$	28.89	30.49	**33.53**	30.98	21.47	22.56	30.09	32.28	4.64	3
STD	14.69	13.94	11.01	17.72	**7.65**	7.73	9.02	9.20	0	5

In this study, two types of screening model are used to explore efficiently and effectively the design space: 1) meta-model based screening model and 2) multi-objective computing budget allocation model; indeed a bi-objective computing budget allocation (BOCBA) approach is used in this case study but let us use the general term "MOCBA" as represented in the proposed framework in chapter 3 for consistency. Besides these screening models, for the operational level decisions, a bottom-up screening model is proposed to further enhance the speed of the overall screening procedure. The results are then compared to a full exhaustive enumeration for purpose of comparisons.

5.3 Phase 2: Screening

In this section, the screening phase of the proposed multi-criteria screening framework is applied to the second case study. In this phase, three screening approaches are considered: 1) A bottom-up screening approach for operational flexibility, 2) A meta-model based screening approach and 3) A computing budget allocation based screening approach. The procedures of the screening approaches are described in the following subsections. The addition of another screening approach demonstrates the generalizability of the proposed framework in Phase 2.

5.3.1 A heuristic schema for operational flexibility

Under each set of demand scenarios, the optimum solution in each operational period can be obtained by optimizing the linear programming (LP) model. Assuming that full flexibility (i.e., all the demand points can receive and deliver LNG) in the operational level is intended, the optimization procedure is called multiple times depending on the number of operational periods and demand scenarios. Let us assume that, under each demand scenario, the optimization solver is called an average of 15 times. Hence, if 2000 demand scenarios are used, the optimization solver will be called 30,000 times. This can be very time consuming. Therefore, a heuristic rebalancing approach is proposed to obtain a good-enough solution for operational level decision-making in a reasonable amount of time.

It should be emphasized that the value added due to operational flexibility can be captured by both meta-model screening approach and multi-objective computing budget allocation. In the heuristic rebalancing schema, LNG fuel produced at sites with unused capacity is evenly distributed among sites with unmet demands. It is important to note that the LP optimization procedure always offers the upper bound for this maximization problem. This is due to the fact that the heuristic procedure does not guarantee the optimal solutions.

Table 5.6 shows the comparison between the LP optimization and the heuristic rebalancing schema in terms of the ENPV and computational runtime for a given design vector. The results suggest that the heuristic algorithm offers good-enough solutions, with a 7.81% gap, and is more than two times faster than the optimization approach.

Table 5.6: Screening operational level decision-making under 2000 demand scenarios

ENPV ($ millions)				**Computational time (Sec.)**			
No operational flexibility	Heuristic	LP	Gap%	No operational flexibility	Heuristic	LP	Efficiency%
17.77	18.50	19.95	7.81%	245.28	7153.08	23125.03	223.29%

The efficiency of the screening model is further enhanced if this kind of screening model (i.e., bottom-up screening model) is combined with the meta-model and computing budget allocation screening approaches that will be explained in the following sections.

5.3.2 A meta-model based screening approach

In this section, the meta-model based screening model is applied to the second case study, the decentralized LNG production system. Table 5.5 shows the parameters used in the meta-model screening approach. As can be seen, a Gaussian process was used in the correlation model and parameter theta was set between 0 and 2. This parameter is a correlation parameter and the DACE model is used to determine the optimum value for its optimal coefficient θ^* of the correlation function.

Using the meta-model screening approach, first a few samples are drawn, using Central Composite Design and Latin Hyper Cube sampling, from the solution space of flexible designs.

Table 5.5: Parameters used in Meta-model screening approach

Meta-model based screening parameters	**Value**
Expected improvement	0.5
Latin Hypercube Design	12
Central Composite Design	18
Correlation model	Gaussian
Theta band	[0 - 2]

Then using the Gaussian model, a simulation surface is created for each objective. The surface is adaptively evolved until a stopping criterion, which is expected improvement, is met. Once response surfaces are created given intended objectives, an enumeration is done using these inexpensive meta-models. Then, a preliminary Pareto front is found and further analysis using a large number of scenarios (i.e., 2000 demand scenarios) is conducted to find True Pareto fronts in phase 3, as done in case study 1.

Unlike exhaustive enumeration that only uses Excel, in the meta-model screening approach both Excel and MATLAB are used. In the MATLAB workspace the DACE model is used to create inexpensive response surface and MATLAB optimization toolboxes are used to perform the EGO procedure. Essentially, optimization toolboxes are used to maximize expected improvement in the DACE model and to find the optimum response surfaces. A represented in chapter 4, Figure 4.9 shows Microsoft Excel and MATLAB interface via spreadsheet link EX® in the meta-model screening approach.

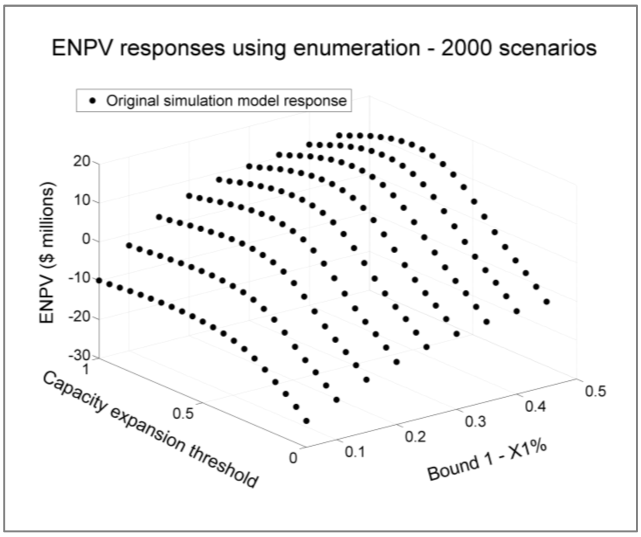
In the EGO procedure, a Kriging meta-model is used to build an inexpensive surrogate response surface. The Kriging method dates back to the early 1960s (Krige, 1960) where its original model was used to find a function that approximates the underground concentration of a valuable mineral. Since then, different types of Kriging meta-models have been developed for complex simulation models (Kleijnen 2009). The Kriging model is an interpolating meta-modeling technique that employs a trend model, F(x), to capture large-scale variations and a systematic departure, Z(x), to capture small-scale variations (Nielsen, Lophaven et al. 2002). Kriging postulation is the combination of a global model and departures in the form of equation 5.13:

$$f(x) = F(x) + Z(x) \tag{5.13}$$

In this equation, f(x) represents the unknown function and F(x) is the global model, while Z(x) represents the localized deviations. In this equation, Z(x) is the realization of a stochastic process with a zero mean and non-zero covariance. A linear polynomial function is used as a trend model and the systematic departure terms follow a Gaussian correlation function. As represented in chapter 4, table 4.7 shows procedure of meta-model screening approach. The screening model is applied to the problem with a uniform solution with all elements of the flexible design vector so that more focus can be given to the details of the framework. As an alternative to an exhaustive search, the screening model is used to find the optimal values of the design vector by efficiently exploring the flexible design solution space.

For visualization purposes, a two-dimensional problem is analyzed first. In the 2D problem with a uniform solution, bound 1 and the threshold value are considered as variables and the other elements of the design vector are set as fixed parameters, bound 2=45% and modular design capacity=25 tons per day. Then, all possible combinations of bound 1 and threshold value are enumerated to obtain the true response of the simulation model in terms of ENPV and Standard deviation as benchmark solutions. In the exhaustive enumeration, the simulation model is run 9×21=189 times, showing all possible flexible design solutions. In the exhaustive search, 2000 demand scenarios are used as the system performance converged to a steady state value with a negligible variation. Figure 5.5 demonstrates the ENPV and standard deviation of the simulation response using the enumeration method.

(a)



(b)

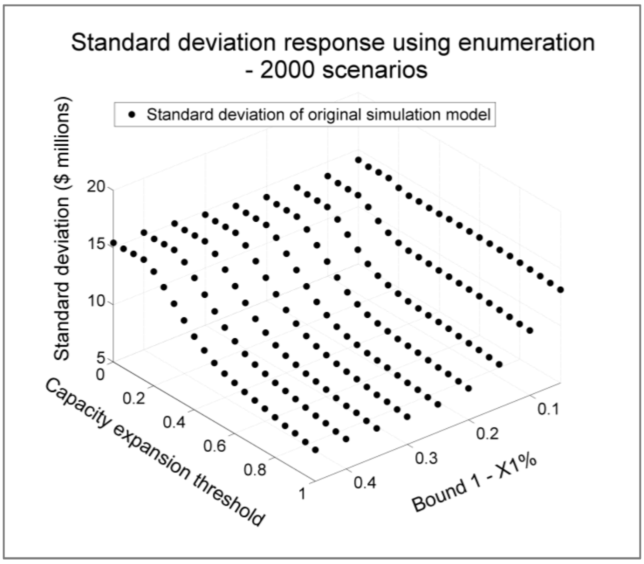
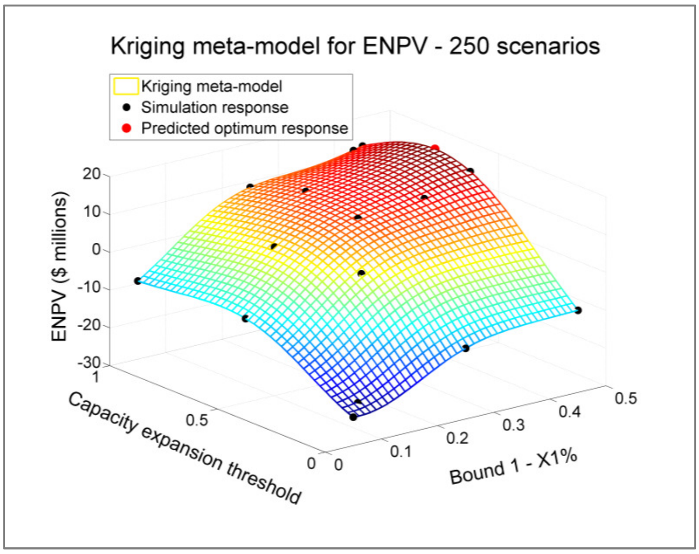


Figure 5.5: Simulation using exhaustive enumeration, 2000 scenarios

Following the exhaustive enumeration method, the EGO based on Kriging meta-modeling was applied to reduce the computational burden. Figure 5.6 demonstrates the response surface for ENPV and standard deviation using the Kriging meta-model.

(a)



(b)

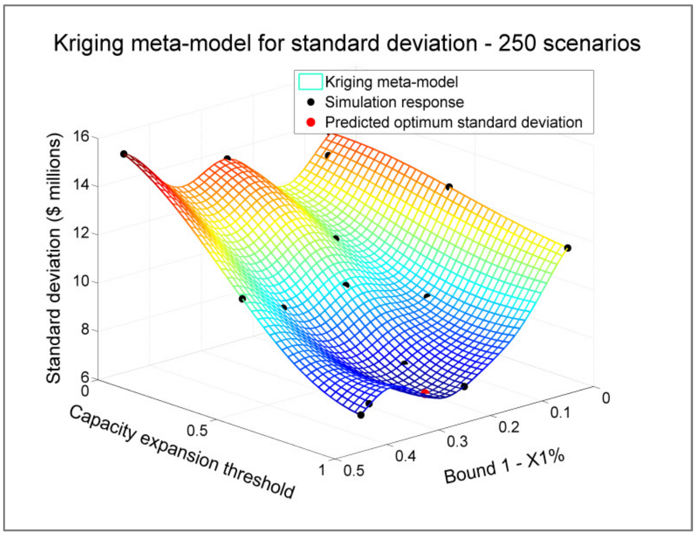


Figure 5.6: Kriging meta-model for ENPV and standard deviation – 250 scenarios

To find the predicted optimum ENPV and standard deviation values, a global multi-start gradient based optimization algorithm in MATLAB was used. While bound 1 and the threshold value are continuous functions varying between 5%-45% and 0%-100% respectively, the screening approach only samples a few points in the simplified design space. Although the two-dimensional analysis is shown for visualization purposes only, in the uniform solution, it is extended to analyze a combination of other decision rules and physical design variables (e.g., bound 2, modular capacity), which will be explained in the following sections.

5.3.3 A computing budget allocation based screening approach

In this section, a computing budget allocation screening model is applied to the second case study, the decentralized LNG production system design. Table 5.6 shows the parameters used in this approach.

Table 5.6: Parameters used in the multi-objective computing budget allocation

MOCBA parameters	Value
Initial Budget Rate	5%
Incremental Budget Rate	10%
Archive keep rate	50%
Minimum archive size	50
Allocation factor	1.2

Using this approach, more budgets are allocated to designs that are close to true Pareto fronts than those are far away from true Pareto front. The process is terminated when the maximum budget is exhausted or the design archive size reaches its minimum acceptable size.

Like the meta-model approach, in the multi-objective computing budget allocation both Excel and MATLAB are used, as shown in Figure 4.11 in chapter 4. Essentially, macros in VBA are used to synthesize flexible designs and simulation is modeled by programming in Excel spreadsheet and VBA. In the MATLAB workspace, Pareto dominance module and MATLAB functions for solving equations are used.

Pareto dominance is used to rank flexible designs in different layers. MATLAB functions for solving equations are used to appropriately allocate budgets to different layers of Pareto fronts. Table 5.7 shows Pseudocode of a multi-objective computing budget allocation model used in the second case study.

Table 5.7: Pseudocode of a multi-objective computing budget allocation

```
Construct initial design archive
Allocate initial budget→MATLAB
Run flexibility simulation→Excel
Conduct Pareto dominance analysis→MATLAB
Sort designs with different frontiers→MATLAB
    Do while (Min_archive size ≤ archive size) or (each design budget ≤ Max_budget)
            Update design archive→MATLAB
            Update simulation replication budget → MATLAB
            Allocate new budgets to designs in different frontiers
            Run flexibility simulation→Excel
            Conduct Pareto dominance analysis→MATLAB
            Sort designs with different frontiers→MATLAB
    End while
Return Pareto front
Conduct analysis using large number of scenarios, with 2000 demand scenarios
Return true Pareto front
```

Assume an experiment with maximum 300 demand scenarios. Given initial budget rate is 5%, initial budget will be 300×5%=15. Therefore all the 3,402 designs are analyzed under 15 demand scenarios. Subsequently, Pareto dominance is conducted and the designs are sorted in the design archive with respect to their Pareto frontier ranks. Now the loop shown in the pseudocode starts until certain criteria are met, $\text{Min}_{\text{archive size}} \leq$ archive size or each design budget $\leq \text{Max}_{\text{budget}}$. Subsequently, the size of the design archive is updated. As Archive keep rate is 50%, only top 50% of flexible designs are kept and the other 50% of the flexible designs are discarded. It should be noted that the archive keep rate was chosen based on trial and error. More research is needed to fine tune this parameter as well as the other parameters used in MOCBA approach. Table 5.8 shows a schematic example of the computing budget allocation approach from a general perspective. As can be seen, all the 3,402 designs are first evaluated 15 times according to the initial simulation budget.

Table 5.8: A schematic example of computing budget allocation

Simulation evaluation	Flexible designs												
	1	2	3	4	5	6	7	...	3,398	3,399	3,400	3,401	3,402
15													
16													
⋮													
300													

Then more simulation evaluation budgets are allocated to the promising flexible designs until the stopping criteria are met. As can be seen, the procedure stops when 300 simulation budgets are allocated to design number 3,398, shown for illustration purpose only. Essentially, this example shows how the problem is structured in Excel spreadsheet. Figure 5.7 shows this transition; Figure 5.7(a) contains 3,402 flexible designs and Figure 5.7(b) contains 1,701 flexible designs.

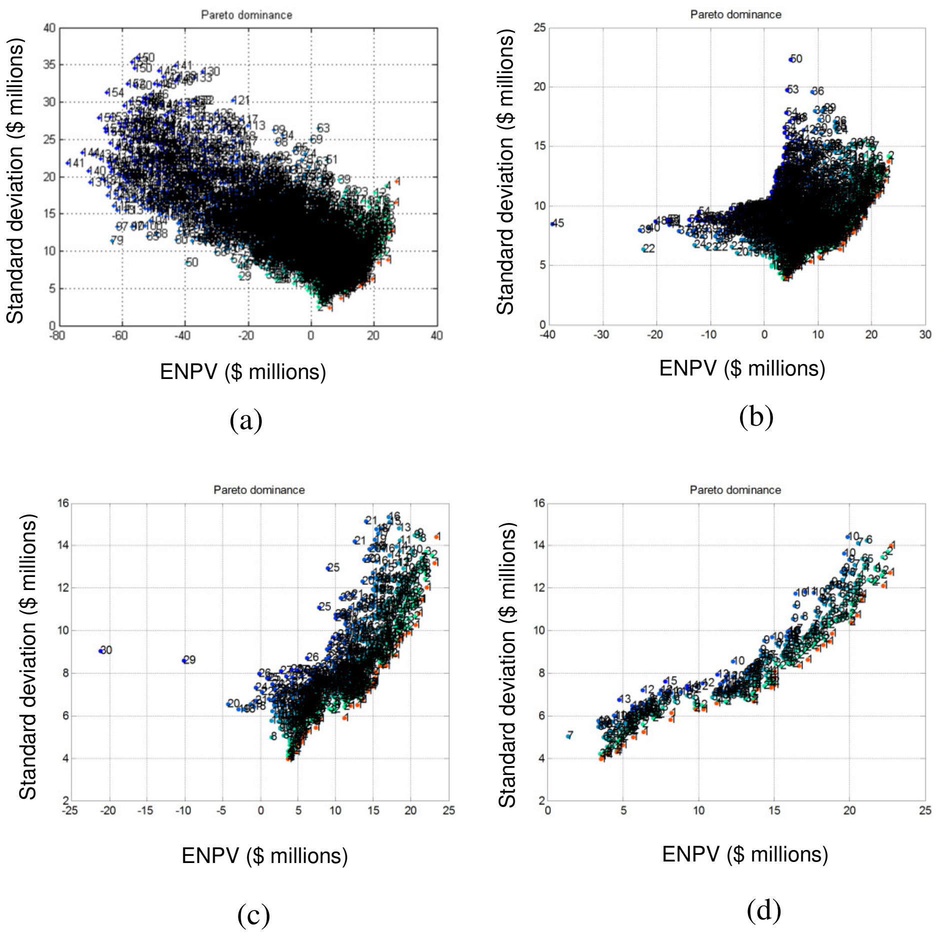


Figure 5.7: Evolution of a design archive in the MOCBA, in an experiment with 300 demand scenarios, from (a) to (d)

Following the procedure in the methodology section, computing simulation budget allocated to different frontiers are updated. Given an updated design archive and an updated incremental simulation budget, Monte Carlo simulation is conducted in Excel. Subsequently Pareto dominance is conducted and all the designs are sorted in terms of different Pareto frontiers. Once the stopping criteria are met, dominant flexible designs are returned as input of phase 3.

5.4 Phase 3: Multi-criteria decision-making analysis

In this section, dominant flexible designs obtained from the screening phase in different computer experiments are further analyzed under large number of scenarios. Subsequently, true Pareto flexible design solutions are generated and the hyper-area is calculated. Once true Pareto fronts are obtained using a large number of sample demand scenarios, a preferred trade-off flexible design solution is chosen based on decision makers' preferences. In this section, the weighted-sum approach described and used before is applied to choose a preferred dominant flexible design among other flexible designs in the true Pareto set.

5.4.1 A meta-model based screening approach

Now, let us consider the design vector with full elements, strategic and tactical flexibility. Figure 5.8 shows the dominant flexible designs using the meta-model screening approach. Enumeration is conducted using inexpensive Kriging meta-models. Then using dominance relation, dominant flexible designs are identified. These dominant flexible designs are further analyzed using large number of scenarios (i.e., 2000 demand scenarios) and hyper-area is calculated using an arbitrary worst case reference point with ENPV=$0M and Standard deviation= $20M.

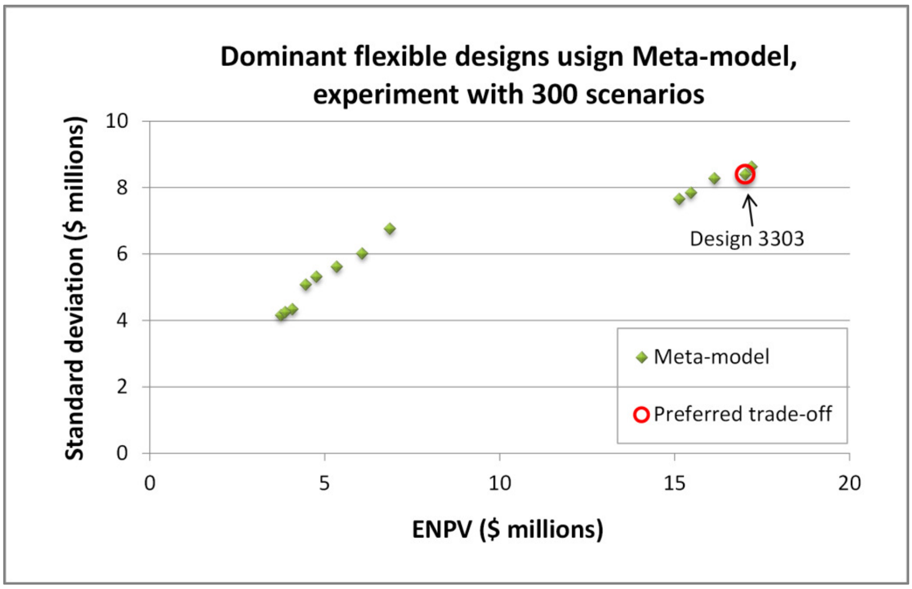


Figure 5.8: Dominant flexible designs using meta-model screening approach

Once dominant flexible designs are obtained using meta-model, a trade-off flexible solution can be found using decision makers' preferences. Assuming the weight for ENPV is 60% and the weight for Standard deviation is 40%, a preferred trade-off flexible design is the design with ENPV=$17.03M and standard deviation=$8.40M, shown in a circle in Figure 5.10. Table 5.9 illustrates the corresponding design vector of the preferred trade-off flexible design.

Table 5.9: Design vector of the preferred trade-off flexible design using MM

Design number	X1	X2	MDC	TV
3303	45%	25%	25	75%

The solution suggests that the system operator should deploy initially capacity based on the following scenarios: 1) IF "the short-term forward looking forecast in year 6 lies in the projected lower (pessimistic) band demand with X1=45% width", THEN "initial capacity should not be deployed and the system operator should wait until demand reaches 75% of the 25 tpd modular capacity"; 2) IF "the short-term forward looking forecast in year 6 lies in the projected base case (most likely) band demand with X2=25% width" THEN "Initial capacity=25"; 3) IF "the short-term forward looking forecast in year 6 lies in the projected upper (optimistic) band demand with X3=1−X1−X2=30% width" THEN "Initial capacity=50". The system operator should use 25 tpd modular design and the capacity should be expanded every time demand reaches 75% of the installed 25 tpd modular capacity.

Post-optimality sensitivity analysis

In this section, a post-optimality sensitivity analysis is performed to assess the effects of changes in input parameters on the value of flexibility for the obtained flexible solution. The effects of these parameters on the value of flexibility are shown in the Tornado diagram in Figure 5.9. The details of the post-optimality sensitivity analysis are provided in Appendix E. The Tornado diagram shows the sensitivity of the value of flexibility subject to different values for the discount rate, learning rate and sharpness volatility. The sharpness volatility, discount rate and learning rate have the most to the least influences on the value of flexibility respectively. The effects of changes in these parameters are analyzed here.

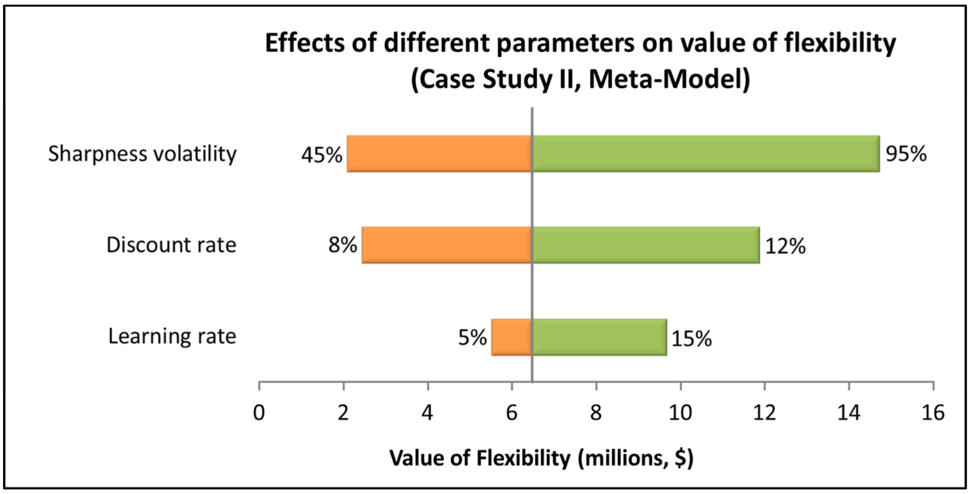


Figure 5.9: Post-optimality sensitivity analysis for the flexible design solution obtained using the meta-model based screening approach, Case study II.

As the sharpness parameter has been recognized as the key demand parameter, it is worthwhile to investigate the effect of different volatilities of this parameter on the designs value and, subsequently, on the value of flexibility. To do so, different values of the sharpness volatility at each geographical site are considered. The values 45%, 70% and 95% correspond to the low, the base and the high for the volatility of the sharpness parameter. When the volatility of the sharpness parameter decreases, the optimum fixed design and the flexible design provide better ENPV while more improvement is observed in the fixed design than the flexible one and consequently the value of flexibility is less than the value obtained under the base sharpness volatility. On the other hand, when the volatility of the sharpness parameter increases, the optimum fixed design and the flexible design provide less ENPV while more decrease is observed especially in the fixed design than the flexible one and consequently the value of flexibility is more than under the base sharpness volatility.

The results suggest that when sharpness volatility is high, although the value of both rigid and flexible designs decreases, the value of flexibility increases. This is similar to the observation made on the first case study in Sections 4.4 and 4.5. The reason for this improvement is that the flexible design provides better value than the fixed design under highly volatile market. When demand is strong, while the fixed design cannot accommodate extra capacity due to its rigid capacity, the flexible designs can acquire more capacity as needed, to meet the stronger-than-expected demand, leading to relatively more improvement in ENPV. On the other hand, when demand is weak, the flexible design is less affected because of the smaller capital investment in unfavorable markets whereas the fixed design incurs huge loss due to the relatively higher upfront investment and higher unused capacity over its lifetime. This improvement in the value of flexibility indicate the ability of flexible design to better capture the upside opportunity of strong demand and better prevent the potential loss of weak demand compared to fixed design.

The Tornado diagram investigates the sensitivity of the value of flexibility subject to changes in learning rate. The changes in learning rate influences the flexible design value and consequently have effect on the value of flexibility. The results suggest that when the learning rate increases (i.e. 15% instead of 10%), the cost of deploying extra modular capacity decreases leading to a higher flexible design value and higher value of flexibility. On the other hand, when there is a low learning rate (i.e. 5% instead of 10%) the flexible design, that uses modular production facility, does not take advantage of cheaper capital investment for extra modular capacity leading to a lower flexible design value and consequently lower value of flexibility.

The Tornado diagram shows the sensitivity of the value of flexibility subject to changes in discount rate. One notices a difference in the results as compared to Case Study I in Sections 4.4 and 4.5, whereby a higher discount rate seems to improve the value of flexibility. As before, in capital-intensive and long-lasting project design, when the discount rate increases the present value of the project design decreases because future cash flow revenues are discounted back in a higher rate to the present time leading to a lower value of project design. On the other hand, when the discount rate decreases future cash flow revenues are discounted back at a lower rate to the present time leading to a higher value of the project design.

The results here show that when the discount rate increases (i.e. 12%) the value of both flexible and fixed designs are decreased but the flexible design is much less affected due to deferring capital investment for the initial capacity deployment leading to a higher value of flexibility compared to the analysis under the base discount rate (i.e. 10%). On the other hand, when the discount rate decreases the value of both flexible and fixed design improves relatively at the same pace leading to a lower value of flexibility. These observations reverse the effect of changes in discount rate observed under case study one where no forward-looking decision rules were applied for determining initial capacity. This may be due to the fact that this system, as opposed the one considered in case study one, is even more modular, and therefore can exploit further the benefits associated to deploying capacity in phases, and over time.

5.4.2 A computing budget allocation based screening approach

To obtain the true Pareto front, analysis with large number of sample scenarios (i.e., 2000 demand scenarios) is conducted. Figure 5.10 shows the dominant flexible designs using MOCBA with an experiment based on 300 scenarios. The preferred flexile design is shown in a circle.

Once the true Pareto front is obtained, the hyper-area is calculated using an arbitrary worst case reference point with ENPV=$0M and Standard deviation= $20M. The Pareto quality of the MOCBA in terms of different computer experiment will be discussed in section 5.6.

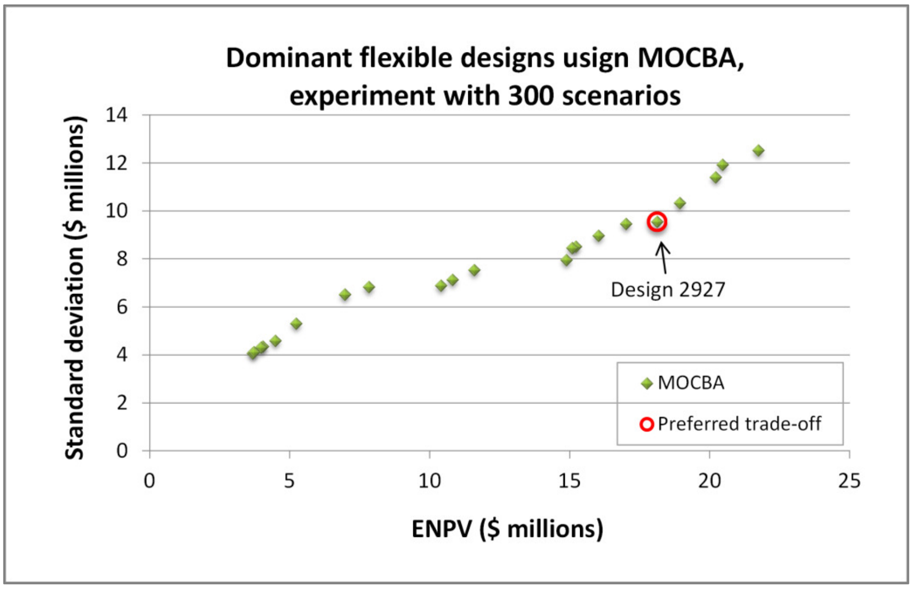


Figure 5.10: Dominant flexible designs using MOCBA approach

Once dominant flexible designs are obtained, a preferred flexible design can be chosen based on decision makers' preferences. Assuming weight 60% for ENPV and weight 40% for standard deviation, a flexible design with ENPV=$18.11M and standard deviation=$9.55M is chosen, shown in a circle in Figure 5.11. Table 5.10 shows the design vector of the preferred flexible design.

Table 5.10: Design vector of the preferred flexible design using MOCBA

Design number	X1	X2	MDC	TV
2927	40%	30%	25	75%

The solution suggests that the system operator should deploy initially capacity based on the following scenarios: 1) IF "the short-term forward looking forecast in year 6 lies in the projected lower (pessimistic) band demand with X1=40% width", THEN "initial capacity should not be deployed and the system operator should wait until demand reaches 75% of the 25 tpd modular capacity"; 2) IF "the short-term forward looking forecast in year 6 lies in the projected base case (most likely) band demand with X2=30% width" THEN "Initial capacity=25"; 3) IF "the short-term forward looking forecast in year 6 lies in the projected upper (optimistic) band demand with X3=1−X1−X2=30% width" THEN "Initial capacity=50". The system operator should use 25 tpd modular design and the capacity should be expanded every time demand reaches 75% of the installed 25 tpd modular capacity.

Post-optimality sensitivity analysis

The post-optimality results for the solution obtained from MOCBA are shown in Figure 5.11. The details of the post-optimality sensitivity analysis are provided in Appendix E. Results show that the sharpness volatility, discount rate and learning rate have the most to the least influences on the value of flexibility respectively. Due to similar explanations as provided in Section 5.4.1, the results show that when more (less) uncertainty is considered in the simulation process via variations in the sharpness parameter, the value of flexibility increases (decreases). The discount rate increases (decreases), the value of flexibility increases (decreases). Also, flexibility becomes more valuable when the learning rate increases due to further exploitation of the modularity.

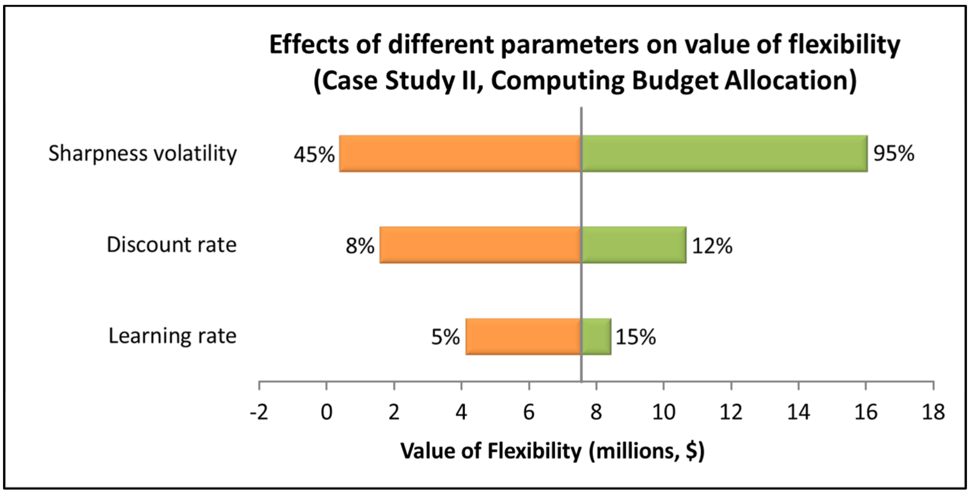


Figure 5.11: Post-optimality sensitivity analysis for the flexible design solution obtained using the computing budget allocation based screening approach, Case study II.

5.5 Exhaustive enumeration

The total number of the solution space combinations is determined by the precision level, which is determined by the step size of design variables and decision rules. The smaller the step size, the larger the number of possible combinations will be and, eventually, the more computationally intensive the exhaustive enumeration will be. Table 5.11 shows the number of flexible design solutions for each site in terms of different precision levels when only strategic and tactical level decisions are considered.

The best flexible design solutions can be obtained by exhaustively exploring the flexible design solution space. To evaluate each flexible design, a Monte Carlo simulation model with a large enough number of scenarios needs to be run, which may take a few seconds, minutes or even hours depending on the complexity of the simulation model. As a result, the enumeration technique can be computationally intensive or even intractable if a high-fidelity simulation model and high-level precision are used. Therefore, a screening model needs to be developed to quickly explore the flexible design solution space.

Table 5.11: Number of flexible design solutions for each site considering strategic and tactical flexibility

Design variables and decision rules' parameters for one location	LB	UB	**High-level precision**		**Mid-level precision**		**Low-level precision**	
			Step size	Steps	Step size	Steps	Step size	Steps
Band 1 - x1%	5%	45%	1%	41	5%	9	20%	3
Band 2 - x2%	5%	45%	1%	41	5%	9	20%	3
Modular design capacity	25	50	25	2	25	2	25	2
Threshold for capacity expansion	0%	100%	1%	101	5%	21	20%	6

Table 5.12 shows the design space of the decentralized LNG production system with mid-level precision. As can be seen, considering mid-level precision, the total number of flexible designs are 3,402 (=9×9×2×21).

Table 5.12: Characterization of the design space for flexibility analysis based on mid-level precision

Option	**Design variables**	**Units**	**Step Size**	**Values**	**Steps**
Strategic flexibility	Band 1 (X1)	% of Projected demand	5	5 to 45	9
	Band 2 (X2)	% of Projected demand	5	5 to 45	9
Tactical flexibility	Modular design capacity (MDC)	Tpd	25	25 to 50	2
	Threshold value (TV)	% of modular design	5	0 to 100	21

It is assumed that when both strategic and tactical flexibility are considered and the operational flexibility is “on”, the added value due to operational flexibility can be added later on. Table 5.13 shows flexible design vectors in a horizontal way. Once different flexible designs are synthesized, Monte Carlo simulation is used to generate different scenarios and analyze the flexible designs under uncertainty.

As a result of different possibilities of design variables and decision rules, different flexible design solutions can be generated. To conduct exhaustive enumeration Excel was used. Essentially, macros developed in VBA were used to synthesize different flexible designs in Excel spreadsheets.

Table 5.13: Different design vectors of flexible designs

Flexible design	Elements of flexible design vectors			
1	$X1_1$	$X2_1$	MDC_1	TV_1
2	$X1_2$	$X2_2$	MDC_2	TV_2
3	$X1_3$	$X2_3$	MDC_3	TV_3
⋮	⋮	⋮	⋮	⋮
n=3,402	$X1_n$	$X2_n$	MDC_n	TV_n

Figure 5.12 shows the interface between Microsoft Excel spreadsheet and macro developed using VBA in an exhaustive enumeration approach.

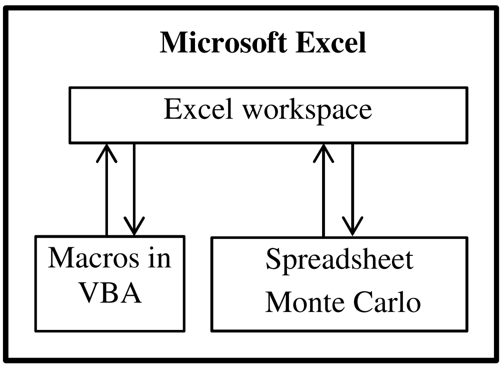


Figure 5.12: Interface between Microsoft Excel spreadsheet and macro developed using VBA in an exhaustive enumeration approach

To measure the performance of the LNG production system design, the performance at each site needs to be evaluated. Hence, the ENPV of the whole system under demand scenario s is calculated using equation 5.14:

$$ENPV_s = ENPV_{location\,(1)} + ENPV_{location\,(2)} + \cdots + ENPV_{location\,(5)} + \mathrm{ENPV_{OP}} \quad (5.14)$$

Table 5.14 shows the pseudocode for exhaustive enumeration approach for decentralized LNG production system design. Essentially dominant flexible designs were further analyzed under 2000 demand scenario to form the true Pareto front. Once dominant flexible designs are obtained, based on 2000 demand scenarios, decision makers can choose a trade-off solution based on their preferences. Assuming weight for ENPV is 60% and weight for Standard deviation is 40%, the preferred trade-off flexible design can be found. Based on decision makers' preferences, a flexible design solution with ENPV=S21.56M and standard deviation=S12.14M is chosen, shown in a circle in Figure 5.13.

Table 5.14: Pseudocode for Exhaustive Enumeration (EE) approach

```
Set input parameters
For Bound 1 = LB_Band1 to UB_Band1 Step_Band1
  For Bound 2 = LB_Band2 to UB_Band2 Step_Band2
    For MDC = LB_MDC to UB_MDC Step_MDC
      For TV = LB_TV to UB_TV Step_TV
                  Synthesize a flexible design vector
                       For i=1 to number of simulation
                           Application.calculate ← Generate a new scenario
                             Calculate NPV
                       Next
                 Calculate ENPV and Standard deviation of the design
      Next
    Next
  Next
Next
Return all design vectors with ENPV and standard deviation
```

Enumerate all flexible designs in objective function space

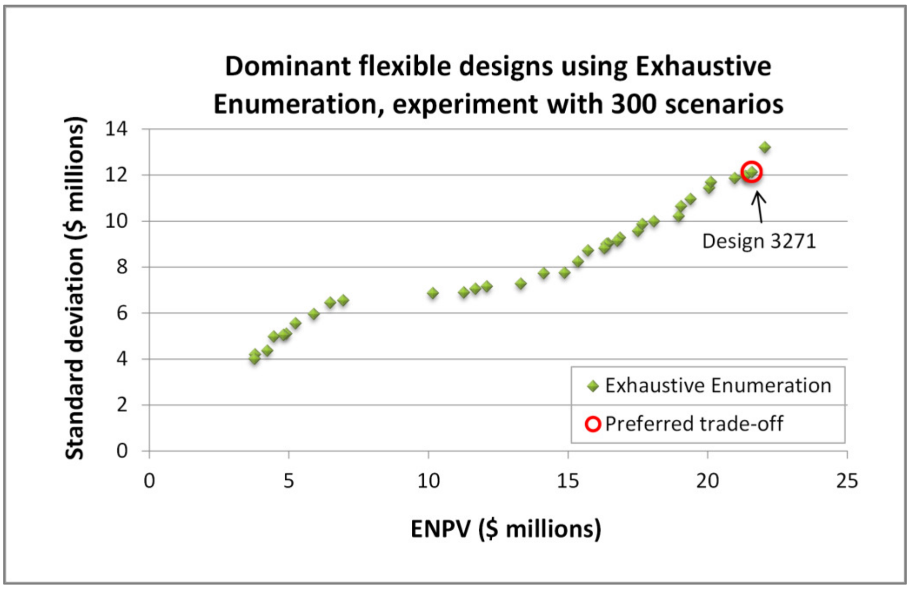


Figure 5.13: Exhaustive enumeration with an experiment with 300 demand scenarios

The corresponding design vector of the flexible deign is shown in Table 5.15.

Table 5.15: Design vector of preferred trade-off flexible design using EE

Design number	X1	X2	MDC	TV
3271	45%	35%	25	65%

The solution suggests that the system operator should deploy initially capacity based on the following scenarios: 1) IF "the short-term forward looking forecast in year 6 lies in the projected lower (pessimistic) band demand with X1=45% width", THEN "initial capacity should not be deployed and the system operator should wait until demand reaches 65% of the 25 tpd modular capacity"; 2) IF "the short-term forward looking forecast in year 6 lies in the projected base case (most likely) band demand with X2=35% width" THEN "Initial capacity=25"; 3) IF "the short-term forward looking forecast in year 6 lies in the projected upper (optimistic) band demand with X3=1−X1−X2=20% width" THEN "Initial capacity=50". The system operator should use 25 tpd modular design and the capacity should be expanded every time demand reaches 65% of the installed 25 tpd modular capacity.

Post-optimality sensitivity analysis

The post-optimality results for the solution obtained from Exhaustive Enumeration are shown in Figure 5.14. The details of the post-optimality sensitivity analysis are provided in Appendix E. Results show that the sharpness volatility, learning rate and discount rate have the most to the least influences on the value of flexibility respectively. Due to similar explanations as provided in Section 5.4.1, the results show that when more (less) uncertainty is considered in the simulation process via variations in the sharpness parameter, the value of flexibility increases (decreases). Also, flexibility becomes more valuable when the learning rate increases due to further exploitation of the modularity. Furthermore, the discount rate increases (decreases), the value of flexibility increases (decreases).

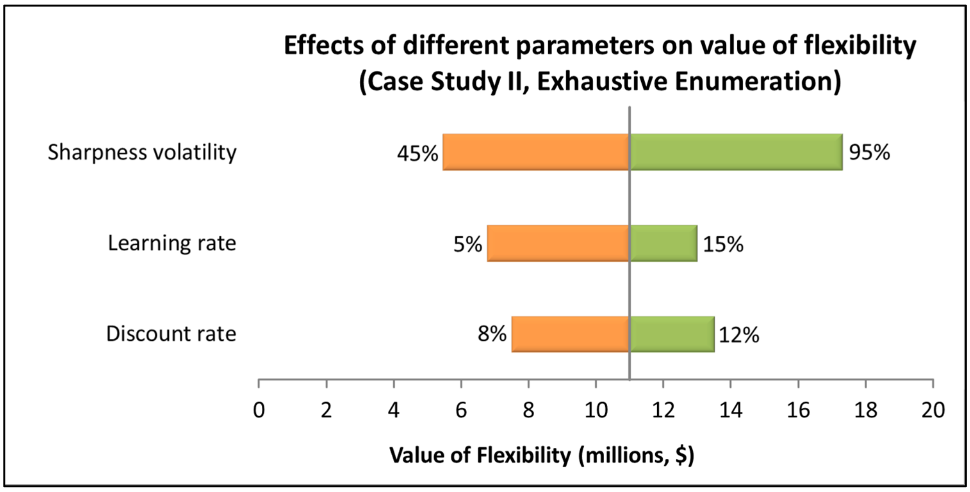


Figure 5.14: Post-optimality sensitivity analysis for the flexible design solution obtained using the exhaustive enumeration approach, Case study II.

5.6 Results and discussion

In this section, results obtained from the proposed screening framework are validated by comparing them with results of an exhaustive enumeration in terms of different computer experiments. In each computer experiment, for different screening approaches as well as the exhaustive enumeration, Pareto quality and simulation evaluation criteria are considered as performance metrics. Figure 5.15 shows dominant flexible designs for case study two, the decentralized LNG production system design, using different screening approaches with experiment based on 300 scenarios.

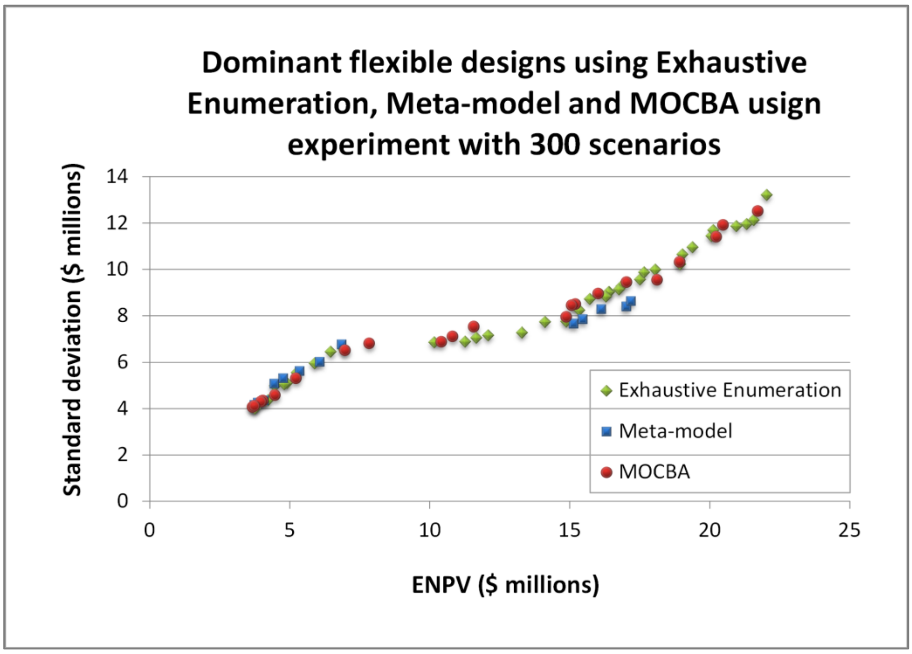


Figure 5.15: Dominant flexible designs using different approaches Meta-model based screening model (MM), Multi- Objective Computing Budget Allocation (MOCBA); Exhaustive Enumeration (EE)

Results obtained from other experiments are provided in Appendix C. As can be seen, Pareto designs using exhaustive enumeration have more spread as compared to meta-model and computing budget allocation based method. As a result, in the exhaustive enumeration, value corresponding to the Pareto quality (i.e., hyper-area) is the highest as compared to the other screening approaches.

Table 5.16 shows the comparison between meta-model (MM), multi-objective computing budget allocation (MOCBA), and exhaustive enumeration (EE) in terms of different performance metrics, the Pareto quality and the number of simulation evaluations. As expected, in terms of Pareto quality, exhaustive enumeration provides better results than meta-model and multi-objective computing budget allocation. As a result, the hyper-area of EE is systematically bigger than MM and MOCBA in terms of different experiments.

The larger the hyper-area the better the Pareto quality and the smaller number of simulation evaluation the more efficient the screening approach. For consistency, an arbitrarily worst case scenario is chosen with ENPV=$0M and Standard deviation=$20M for calculation of hyper-area in all the experiments.

Table 5.16: Comparison between MM, MOCBA, and EE in terms of different performance metrics, Pareto quality and maximum budget allocation

Experiments	**Pareto quality (hyper-area)**			**Number of simulation evaluation**		
	MM	MOCBA	EE	MM	MOCBA	EE
50	240	259	273	1,700	17,570	170,100
100	234	263	268	3,300	34,993	340,200
150	241	269	276	5,100	56,237	510,300
200	220	271	273	6,400	71,708	680,400
250	233	269	274	8,250	93,503	850,500
300	230	270	276	9,600	111,266	1,020,600

Let us compare the results in terms of different experiments. It should be noted that although different scenarios are considered in different experiments (i.e., 50 to 300 simulation evaluations), final true Pareto fronts are analyzed under the same analysis with large enough number of scenarios (i.e., 2000 demand scenarios). When the number of simulations in different experiments increases, the number of required simulation evaluations increases. By increasing the number of simulations in different experiments, however, the hyper-area does not strictly increase for the reasons explained in Section 4.6.

Now let us compare the results in terms of different screening approaches. For Pareto quality, multi-objective computing budget allocation (MOCBA) systematically offers better hyper-areas as compared to meta-model based screening approach, but requires more computations. This is similar to the results observed in case study 1. As expected, exhaustive enumeration offers the best Pareto quality among the other approaches.

For illustration purpose, let us compare the results in terms of different screening approaches with respect to a particular computer experiment. Considering the experiment with 50 sample scenarios, see the first row in Table 5.17, the meta-model and computing budget allocation approaches provide dominant flexible design solutions with 12% (i.e., (273-240)/273×100) and 5% (i.e., (273-259)/259)×100) Pareto quality gap (hyper-area) respectively as compared to the exhaustive enumeration. Furthermore, meta-model and computing budget allocation screening approaches require only 1% (i.e., 1,700/170,100) and 10.3% (i.e., 17,570/170,100) of the number of simulation evaluations, respectively, required in the exhaustive enumeration approach. In sum, there is indeed a trade-off between these two screening approaches in terms of expected Pareto quality and number of simulation evaluation.

Table 5.17 shows the comparison between MM, MOCBA, and EE in terms of computational runtime. All screening analyses were performed on a Windows 7 platform with 8 GB RAM and 3.3 GHz processing speed. Assuming each simulation evaluation takes one second, computational runtime for all screening methods are calculated.

Table 5.17: Comparison between MM, MOCBA, and EE in terms of computational runtime

Experiments	**Computational runtime (hours)**		
	MM	MOCBA	EE
50	0.47	4.88	47.25
100	0.92	9.72	94.5
150	1.42	15.62	141.75
200	1.78	19.92	189
250	2.29	25.97	236.25
300	2.67	30.91	283.5

As can be seen, by increasing the number of scenarios in the computer experiments the computational runtime proportionally increases. Exhaustive enumeration requires the most computational effort while the meta-model based screening method needs the least computational resource.

Table 5.18 shows the summary of results for the second case study where the flexible design with no operational flexibility is investigated considering weight 60% for ENPV and weight 40% for standard deviation for illustration purposes, in an experiment with 300 sample scenarios.

The Table provides value of flexibility when different screening approaches as well as the exhaustive enumeration approached are used. The value of flexibility using MM is calculated as $ENPV_{MM} - ENPV_{Fixed}$ = \$17.03M − \$10.56M = \$6.47M, the value of flexibility using MOCBA is calculated as $ENPV_{MOCBA} - ENPV_{Fixed}$ = \$18.11M− \$10.56M = \$7.55M and the value of flexibility using EE is calculated as $ENPV_{EE} - ENPV_{Fixed}$ = \$21.56M− \$10.56M = \$11M. As can be seen, EE provides the best value of flexibility with \$11M.

Table 5.18: Summary of results for case study two, flexible design with no operational flexibility considering W1=60% and W2=40% in an experiment with 300 scenarios

Criteria	**Computational runtime (hours)**		
	MM	MOCBA	EE
Design vector number	3305	2927	3271
Value of flexibility ($M)	6.47	7.55	**11**
Runtime (hours)	**2.67**	30.91	283.5

Figure 5.16 shows the cumulative density function of the preferred flexible designs resulted from the proposed screening framework, exhaustive enumeration and the fixed benchmark design. As can be seen, all the flexible designs can reduce the downside risk and capture the upsides opportunities. Decision-makers can feed the design(s) to a high-fidelity model to further investigate the design in a greater detail.

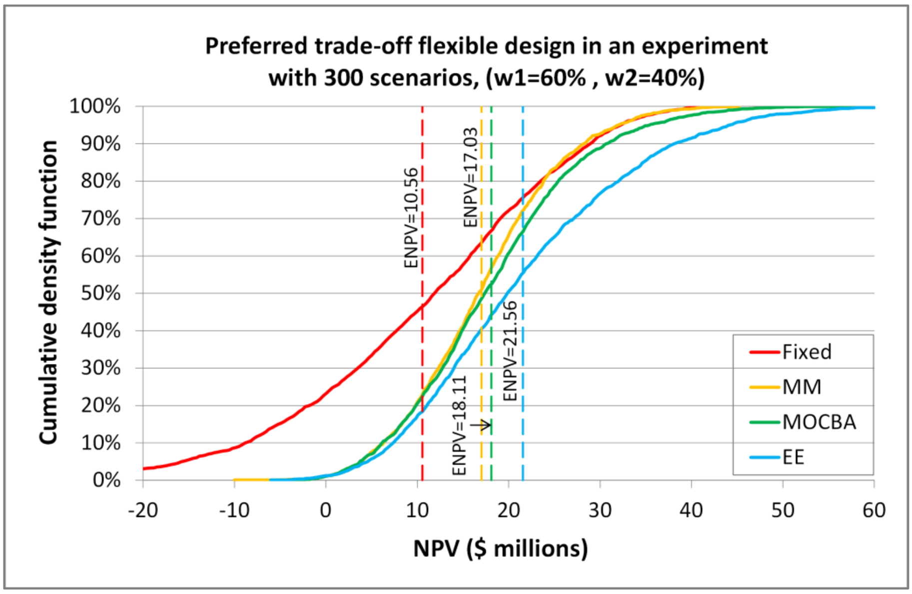


Figure 5.16: CDFs for preferred trade-off flexible designs for case study two in a computer experiment with 300 scenarios, w1=60% and w2=40%

5.7 Summary

This case study has proposed and applied an integrated multi-criteria screening framework to efficiently explore the solution space of flexible design and management strategies and effectively provide multi-criteria decision-making support in complex engineering systems. The proposed methodology is applied to the analysis of a real-world, decentralized on-shore LNG supply chain production design. The results demonstrate promising improvement in economic lifecycle performance by exploiting ideas of flexibility in comparison to a baseline design concept developed from standard design and evaluation approaches.

The results of the case study obtained using the proposed methodology can be explained to management, laymen, and policy-making audiences. the flexible design solution includes these decision variables: X1, X2, MDC and TV. Once the optimum values are obtained, the solution can be explained to laymen and a team of experts with diverse backgrounds. The solution suggests that the system operator should deploy initially capacity based on the following scenarios: 1) IF "the short-term forward looking forecast in year 6 lies in the projected lower (pessimistic) band demand with X1 width", THEN "initial capacity should not be deployed and the system operator should wait until demand reaches the amount TV of the MDC modular capacity"; 2) IF "the short-term forward looking forecast in year 6 lies in the projected base case (most likely) band demand with X2 width" THEN "Initial capacity=25"; 3) IF "the short-term forward looking forecast in year 6 lies in the projected upper (optimistic) band demand with X3=1−X1−X2 width" THEN "Initial capacity=50". The system operator should use modular design with capacity MDC and the capacity should be expanded every time demand reaches the amount TV of the installed MDC modular capacity.

Observations from the case study show that the screening approach reduces significantly computational time as compared to the full exhaustive search (0.1%

for MM and 11% for MOCBA). The MM and MOCBA approaches find flexible design solutions that recognize 59% and 69% of the value of flexibility identified under the full exhaustive search. This may represent a good tradeoff for decision-makers, depending on the amount of time and computational resources available for the analysis. Even if the value of flexibility is only recognized at about two-thirds the value from the exhaustive, it still represents 61% and 71% performance improvements as compared to the benchmark design respectively, which is significant given the multi-million dollar investment required. The recommended design can then be used for further high fidelity analysis, depending on the analyst's needs.

Chapter 6 Conclusion and Future Work

6.1 Introduction

This research has proposed an integrated multi-criteria screening framework to efficiently explore the solution space of flexible design and management strategies and effectively provide multi-criteria decision-making support in complex engineering systems. The proposed methodology covers two approaches: 1) a meta-model based screening approach; 2) a computing budget allocation based screening approach. For verification purpose, results obtained from these screening approaches were compared with the results obtained from the exhaustive enumeration. Essentially, the proposed methodology extends an existing three-step simulation based analysis for uncertainty and flexibility to account for screening and multi-criteria exploration of the flexible design space. The significance of the proposed framework is that for the first time, screening and multi-criteria approaches have been integrated in the context of flexibility in engineering systems design where different types of flexibility exist. To show the validity of the methodology, it has been applied to the designs of two variants of a real-world on-shore LNG production infrastructure system: a centralized and a decentralized one.

In the first phase of the methodology, problem modeling, attempts were made to demonstrate the economic value of flexibility in the long-term design and deployment of production facilities subject to demand growth uncertainty. Results demonstrated promising improvement on economic lifecycle performances where ideas of flexibility are exploited in the different levels of the project domain. This approach proves to be superior to a baseline design concept developed from standard design and evaluation approaches. The significance of the approach used in the first phase is that it motivates the use of flexibility in engineering design as a paradigm to deal with uncertainty affecting the lifecycle performance of engineering systems. In this respect, the study represents an argument for a shift in the design paradigm, away from the frequent focus on economies of scale and on to the development and deployment of unitary large facilities that embody this advantage. The concepts introduced in the problem modeling phase are general and can be applied to other distributed engineering systems sharing similar characteristics. However, consideration of flexibility adds another layer of complexity to the analytical problem making the simulation model computationally intensive.

To overcome the computational issue, screening was developed to efficiently explore flexible design strategies. Observations on the case studies showed that the screening model offers better performance than a full exhaustive search of the design space in terms of the number of evaluations required and of the simulation runtime, while providing good enough flexible design solutions in terms of lifecycle performance evaluation. These findings are significant as this approach enables decision-makers and practitioners to explore flexible design strategies at a fraction of the computational cost, while finding good enough solutions as compared to a full exhaustive search that may require hours, if not days, of computations on standard computers. The output from such analysis can then be fed into a higher fidelity model, if needed, for the more detailed and subsequent phase of the design analysis.

As decision-making typically involves several objectives, a multi-criteria decision-making using trade-space approach was introduced in the following step to further assist the decision-making process. In the proposed methodology, the multi-criteria decision-making approach was developed to evaluate flexible design strategies subject to different objectives and decision-makers' preferences. The results suggest that when dominant flexible designs are identified and classified into number of distinct flexible designs, a better decision-making platform is provided than a single criterion analysis. Using a multi-criteria decision-making approach hence is significant as generating different design solutions based on multiple objectives helps designers avoid starting with point designs, and allow them to recognize better design solutions.

6.2 Main contributions

This thesis, as a practical evaluation procedure, aims to facilitate the decision-making process, especially when computational resources are limited and the designer must consider multiple decision-making preferences and criteria. The proposed three-phase framework can be applied to evaluate flexibility in complex engineering systems design. The integrated multi-criteria screening framework consists of: 1) developing a simulation framework to evaluate flexibility in engineering systems design under uncertainty, accounting for both design variables and managerial decision rules; 2) developing a screening models based on meta-modeling approach and/or computing budget allocation to lessen the computational effort of simulations by balancing exploration and exploitation of design space (with some attention given to bottom-up heuristics-based simplifications in case study 2); and 3) applying a multi-criteria model to provide distinct dominant flexible designs consistent with decision-makers' preferences.

The proposed three-phase framework gives guidance to analysts to 1) consider flexibility systematically as a value-enhancing paradigm in the face of uncertainty, 2) speed up the analytical process, and 3) account for the fact that multiple decision criteria might have to be considered. Essentially, each phase is adding value upon each other. This is how the complete value is added, and the proposed methodology helps decision-makers make better design decisions, and system operators make better decisions in operations. As a result of saving time in the analytical process, systems designers and stakeholders can start analyzing the flexible system design in detail earlier than when an exhaustive enumeration approach is used. In addition, by considering multiple objectives and decision makers' preferences, the flexible design offered by the proposed framework would satisfy systems designers and stakeholders' preferences, and help identify a system that represents a good tradeoff between the decision makers' possibly conflicting objectives.

6.3 Recommendations

In this thesis, to explore the flexible design space efficiently and effectively two screening approaches were proposed: 1) A meta-model based screening approach; 2) A computing budget allocation based screening approach. Results show that if there are less limitations on computational resources, the computing budget allocation based can provide good-enough solutions in terms of measuring the economic benefits of flexibility. On the other hand, if there are strict limitations on computational resources, the meta-model based screening approach can provide good-enough solutions using the least computational cost. The exhaustive enumeration provides the best results in terms of the Pareto quality. In reality, however, this approach can be intractable from a computational standpoint. The framework provides the freedom to the decision makers to choose an appropriate screening method subject to the expected accuracy of results, and available computational resources.

Table 6.1 summarizes the results of the two case studies considering for illustrative purposes 60% weight for ENPV and 40% weight for standard deviation in a computer experiment with 300 scenarios.

Table 6.1: Summary of results for two case studies considering W1=60% and W2=40% in an computer experiment with 300 scenarios

Case study	**Criteria**	**Exploration of flexible design space**		
		MM	MOCBA	EE
Centralized LNG production system	Design vector number	601	2305	2592
	Value of flexibility ($M)	5.79	4.66	**9.95**
	Runtime (hours)	**5.00**	45.01	495.00
Decentralized LNG production system	Design vector number	3305	2927	3271
	Value of flexibility ($M)	6.47	7.55	**11**
	Runtime (hours)	**2.67**	30.91	283.5

Results show that in case study one MM has better performance than MOCBA while in case study two MOCBA has better performance than MM in terms of measuring the value of flexibility, as compared to the value determined by the exhaustive enumeration analysis. Results show that MM requires the least amount of computational resources among all approaches in two case studies. In sum, the choice of design space exploration approaches depends on whether the analyst wants to reduce computational burden at the expense of the solution quality, or emphasize quality at the expense of additional computational resources.

In case study one, while MM and MOCBA requiring respectively 1% and 9% of the computational runtime, the MM and MOCBA find flexible design solutions that recognize 58% and 47% of the value of flexibility identified under the full exhaustive search. This may represent a good tradeoff for decision-makers, depending on the amount of time and computational resources available for the analysis. Even if the value of flexibility is only recognized at about half the value from the exhaustive, it still represents 41% and 33% performance improvements as compared to the benchmark design, which is significant given the multi-million dollar investment required. Figures 6.1 represents the cumulative density function for preferred trade-off flexible designs for case study one in a computer experiment with 300 scenarios considering w1=60%, w2=40%.

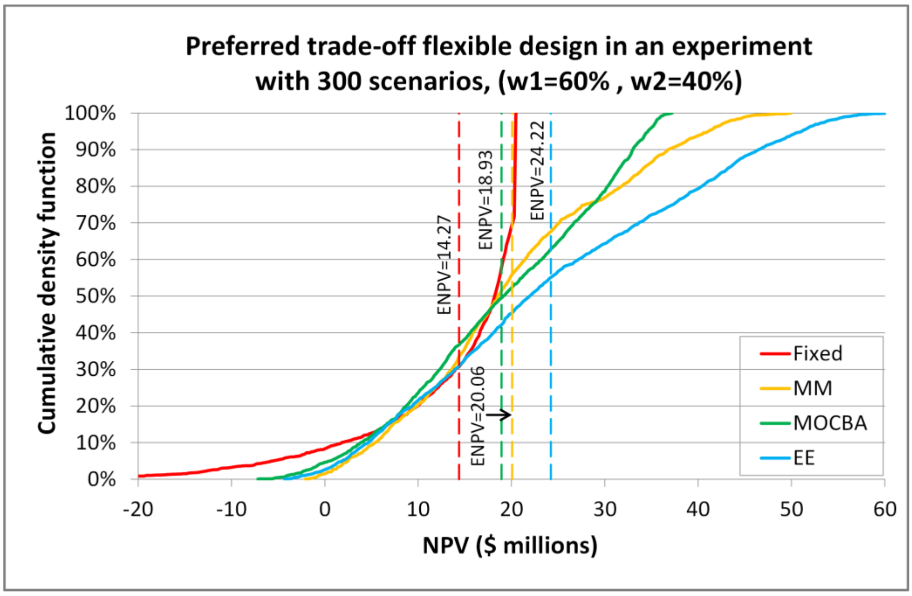


Figure 6.1: CDFs for preferred trade-off flexible designs for case study one in a computer experiment with 300 scenarios, w1=60%, w2=40%

The analyst can choose a flexible design in terms of different economic performance metrics such as ENPV, value at risk, value at gain and standard deviation in a multi-criteria decision-making table. The recommended design can then be used for further high fidelity analysis, depending on the analyst's needs.

In case study two, observations from the case study show that the screening approach reduces significantly computational time as compared to the full exhaustive search (0.1% for MM and 11% for MOCBA). The MM and MOCBA approaches find flexible design solutions that recognize 59% and 69% of the value of flexibility identified under the full exhaustive search. This may represent a good tradeoff for decision-makers, depending on the amount of time and computational resources available for the analysis. Even if the value of flexibility is only recognized at about two-thirds the value from the exhaustive, it still represents 60% and 70% performance improvements as compared to the benchmark design, which is significant given the multi-million dollar investment required.

Figures 6.2 represents the cumulative density function for preferred trade-off flexible designs for case study two in a computer experiment with 300 scenarios considering w1=60%, w2=40%. The analyst can choose a flexible design in terms of different economic performance metrics such as ENPV, value at risk, value at gain and standard deviation in a multi-criteria decision-making table. The recommended design can then be used for further high fidelity analysis, depending on the analyst's needs.

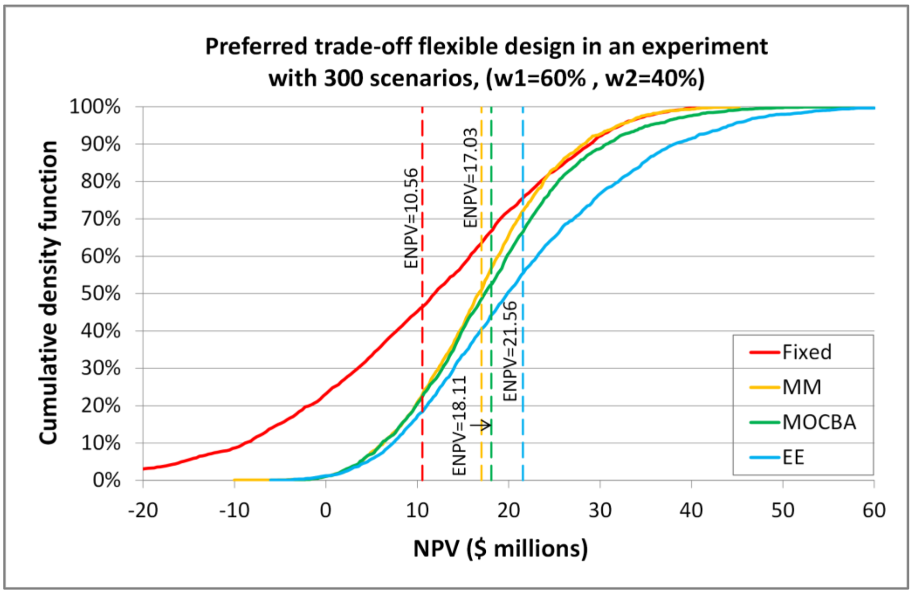


Figure 6.2: CDFs for preferred trade-off flexible designs for case study two in a computer experiment with 300 scenarios, w1=60% and w2=40%

6.4 Results validity, limitations and future work

Results validity, limitations and future work are discussed in this section.

6.4.1 Results validity

Validity of the results is discussed here along the three angles: 1) External validity; 2) Internal validity and 3) Reliability.

The external validity of the results refers to what extent the obtained results can be generalized to other contexts and systems. As the literature review in Chapter 2 shows, the methodology of the three-step simulation based flexibility analysis can be applied to different domains, see Table 2.1. As simulation is the core part of the proposed screening-based framework, it is reasonable to assume that the proposed screening methodology could be applied in different domains as well. While the proposed methodology was applied to two variants of an LNG infrastructure system to provide support to the above claim, more work is needed to fully validate and guarantee generalizability of the proposed framework, and to determine to what extent it generalizes to other classes of engineering systems.

Internal validity is discussed here to show how one can trust the procedure and the cause and effect relationships represented in the proposed framework. Essentially, flexibility is worthwhile to consider and improves performance, and that the proposed framework can do that faster. First, an economic model was developed from data collected based on close interactions with industry collaborators, cost and market information from publicly available sources, and it was relied on standard methods used for analysis (simulation, optimization, DCF). Second, the speed of the proposed approach using the same computer for all experiments and across all three methods (MM, MOCBA, and EE) were compared.

Reliability of the results is discussed here to show how repeatable the experiments are. The same underlying assumptions for the simulation processes were used when all three methods were compared and a large set of simulation samples were used, thus reinforcing the statistical validity.

6.4.2 Limitations and future work

Although the proposed multi-criteria screening framework has addressed the identified research gaps in the literature, several interesting and challenging directions remain to be considered for future extensions.

Problem modeling

In the problem modeling phase, the demand sites and location of the plants are assumed to be pre-decided. These considerations determine the distances between plants and demand points and thus further determine the transportation costs. Hence, one possible future research direction is to extend the strategic decisions to determine the optimal plant set-up, namely identifying a location based on observed LNG demand in many candidate production sites. This is closer to how, in reality, plant investment decisions are made. Also, set-covering principles from operations research area may be employed to address this problem. Another possible avenue for future work is to extend the strategic level decisions of the problem so that the location of the facility can be decided in this phase.

While the proposed multi-criteria screening framework was applied to LNG production system design, it could be applied to other engineering systems with different types of flexibility. For the operational flexibility, only the rebalancing schema was used; different types of operational screening models could be used to efficiently explore the operational solution space.

The proposed framework is developed to address the computational complexity associated with exploring large number of flexible design solutions for complex engineering systems, which is already motivated in the literature focusing on flexibility in engineering design (e.g. Lin, de Weck et al. (2012)). In this study, only exogenous market-related uncertainty is considered, while other uncertainty sources can also be considered in the simulation model. When the number of uncertainty factors increases, the computational complexity of the simulation model increases as well. As a result, the enumeration of different flexible designs can be computationally intensive or even intractable when simulating each flexible design, which may take several hours if not days. Therefore, the increased computational complexity even further motivates us to apply meta-modeling and computing budget allocation based screening approaches, especially when the computational resources are limited. An extensive study considering multiple uncertainty sources and real option strategies can be considered as an opportunity for future improvement and work.

It was also assumed that the number of design vector combinations was of a size such that an exhaustive search was still feasible – even though taking days of computations. In many complex systems, however, exhaustive search could be computationally intractable. To address this issue, an optimization mechanism could be coupled with a meta-modeling approach to overcome the combinatorial complexity of the flexible design space. In other words, the design space with different types of flexibility can be combinatorial, and combinatorial space grows large easily. Therefore evolutionary algorithms such as genetic algorithm and scatter search among others could be used to augment the current framework to efficiently explore large number of flexible design solutions.

Meta- modeling approach

In the meta-model approach, while the multi-criteria phase was done sequentially after the screening phase in this research, by merging the screening phase and multi-criteria decision-making technique, the results of the trade-off solutions could be further improved. The current meta-model based screening approach samples from the design space to separately improve the response surface for each objective function (i.e. ENPV or standard deviation). In multi-objective optimization, however, samples should be drawn from the design space to improve the trade-off flexible solutions with respect to different objectives. Hence, a multi-objective version of the meta-modeling approach could be applied in the future research to improve the Pareto front solutions. Although a Kriging meta-model in the DACE model for deterministic simulation was used in this study, further research is required to investigate the application of the stochastic version of the Kriging meta-model for current stochastic simulation for uncertainty and flexibility.

Computing budget allocation approach

Furthermore, the current computing budget allocation analysis requires a predefined set of input parameters and these parameters need to be fine-tuned for better performance. More work may focus on exploring other combinations of parameters, and determine how this may affect the results. While a heuristic multi-objective computing budget allocation based screening model was developed in this study, an optimal computing budget allocation (OCBA) can be applied to see the effects of the optimal simulation budget allocation feature. Essentially in OCBA, an optimal ratio is defined and calculated to determine the optimal simulation budget allocation for stochastic simulations, at each iteration of the algorithm.

Bibliography

Allen, T., D. Mcgowan, J. Moses, et al. (2002). "ESD terms and definitions." Journal of Project Management, from http://esd.mit.edu/WPS/esd-wp-2002-01.pdf.

Andersson, H., M. Christiansen and K. Fagerholt (2010). Transportation planning and inventory management in the LNG supply chain. Energy, natural resources and environmental economics, Springer**:** 427-439.

Babajide, A. (2007). Real options analysis as a decision tool in oil field developments, Massachusetts Institute of Technology.

Babajide, A., R. de Neufville and M. A. Cardin (2009). "Integrated method for designing valuable flexibility in oil development projects." SPE Projects Facilities & Construction **4**(2).

Barman, B. (2007). A streamlined real options model for Real Estate Development. Master's degree, Massachusetts Institute of Technology.

Bartolomei, J. E., D. Hastings, R. De Neufville, et al. (2006). Screening for real options 'in'an engineering system: a step towards flexible weapon system development'. Part I: the use of design matrices to create an end-to-end representation of a complex socio-technical system, paper presented at the INCOSE Conference on System Engineering Research, Los Angeles, CA.

Black, F. and M. Scholes (1973). "The pricing of options and corporate liabilities." Journal of Political Economy **81**(3): 637-654.

Bradstreet, L., L. While and L. Barone (2008). "A fast incremental hypervolume algorithm." Evolutionary Computation, IEEE Transactions on **12**(6): 714-723.

Brealey, R. and S. Myers (2000). Principles of corporate finance, Boston: Irwin:'McGraw-Hill.

Browning, T. R. and E. C. Honour (2008). "Measuring the life-cycle value of enduring systems." Systems Engineering **11**(3): 187-202.

Cardin, M.-A. (2007). Facing reality: design and management of flexible engineering systems Master of Science Thesis in Technology and Policy, Massachusetts Institute of Technology.

Cardin, M.-A., R. de Neufville and V. Kazakidis (2008). "Process to improve expected value of mining operations." Mining Technology **117**(2): 65-70.

Cardin, M.-A., G. L. Kolfschoten, D. D. Frey, et al. (2013). "Empirical evaluation of procedures to generate flexibility in engineering systems and improve lifecycle performance." Research in Engineering Design **24**(3): 277-295.

Cardin, M.-A., M. Ranjbar-Bourani, Y. Deng, et al. (2013). "Quantifying the value of flexibility in oil and gas projects: a case study of centralized vs. decentralized LNG production systems." Keppel Offshore & Marine Technology Centre, Technology Review 2013.

Cardin, M.-A. (2014). "Enabling flexibility in engineering systems: a taxonomy of procedures and a design framework." ASME Journal of Mechanical Design **136**(1).

Cardin, M.-A., M. Ranjbar-Bourani and R. de Neufville (2015). "Improving the lifecycle performance of engineering projects with flexible strategies: example of on-shore LNG production design." Systems Engineering **18**(3): 253-268.

Chambers, R.-D. (2007). Tackling uncertainty in airport design: a real options approach, Technology and Policy, MIT.

Cox, J. C., S. A. Ross and M. Rubinstein (1979). "Options pricing: a simplified approach." Journal of Financial Economics **7**(3): 229-263.

Czyzżak, P. and A. Jaszkiewicz (1998). "Pareto simulated annealing—a metaheuristic technique for multiple-objective combinatorial optimization." Journal of Multi-Criteria Decision Analysis **7**(1): 34-47.

de Neufville, R. and A. Pirnar (1999). "A dynamic technology strategy for Xerox to respond to the threat of high-tech commoditisation." International Journal of Technology Management **18**(1): 73-92.

de Neufville, R. (2000). "Dynamic strategic planning for technology policy." International Journal of Technology Management **19**(3): 225-245.

de Neufville, R., S. Scholtes and T. Wang (2006). "Real options by spreadsheet: parking garage case example." Journal of infrastructure systems **12**(2): 107-111.

de Neufville, R. (2008). "Building airport systems for the next generation." The Bridge, Journal of the National Academy of Engineering, Special Issue on Transportation Infrastructure: pp.41-46-pp.41-46.

de Neufville, R., K. Hodota, J. Sussman, et al. (2008). "Real options to increase the value of intelligent transportation systems." Transportation Research Record: Journal of the Transportation Research Board **2086**(-1): 40-47.

de Neufville, R., Y. S. Lee and S. Scholtes (2008). Using flexibility to improve value-for-money in hospital infrastructure investments. First International Conference on Infrastructure Systems and Services: Building Networks for a Brighter Future (INFRA), IEEE.

de Neufville, R. and S. Scholtes (2011). Flexibility In Engineering Design. Cambridge, MA, United States, MIT Press.

de Weck, O. L., R. de Neufville and M. Chaize (2004). "Staged deployment of communications satellite constellations in Low Earth Orbit." Journal of Aerospace Computing, Information, and Communication **1**: 119-136.

Deb, K. (2001). Multi-Objective Optimization using Evolutionary Algorithms, John Wiley & Sons Chichester.

Deb, K. and S. Tiwari (2005). Omni-optimizer: a procedure for single and multi-objective optimization. Evolutionary Multi-Criterion Optimization, Springer.

Deb, K. (2014). Multi-objective optimization. Search methodologies, Springer**:** 403-449.

Dixit, A. K. and R. S. Pindyck (1994). Investment under Uncertainty. NJ, United States, Princeton University Press.

ECS. (2011, June). "Western Australia natural gas demand and supply - a forecast." Report for the DomGas Alliance, from http://www.latentpet.com/_content/documents/575.pdf.

Engel, A. and T. R. Browning (2008). "Designing systems for adaptability by means of architecture options." Systems Engineering **11**(2): 125-146.

Fitzgerald, M. E., A. M. Ross and D. H. Rhodes (2012). Assessing uncertain benefits: a valuation approach for strategic changeability (VASC). INCOSE International Symposium, Citeseer.

Frey, D. D. and H. Wang (2006). "Adaptive One-Factor-at-a-Time experimentation and expected value of improvement." Technometrics **48**(3): 418-431.

Friedman, J. H. (1991). "Multivariate adaptive regression splines." The annals of statistics: 1-67.

Georgiadis, D. R., T. A. Mazzuchi and S. Sarkani (2013). "Using multi criteria decision making in analysis of alternatives for selection of enabling technology." Systems Engineering **16**(3): 287-303.

GLE. (2011, November 2011). "GLE position paper: GLE's view on small scale LNG." Gas LNG Europe, from www.gie.eu.

GLE (2013). GLE Position Paper: Overcoming barriers in the Small Scale LNG development. Gas LNG Europe, Gas Infrastructure Europe: 10.

Greden, L., R. de Neufville and L. Glicksman (2005). Management of technology investment risk with real options-based design: a case study of an innovative building technology. 9 th Annual Real Options Conference, Citeseer.

Greden, L. V. (2005). Flexibility in building design: A real options approach and valuation methodology to address risk, Massachusetts Institute of Technology.

Grierson, D. E. (2008). "Pareto multi-criteria decision making." Advanced Engineering Informatics **22**(3): 371-384.

Grønhaug, R. and M. Christiansen (2009). Supply chain optimization for the Liquefied Natural Gas business. Innovations in Distribution Logistics, Springer**:** 195-218.

Guma, A. C. (2008). A real options analysis of a vertically expandable real estate development. Master's degree, Massachusetts Institute of Technology.

Guma, A. C., J. Pearson, K. Wittels, et al. (2009). "Vertical phasing as a corporate real estate strategy and development option." Journal of Corporate Real Estate **11**(3): 144-157.

Gupta, A. P. (2011). Governance mechanisms for infrastructure public-private partnerships: focus on India, Massachusetts Institute of Technology.

Güyagüler, B. (2002). Optimization of well placement and assessment of uncertainty. Doctor of Philosophy Dissertation, Stanford University.

Hassan, R., R. de Neufville and D. McKinnon (2005). Value-at-risk analysis for real options in complex engineered systems. Systems, Man and Cybernetics, 2005 IEEE International Conference on.

Hassan, R. and R. de Neufville (2006). Design of engineering systems under uncertainty via real options and heuristic optimization. Real Options Conference. New York, NY, United States.

Hong, L. J. and B. L. Nelson (2006). "Discrete optimization via simulation using COMPASS." Operations Research **54**(1): 115-129.

Horn, J. (1996). "Multicriteria decision making and evolutionary computation."

Hsu, C., J. Cho, L. Yee, et al. (1995). "Core information model: a practical solution to costly integration problems." Computers & Industrial Engineering **28**(3): 523-544.

Hu, J. and M.-A. Cardin (2015). "Generating flexibility in the design of engineering systems to enable better sustainability and lifecycle performance." Research in Engineering Design **26**(2): 121-143.

Jacoby, H. and D. Loucks (1972). "The combined use of optimization and simulation models in river basin planning." Water Resources Research **8**(6): 1401-1414.

Jaszkiewicz, A. (2004). "A comparative study of multiple-objective metaheuristics on the bi-objective set covering problem and the Pareto memetic algorithm." Annals of Operations Research **131**(1-4): 135-158.

Jones, D. R., M. Schonlau and W. J. Welch (1998). "Efficient global optimization of expensive black-box functions." Journal of Global Optimization **13**(4): 455-492.

Jones, D. R. (2001). "A taxonomy of global optimization methods based on response surfaces." Journal of Global Optimization **21**(4): 345-383.

Julka, N., T. Baines, B. Tjahjono, et al. (2007). "A review of multi-factor capacity expansion models for manufacturing plants: Searching for a holistic decision aid." International Journal of Production Economics **106**(2): 607-621.

Justesen, P. D. (2010). Distinct candidates optimization: a novel approach to applied evolutionary multi-and many-objective optimization, Ph. D. thesis, 2010. Dept. of Computer Science, Aarhus University, www. cs. au. dk/~ juste/MOEA/main2. pdf.

Kalligeros, K. C. (2006). Platforms and real options in large-scale engineering systems. Doctor of Philosophy Dissertation, Massachusetts Institute of Technology.

Kalligeros, K. C., O. de Weck, R. de Neufville, et al. (2006). Platform identification using design structure matrices. Sixteenth Annual International Symposium of the International Council On Systems Engineering (INCOSE), INCOSE.

Kazakidis, V. and M. Scoble (2003). "Planning for flexibility in underground mine production systems." Mining Engineering **55**(8): 33-38.

Kim, I. Y. and O. De Weck (2006). "Adaptive weighted sum method for multiobjective optimization: a new method for Pareto front generation." Structural and Multidisciplinary Optimization **31**(2): 105-116.

Kleijnen, J. P. (2009). "Kriging metamodeling in simulation: A review." European Journal Of Operational Research **192**(3): 707-716.

Kumar, S., H.-T. Kwon, K.-H. Choi, et al. (2011). "Current status and future projections of LNG demand and supplies: A global prospective." Energy Policy **39**(7): 4097-4104.

Lee, L. H., E. P. Chew, S. Teng, et al. (2010). "Finding the non-dominated Pareto set for multi-objective simulation models." IIE Transactions **42**(9): 656-674.

Lee, L. H., E. P. Chew and H. Li (2011). Multi-objective compass for discrete optimization via simulation. Simulation Conference (WSC), Proceedings of the 2011 Winter, IEEE.

Lee, Y. S. (2007). Flexible design in Public Private Partnerships: a PFI case study in the National Health Service. Master's Dissertation, University of Cambridge.

Lin, J. (2009). Exploring flexible strategies in engineering systems using screening models - applications to offshore petroleum projects Doctoral Dissertation in Engineering Systems, Massachusetts Institute of Technology.

Lin, J., O. de Weck, R. de Neufville, et al. (2009). Designing capital-intensive systems with architectural and operational flexibility using a screening model. Complex sciences, Springer**:** 1935-1946.

Lin, J., O. de Weck and D. MacGowan (2012). "Modeling epistemic subsurface reservoir uncertainty using a reverse Wiener jump–diffusion process." Journal of Petroleum Science and Engineering **84–85**(0): 8-19.

Lister, M. J. (2007). Towards a new real estate: innovative financing for a better built environment. Master's degree, Massachusetts Institute of Technology.

Longstaff, F. A. and E. S. Schwartz (2001). "Valuing American options by simulation: A simple least-squares approach." Review of Financial studies **14**(1): 113-147.

Mangin, C. G. E., R. de Neufville, F. Field Iii, et al. (1995). "Defining markets for new materials: Developing a utility methodology with case application." Resources Policy **21**(3): 169-178.

Markowitz, H. M. (1991). "Foundations of portfolio theory." The Journal of Finance **46**(2): 469-477.

Maseda, L. J. (2008). Real option analysis of flexibility in a hospital emergency department expansion project: a systems approach, Massachusetts Institute of Technology.

Masunaga, S. (2007). A comparative study of real options valuation methods: economics-based approach vs. engineering-based approach. Master's degree, Massachusetts Institute of Technology.

Matheron, G. (1963). "Principles of geostatistics." Economic geology **58**(8): 1246-1266.

McConnell, J. B. (2007). A life-cycle flexibility framework for designing, evaluating and managing "complex" real options: Case studies in urban transportation and aircraft systems. Doctor of Philosophy Dissertation, Engineering Systems Division, MIT.

Meckesheimer, M., R. R. Barton, T. Simpson, et al. (2001). "Metamodeling of combined discrete/continuous responses." AIAA journal **39**(10): 1950-1959.

Mikaelian, T., D. J. Nightingale, D. H. Rhodes, et al. (2011). "Real options in enterprise architecture: A holistic mapping of mechanisms and types for uncertainty management." IEEE Transactions on Engineering Management **54**(3): 457-470.

Mittal, G. (2004). Real options approach to capacity planning under uncertainty, Massachusetts Institute of Technology.

Morgado, F., S. S. Nagaralu, R. Macairio, et al. (2011). Value of options in airport expansion - Example of AICM. Proceedings of the European Regional Science Association, 51st European Congress, Barcelona, Spain, European Regional Science Association.

Nebro, A., J. Durillo, C. Coello Coello, et al. (2008). A study of convergence speed in multi-objective metaheuristics. Parallel Problem Solving from Nature – PPSN X. G. Rudolph, T. Jansen, S. Lucas, C. Poloni and N. Beume, Springer Berlin Heidelberg. **5199:** 763-772.

Neely III, J. E. and R. de Neufville (2001). "Hybrid real options valuation of risky product development projects." International Journal of Technology, Policy and Management **1**(1): 29-46.

Nielsen, H. B., S. N. Lophaven and J. Søndergaard (2002). "DACE, a MATLAB Kriging toolbox." Technical University of Denmark, http://www. imm. dtu. dk/~ hbn/dace.

Nilchiani, R. and D. E. Hastings (2007). "Measuring the value of flexibility in space systems: A six-element framework." Systems Engineering **10**(1): 26-44.

Ohama, D. (2008). Using design flexibility and real options to reduce risk in Private Finance Initiatives: the case of Japan, Massachusetts Institute of Technology.

Olewnik, A. and K. Lewis (2006). "A decision support framework for flexible system design." Journal of Engineering Design **17**(1): 75-97.

Özelkan, E. C., A. D'Ambrosio and S. G. Teng (2008). "Optimizing liquefied natural gas terminal design for effective supply-chain operations." International Journal of Production Economics **111**(2): 529-542.

Pearson, J. R. and K. S. Wittels (2008). Real options in action: vertical phasing in commercial real estate development. Master of Science in Real Estate Development Massachusetts Institute of Technology.

Petkova, B. (2007). Strategic planning for rail system design: An application for portuguese high speed rail, Master's Thesis, Industrial Engineering and Management, University of Groningen. Groningen, Netherlands.

Pochard, S. (2003). Managing risks of supply-chain disruptions: dual sourcing as a real option, Massachusetts Institute of Technology. .

Quispez-Asin, N. (2007). Hybrid lattice and decision analysis of real options: Application to a supply chain strategy, Massachusetts Institute of Technology.

Ramirez, N. (2002). Valuing flexibility in infrastructure developments: the Bogota water supply expansion plan, Citeseer.

Ranjbar-Bourani, M., M.-A. Cardin, W. S. Chong, et al. (2013). An integrated screening framework to analyze flexibility in engineering systems design. International Conference on Engineering Design, Seoul, Korea, The Design Society.

Raphael, B. (2011). "Multi-criteria decision making for collaborative design optimization of buildings." Built Environment Project and Asset Management **1**(2): 3-3.

Rivey, D. (2007). A practical method for incorporating Real Options analysis into US federal benefit-cost analysis procedures, Massachusetts Institute of Technology.

Roques, F. A., W. J. Nuttall, D. M. Newbery, et al. (2006). "Nuclear power: a hedge against uncertain gas and carbon prices?" The Energy Journal: 1-23.

Ross, A., N. P. Diller, D. Hastings, et al. (2002). Multi-attribute tradespace exploration in space system design. 53rd International Astronautical Congress, Houston,Texas.

Ross, A. (2006). Managing unarticulated value: changeability in multi-attribute tradespace exploration Doctoral Dissertation in Engineering Systems, Massachusetts Institute of Technology.

Ross, A. M. and D. E. Hastings (2005). The tradespace exploration paradigm. INCOSE International Symposium 2005, Rochester, NY.

Ross, A. M. (2006). Managing unarticulated value: changeability in multi-attribute tradespace exploration. Doctor of Philosophy Dissertation, Massachusetts Institute of Technology. .

Ross, A. M. and D. H. Rhodes (2008). Using natural value-centric time scales for conceptualizing system timelines through epoch-era analysis. INCOSE International Symposium, Utrecht, the Netherlands.

Ross, A. M., D. H. Rhodes and D. E. Hastings (2008). "Defining changeability: Reconciling flexibility, adaptability, scalability, modifiability, and robustness for maintaining system lifecycle value." Systems Engineering **11**(3): 246-262.

Rouse, W. B., C. W. Howard, W. E. Carns, et al. (2000). "Technology investment advisor: An options-based approach to technology strategy." Information, Knowledge, Systems Management **2**(1): 63-81.

Ryan, E. T., D. R. Jacques and J. M. Colombi (2013). "An ontological framework for clarifying flexibility-related terminology via literature survey." Systems Engineering **16**(1): 99-110.

Sacks, J., W. J. Welch, T. J. Mitchell, et al. (1989). "Design and analysis of computer experiments." Statistical science **4**(4): 409-423.

Savage, S. L. (2009). The Flaw of Averages: Why We Underestimate Risk in the Face of Uncertainty, John Wiley and Sons.

Sullivan, W. G., E. M. Wicks, C. P. Koelling, et al. (2009). Engineering economy, Pearson Prentice Hall.

Sussman, J. M. and J. B. McConnell (2007). A life-cycle flexibility framework for designing, evaluating and managing" complex" real options: case studies in urban transportation and aircraft systems, Massachusetts Institute of Technology.

Taboada, H. A., F. Baheranwala, D. W. Coit, et al. (2007). "Practical solutions for multi-objective optimization: An application to system reliability design problems." Reliability Engineering & System Safety **92**(3): 314-322.

Trigeorgis, L. (1996). Real Options: Managerial Flexibility and Strategy in Resource Allocation, MIT Press.

Tsui, M. (2005). Valuing innovative technology R&D as a real option: Application to fuel cell vehicles. Master's degree, Massachusetts Institute of Technology.

Ulungu, E., J. Teghem, P. Fortemps, et al. (1999). "MOSA method: a tool for solving multiobjective combinatorial optimization problems." Journal of Multi-Criteria Decision Analysis **8**(4): 221-236.

Van Groenendaal, W. J. H. and J. P. C. Kleijnen (1998). Identifying important factors in deterministic investment problems using design of experiments, IEEE Computer Society Press.

Viscito, L., D. Chattopadhyay and A. M. Ross (2009). Combining Pareto trace with filtered outdegree for identifying valuably flexible systems.

Viscito, L. and A. M. Ross (2009). Quantifying flexibility in tradespace exploration: value weighted filtered outdegree, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Dr., Suite 500 Reston VA 20191-4344 USA.

Wang, T. (2003). Analysis of real options in hydropower construction projects - a case study in china. Master's degree, Massachusetts Institute of Technology.

Wang, T. and R. de Neufville (2004). Building real options into physical systems with stochastic mixed-integer programming. Proceedings of the 8th Real Options Annual International Conference, Citeseer.

Wang, T. (2005). Real options in projects and systems design - identification of options and solutions for path dependency Doctoral Dissertation in Engineering Systems, Massachusetts Institute of Technology.

Yang, Y. (2009). A screening model to explore planning decisions in automotive manufacturing systems under demand uncertainty. Doctor of Philosophy Dissertation, Massachusetts Institute of Technology.

Zhang, N. (2010). Apply option-thinking in long term infrastructure investment: the case of commercial real estate. Master's degree, Massachusetts Institute of Technology.

Zhang, S. X. and V. Babovic (2011). "An evolutionary real options framework for the design and management of projects and systems with complex real options and exercising conditions." Decision Support Systems **51**(1): 119-129.

Zitzler, E., L. Thiele, M. Laumanns, et al. (2003). "Performance assessment of multiobjective optimizers: an analysis and review." Evolutionary Computation, IEEE Transactions on **7**(2): 117-132.

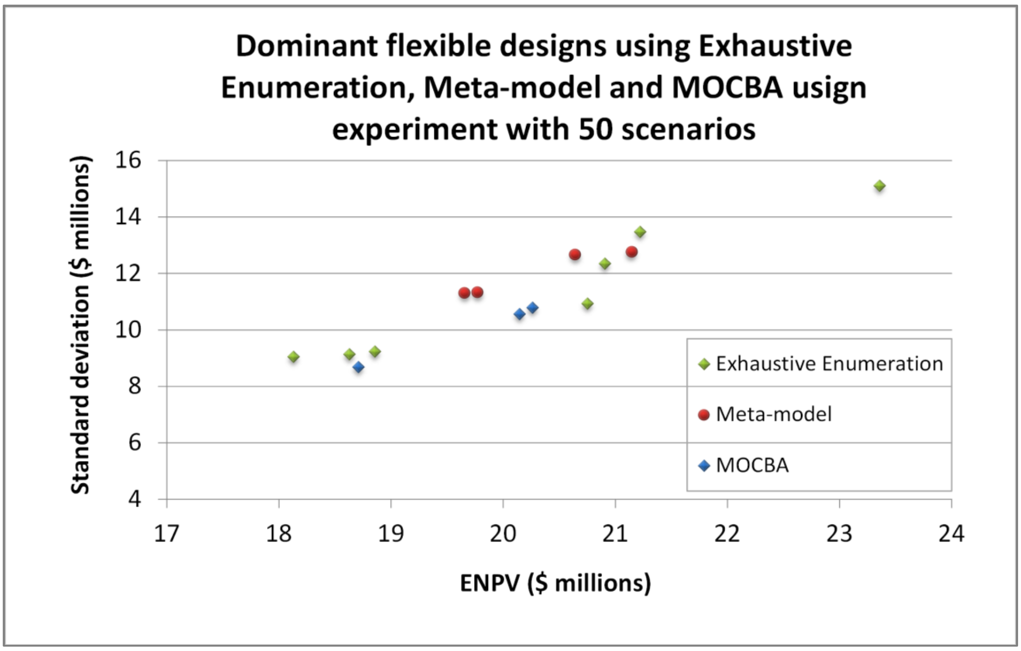
Appendix A: Multi-Criteria Decision-Making Table for Case Study I

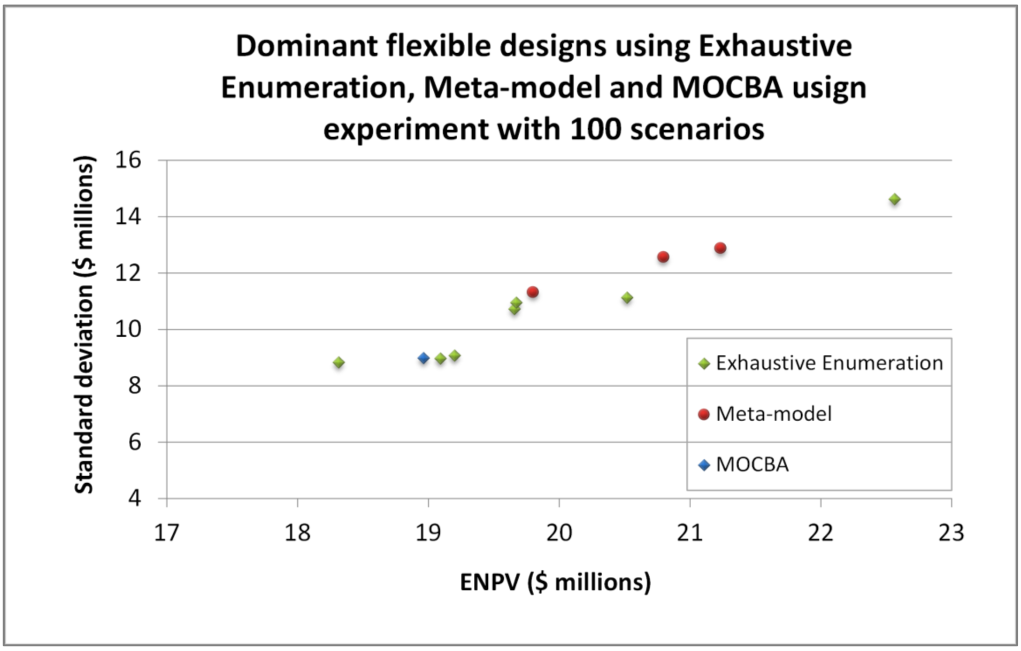
α=1	on-shore LNG production system design												
	Fixed design	Flexible 1: no move			Flexible 2: with move			Best design			Value of flexibility		
		Learning rate			Learning rate			Learning rate			Learning rate		
Criteria	(25 tpd)	0%	10%	20%	0%	10%	20%	0%	10%	20%	0%	10%	20%
ENPV	0.87	20.69	36.93	50.92	**23.29**	**43.17**	**59.00**	Flexible 2	Flexible 2	Flexible 2	22.42	42.31	58.13
VaR	0.89	**5.40**	10.82	15.71	3.74	**11.06**	**16.47**	Flexible 1	Flexible 2	Flexible 2	4.51	10.17	15.58
VaG	0.89	34.54	63.17	85.65	**45.78**	**80.09**	**108.29**	Flexible 2	Flexible 2	Flexible 2	44.90	79.20	107.41
STD	**0.14**	10.57	18.91	25.30	15.79	25.31	33.35	Fixed	Fixed	Fixed	0.00	0.00	0.00
Capex	**25.00**	27.50	27.50	27.50	27.5	27.5	27.5	Fixed	Fixed	Fixed	N/A	N/A	N/A

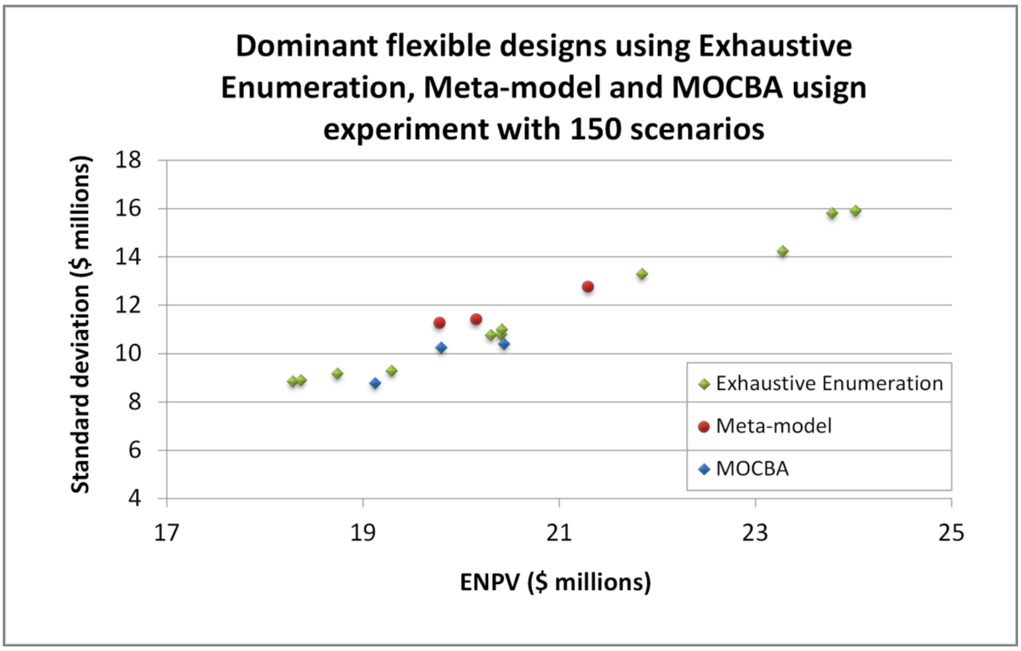
α=0.90	on-shore LNG production system design												
	Fixed design	Flexible 1: no move			Flexible 2: with move			Best design			Value of flexibility		
		Learning rate			Learning rate			Learning rate			Learning rate		
Criteria	(125 tpd)	0%	10%	20%	0%	10%	20%	0%	10%	20%	0%	10%	20%
ENPV	**36.76**	20.69	36.93	50.92	23.29	**43.17**	**59.00**	Fixed	Flexible 2	Flexible 2	0.00	6.41	22.24
VaR	2.66	**5.40**	10.82	15.71	3.74	**11.06**	**16.47**	Flexible 1	Flexible 2	Flexible 2	2.73	8.40	13.80
VaG	**59.18**	34.54	63.17	85.65	45.78	**80.09**	**108.29**	Fixed	Flexible 2	Flexible 2	0.00	20.90	49.11
STD	**23.32**	**10.57**	**18.91**	25.30	15.79	25.31	33.35	Flexible 1	Flexible 1	Fixed	12.75	4.42	0.00
Capex	77.13	**27.50**	**27.50**	**27.50**	**27.5**	**27.5**	**27.5**	Flexible	Flexible	Flexible	N/A	N/A	N/A

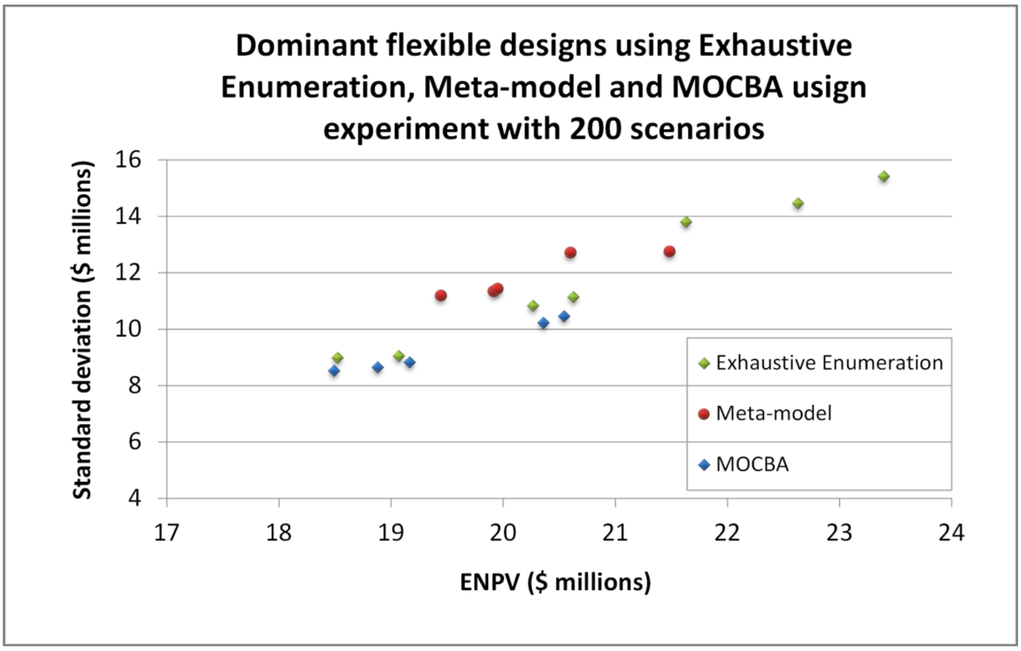
α=0.85	on-shore LNG production system design												
	Fixed design	Flexible 1: no move			Flexible 2: with move			Best design			Value of flexibility		
		Learning rate			Learning rate			Learning rate			Learning rate		
Criteria	(175 tpd)	0%	10%	20%	0%	10%	20%	0%	10%	20%	0%	10%	20%
ENPV	**60.11**	20.69	36.93	50.92	23.29	43.17	59.00	Fixed	Fixed	Fixed	0.00	0.00	0.00
VaR	-1.29	**5.40**	10.82	15.71	3.74	**11.06**	**16.47**	Flexible 1	Flexible 2	Flexible 2	6.69	12.35	17.76
VaG	**104.54**	34.54	63.17	85.65	45.78	80.09	**108.29**	Fixed	Fixed	Flexible 2	0.00	0.00	3.75
STD	40.03	**10.57**	**18.91**	**25.30**	15.79	25.31	33.35	Flexible 1	Flexible 1	Flexible 1	29.46	21.13	14.73
Capex	80.65	**27.50**	**27.50**	**27.50**	**27.5**	**27.5**	**27.5**	Flexible	Flexible	Flexible	N/A	N/A	N/A

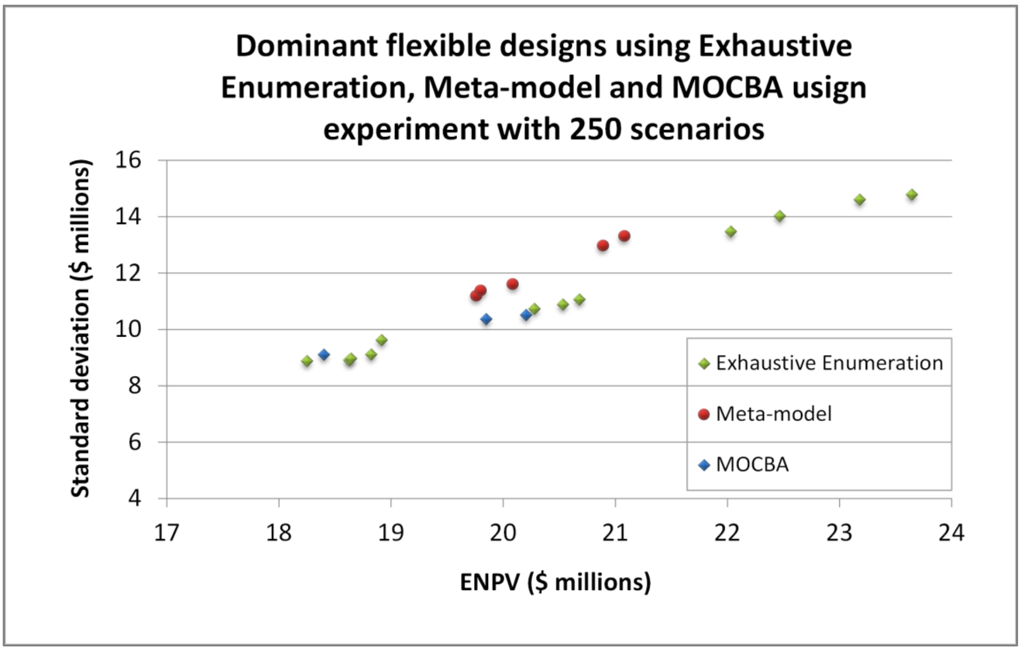
Appendix B: Pareto Front for Case Study I



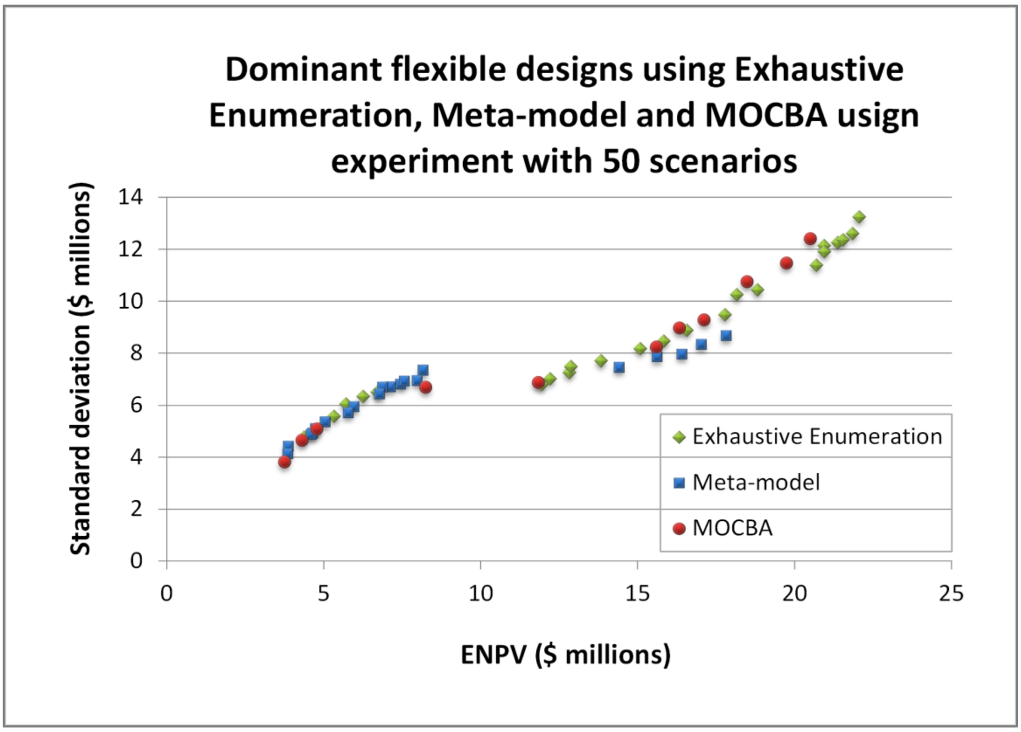


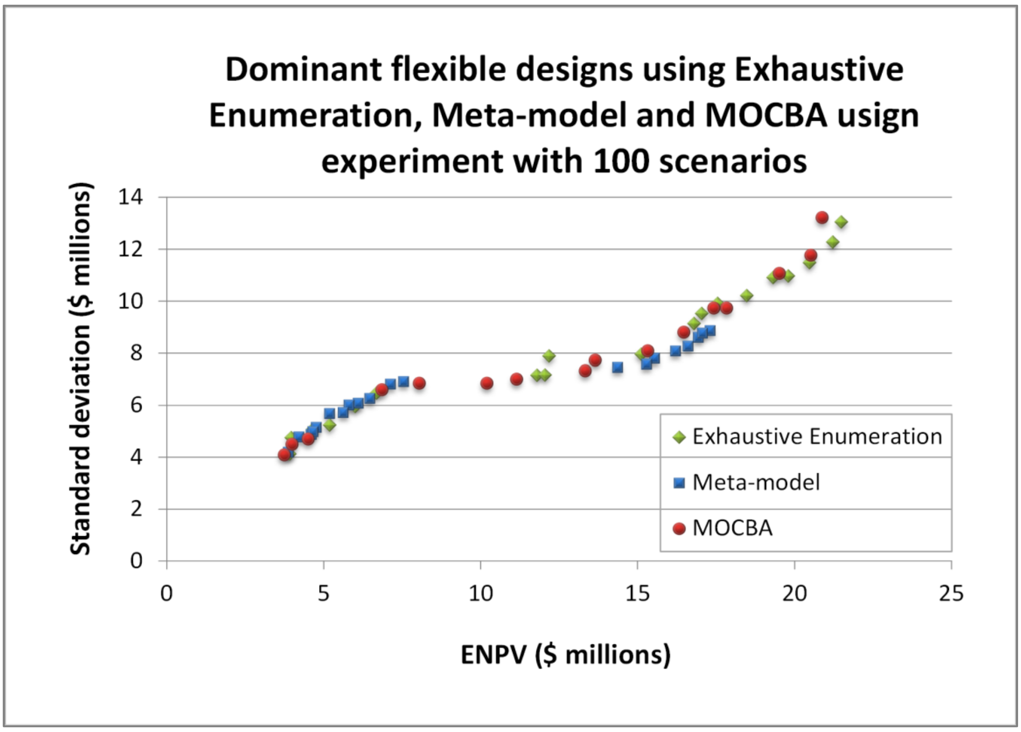

Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 150 scenarios
Standard deviation ($ millions)
18
16
14
12
10
8
6
4
17
19
21
23
25
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA

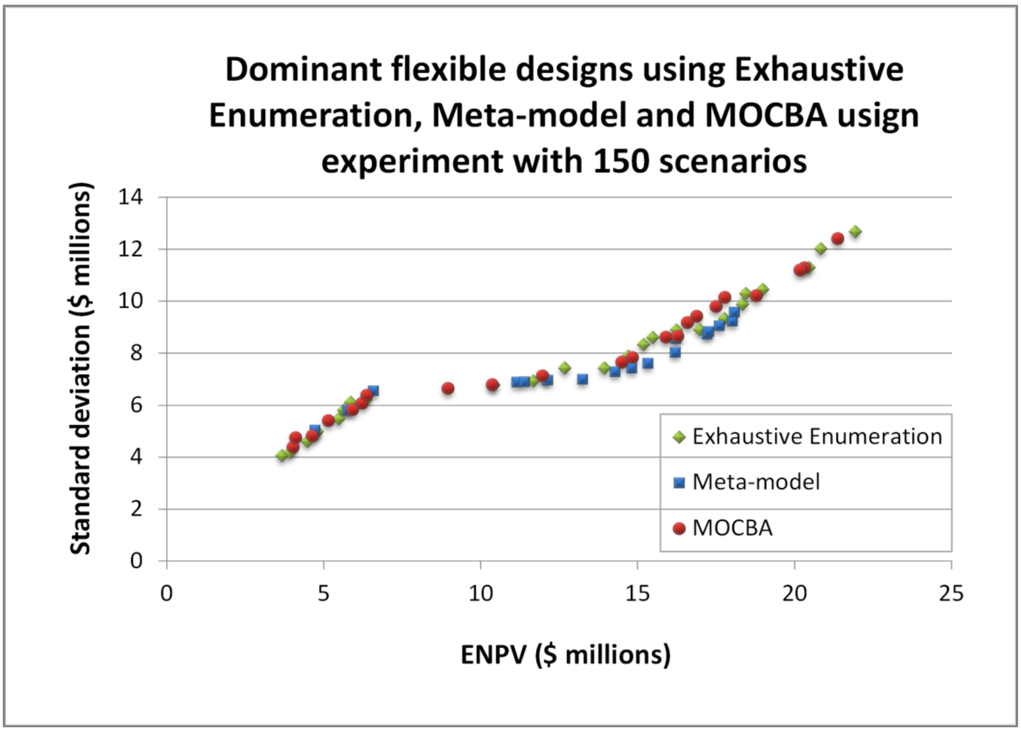

Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 200 scenarios
Standard deviation ($ millions)
16
14
12
10
8
6
4
17
18
19
20
21
22
23
24
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA

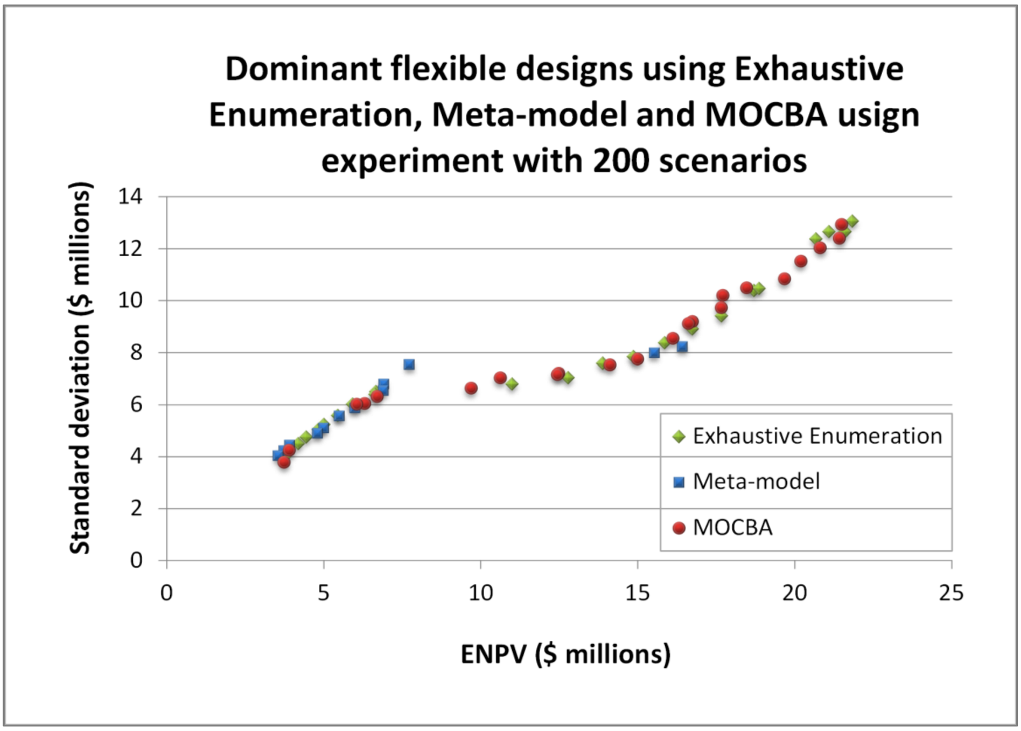

Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 250 scenarios
Standard deviation ($ millions)
16
14
12
10
8
6
4
17
18
19
20
21
22
23
24
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA

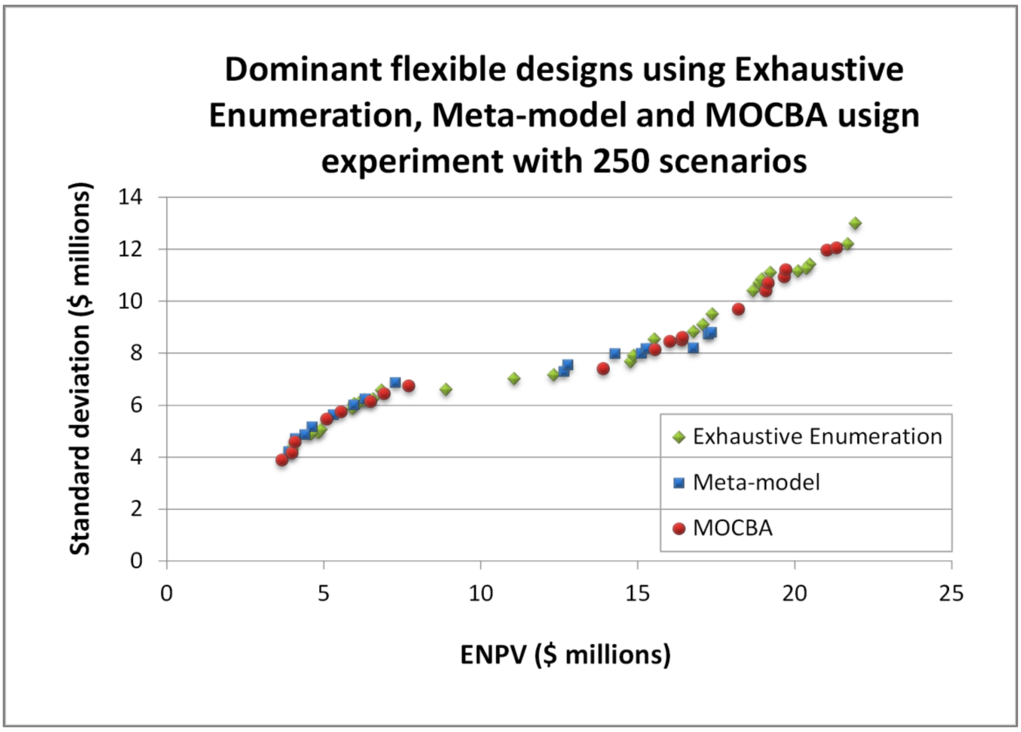
Appendix C: Pareto Front for Case Study II






Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 150 scenarios
Standard deviation ($ millions)
14
12
10
8
6
4
2
0
0
5
10
15
20
25
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA


Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 200 scenarios
Standard deviation ($ millions)
14
12
10
8
6
4
2
0
0
5
10
15
20
25
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA



Dominant flexible designs using Exhaustive Enumeration, Meta-model and MOCBA usign experiment with 250 scenarios
Standard deviation ($ millions)
14
12
10
8
6
4
2
0
0
5
10
15
20
25
ENPV ($ millions)
Exhaustive Enumeration
Meta-model
MOCBA

Appendix D: Post-Optimality Sensitivity Analysis for Case Study I

Case Study I: Sensitivity Analysis for Solution Obtained using Exhaustive Enumeration

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
	Low	Base	High	Low			Base			High			
				Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Discount rate	12%	10%	8%	5.20	2.12	3.09	24.22	14.27	9.95	48.33	30.32	18.02	14.93
Learning rate	0%	0%	5%	24.22	14.27	9.95	24.22	14.27	9.95	33.10	14.54	18.57	8.62
Sharpness volatility	45%	70%	95%	25.31	16.49	8.83	24.22	14.27	9.95	21.69	10.06	11.63	2.80

Case Study I: Sensitivity Analysis for Solution Obtained using Meta-Model

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
	Low	Base	High	Low			Base			High			
				Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Discount rate	12%	10%	8%	3.84	2.11	1.74	20.06	14.27	5.79	39.93	30.20	9.73	8.00
Learning rate	0%	0%	5%	20.06	14.27	5.79	20.06	14.27	5.79	27.46	14.64	12.82	7.03
Sharpness volatility	45%	70%	95%	20.64	16.46	4.18	20.06	14.27	5.79	17.40	10.40	7.00	2.82

Case Study I: Sensitivity Analysis for Solution Obtained using Computing Budget Allocation

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
	Low	Base	High	Low			Base			High			
				Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Discount rate	12%	10%	8%	2.34	1.81	0.53	21.24	16.49	4.75	42.43	30.19	12.24	11.71
Learning rate	0%	0%	5%	21.24	16.49	4.75	21.24	16.49	4.75	29.49	14.72	14.77	10.02
Sharpness volatility	45%	70%	95%	19.80	16.59	3.21	21.24	16.49	4.75	16.81	10.34	6.47	3.26

Appendix E: Post-Optimality Sensitivity Analysis for Case Study II

Case Study II: Sensitivity Analysis for Solution Obtained using Exhaustive Enumeration

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
				Low			Base Case			High			
	Low	Base	High	Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Sharpness volatility	45%	70%	95%	22.84	17.40	5.44	21.56	10.56	11.00	20.77	3.48	17.29	11.85
Learning rate	5%	10%	15%	18.06	11.31	6.76	21.56	10.56	11.00	23.94	10.95	12.99	6.23
Discount rate	8%	10%	12%	43.97	36.49	7.48	21.56	10.56	11.00	4.66	-8.83	13.50	6.02

Case Study II: Sensitivity Analysis for Solution Obtained using Meta-Model

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
				Low			Base			High			
	Low	Base	High	Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Sharpness volatility	45%	70%	95%	19.44	17.36	2.08	17.03	10.56	6.47	18.94	4.23	14.71	12.63
Discount rate	8%	10%	12%	39.39	36.97	2.43	17.03	10.56	6.47	3.89	-7.98	11.88	9.45
Learning rate	5%	10%	15%	16.10	10.60	5.50	17.03	10.56	6.47	20.63	10.95	9.68	4.18

Case Study II: Sensitivity Analysis for Solution Obtained using Computing Budget Allocation

Input Variable	Input Value			Output Value of Flexibility ($M)									Swing ($M)
				Low			Base			High			
	Low	Base	High	Flexible	Fixed	VoF	Flexible	Fixed	VoF	Flexible	Fixed	VoF	
Sharpness volatility	45%	70%	95%	17.79	17.42	0.37	18.11	10.56	7.55	18.31	2.30	16.02	15.65
Discount rate	8%	10%	12%	38.73	37.15	1.58	18.11	10.56	7.55	2.20	-8.46	10.67	9.09
Learning rate	5%	10%	15%	15.16	11.04	4.11	18.11	10.56	7.55	19.64	11.21	8.43	4.32

Appendix F: Mathematical representation of the DCF model for Case Study I

To have a better understanding of the detailed relations among the components of the simulation model for case study I, a mathematical representation of the DCF model is presented. First, a deterministic DCF model is built and then by taking uncertainty into account the DCF model under uncertainty is proposed. Finally, by incorporating decision rules into the DCF model under uncertainty, the flexible DCF model is presented. Table 1 shows the solution representation of the flexible design for case study 1.

Table 1: Solution representation of the flexible design for case study I

InCap	MDC	MsiteTV	MoveTV	Cover	DsiteTV

Decision rules, design variables

$InCap_{Msite}$ Initial capacity of LNG at the main production site (tpd)

MDC Modular design capacity of LNG used in the system design (tpd)

$MsiteTV$ Percentage of the modular design capacity for capacity expansion decision rule used at the main production site (%)

$MoveTV$ Percentage of the modular design capacity to consider the time for the first capacity deployment at demand sites in the relevant decision rule embedded at each demand site (%)

$Cover$ The coverage distance from the main production site where demand sites located beyond this coverage distance are considered for the first capacity deployment in the relevant decision rule embedded at each demand site (%)

$DsiteTV$ Percentage of the modular design capacity for capacity expansion decision rule used at the demand site with installed capacity (%)

$CAP_{Msite,t,s}$ Capacity of LNG at the main production in year *t* under demand scenario *s* (tpd)

$CAP_{l,t,s}$ Capacity of LNG at the demand site *l* in year *t* under demand scenario *s* (tpd)

$SQ_{l,t,s}$ Sale quantity of LNG for the demand site *l* in year *t* under demand scenario *s* (tpd)

Equation 1 shows how the margin of selling one unit LNG is calculated. In this function, an escalation factor (*ESCF*) is used to consider the increasing trend of selling price (*SP*) and gas purchase (*GP*) during the entire study period, where it is assumed to be 3% per year.

$$Margin_t = ESCF \times (SP_t - GP_t) \quad (1)$$

The capacity expansion decision rule embedded at the main production site is presented in equation 2, where the *DRMEXP* shows the decision rule for the main production site capacity expansion. The decision rule takes value 1 if the realized aggregate demand at main production site in year *t* under demand scenario *s* is greater than or equal to the threshold value *MsiteTV* multiplied by the modular capacity *MDC,* where *RAD* is the realized aggregate demand. Otherwise the decision rule takes value zero.

$$DRMEXP_{Msite,t,s} = \begin{cases} 1 & \text{If } RAD_{Msite,t,s} \geq (MsiteTV \times MDC) \quad \forall\, t, s \\ 0 & \text{Otherwise} \end{cases} \quad (2)$$

At the main production site, time to build for the first plant is 3 years while one decides to expand capacity in year t, extra capacity will be available for production in year t+1.

The first capacity deployment at demand site *l* is presented in equation 3, where *DRFCD* shows the decision rule for the first capacity deployment. The decision rule takes value 1 if the realized demand at demand site *l*, in year *t* under demand scenario *s* is greater than or equal to the threshold value *MoveTV* multiplied by the modular capacity MDC and the distance from the demand site l to the main production site is more than or equal to the coverage distance *Cover*, where RD is the realized demand and $Dist_l$ shows the distance from the main production site to the demand site *l*. Otherwise, the decision rule takes value zero.

$$DRFCD_{l,t,s} = \begin{cases} 1 & \text{If } ((RD_{l,t,s} \geq (MoveTV \times MDC) \text{ } and \text{ } (Dist_l \geq Cover)) \quad \forall\, l,t,s \\ 0 & \text{Otherwise} \end{cases} \tag{3}$$

At demand site *l*, time to build for the first plant is 2 years while one decides to expand capacity at any demand site in year t, extra capacity will be available for production in year t+1.

The capacity expansion decision rule embedded at each demand site is presented in equation 4, where DRDEXP shows the capacity expansion decision rule for demand sites. The decision rule takes value 1 if the realized demand at demand site *l*, in year *t* under demand scenario *s* is greater than or equal to the threshold value *DsiteTV* multiplied by the modular capacity *MDC* and the capacity of the demand site *l* is bigger than zero. Otherwise, the decision rule takes value zero.

$$DRDEXP_{l,t,s} = \begin{cases} 1 & \text{If } ((RD_{l,t,s} \geq (DsiteTV \times MDC) \text{ } and \text{ } \left(CAP_{l,t,s} > 0\right)) \quad \forall\, l,t,s \\ 0 & \text{Otherwise} \end{cases} \tag{4}$$

Equation 5 guarantees that sale quantity of LNG at demand site *l* in year t under demand scenario *s* is less than or equal to the capacity installed at demand site *l* in year *t* under scenario *s*.

$$SQ_{l,t,s} \leq CAP_{l,t,s} \qquad \forall\, l,t,s \tag{5}$$

The objective function is NPV which is calculated based on discounted cash flow of costs and revenues. The general form of the objective function is demonstrated in equation 6, where $TR_{t,s}$ shows the total revenue in year *t* under scenario *s,* $TC_{t,s}$

shows the total cost in year *t* under scenario *s* and $d_{t,s}$ shows the sum of all noncash, or book, costs such as depreciation during year *t* under scenario *s*. Essentially in equation 6 an After Tax Cash Flows (ATCFs) analysis is used in place of a Before Tax Cash Flows (BTCFs) approach by including expenses (or savings) to income taxes and then making equivalent worth calculations using the after-tax MARR (Sullivan, Wicks et al. 2009).

$$NPV_s = \sum_{t=1}^{T} \frac{(1 - Tax)\left(TR_{t,s} - TC_{t,s}\right) + Tax\ d_{t,s}}{(1 + r)^t} \quad \forall\, s \tag{6}$$

Equation 7 calculates the total revenue obtained by selling LNG in year *t* under scenarios *s* and the salvage value of the design alternative.

$$TR_{t,s} = \sum_{l=1}^{L} SQ_{l,t,s} \times Margin_t \quad \forall\, t, s \tag{7}$$

Equation 8 shows the components of the total cost including the CAPEX, OPEX and transportation cost in year *t* under scenario *s*, where $TRNC_{t,s}$ is the total transportation cost in year *t* under scenario *s*.

$$TC_{t,s} = CAPEX_{t,s} + OPEX_{t,s} + TRNC_{t,s} \tag{8}$$

Equation 9 is considered to calculate the CAPEX of the project in year *t=0* under scenario *s* while equation 10 is considered to calculate the CAPEX of the project in year *t* under scenario *s*.

$$CAPEX_{t,s} = \left\lceil \frac{InCap_{Msite}}{MDC} \right\rceil \times CAPEX_{MDC} \ \forall\, t = 0, s \tag{9}$$

$$\begin{aligned} CAPEX_{t,s} = {} & \left(DRMEXP_{Msite,t,s} \times CAPEX_{MDC}\right) \\ & + \sum_{l=1}^{L} \left(DRFCD_{l,t,s} + DRDEXP_{l,t,s}\right) \times CAPEX_{MDC} \quad \forall\, t > 0, s \end{aligned} \tag{10}$$

Equation 11 is considered to calculate the operational cost of the project in year *t* under scenario *s*, where $CAP_{l,t,s}$ is the capacity in demand site l in year *t* under scenario *s*.

$$OPEX_{t,s} = \left\lceil \frac{CAP_{Msite,t,s}}{MDC} \right\rceil \times OPEX_{MDC} + \sum_{l=1}^{L} \left(\left\lceil \frac{CAP_{l,t,s}}{MDC} \right\rceil \times OPEX_{MDC} \right) \quad \forall\, t, s \tag{11}$$

Equation 12 represents how the transportation cost is calculated, where C_l is the cost of transporting one tone of LNG from the main production site to demand site *l* in year *t* under scenario *s*. The equation indicates that when new production facility is deployed at demand site, the corresponding transportation cost decreases as the demand is met by the LNG produced at the same demand site.

$$TRNC_{t,s} = \sum_{l=1}^{L} (max(0, SQ_{l,t,s} - CAP_{l,t,s}) \times C_l) \quad \forall\, t, s \tag{12}$$

To generate the distribution of NPV outcomes, Monte Carlo simulation, which allows one to consider a large enough number of scenarios (e.g. 2000), is used.

Appendix G: Mathematical representation of the DCF model for Case Study II

To have a better understanding of detailed relations among the components of the simulation model for case study II, a mathematical representation of the DCF is presented. First, a deterministic DCF model is built and then by taking uncertainty into account the DCF model under uncertainty is proposed. Finally, by incorporating decision rules into the DCF model under uncertainty the flexible DCF model is presented. Table 1 shows the solution representation of the flexible design for case study II.

Table 1: Solution representation of the flexible design for case study II

X1	X2	MDC	TV

Decision rules and design variables

$InCap_l$	Initial capacity of LNG at demand site *l* (tpd)
$SDF_{l,t,s}$	Short-term forward looking demand forecast at demand site *l* in year *t* under scenario *s* (tpd)
$RD_{l,t,s}$	Realized demand at demand site *l* in year *t* under scenario *s* (tpd)
MDC	Modular design capacity of LNG used in the system design (tpd)
TV_l	Percentage of the modular design capacity for capacity expansion decision rule used at demand site *l* (%)
$USC_{l,t,s}$	Unused capacity at demand site *l* in year *t* under scenario *s* (tpd)
$UMD_{l,t,s}$	Unmet demand at demand site *l* in year *t* under scenario *s* (ton)
$x_{i,j,t,s}$	Amount of LNG to be transferred from demand site *i* with unused capacity to demand site *j* with unmet demand in year *t* under scenario *s* (tpd)

$CAP_{l,t,s}$	Capacity of LNG production facility at demand site *l* in year *t* under scenario *s* (tpd)
$SQ_{l,t,s}$	Sale quantity of LNG facility for the demand site *l* in year *t* under demand scenario *s* (tpd)
$TRSC_{t,s}$	Total transportation cost incurred by enabling operational flexibility in year *t* under scenarios *s*
$TRO_{t,s}$	Total revenue generated by enabling operational flexibility in year *t* under scenario *s*
$TCO_{t,s}$	Total cost incurred by enabling operational flexibility, comprising total gas purchase cost and transportation cost, in year *t* under scenario *s*
$VAO_{t,s}$	The value added by enabling operational flexibility in year *t* under demand scenario *s*

Equation 1 shows the three decision rules used in the simulation model that are as follows: 1) IF "realized demand in year of forecast t <= bound 1" THEN "Initial capacity = 0"; 2) IF "realized demand in year of forecast t > bound 1" AND "realized demand in year of forecast t <= bound 2" THEN "Initial capacity = 25"; and 3) IF "realized demand in year of forecast t > bound 2" THEN "Initial capacity = 50", where bound 1, bound 2 and year of forecast t are parameters of the decision rules.

$$InCap_{l,s} = \begin{cases} 0 & \text{If } SDF_{t,s} \leq Bound1 \;\; \forall\, t,s \\ 25\ tpd & \text{If } (SDF_{t,s} \geq Bound1 \; and \; SDF_{t,s} \leq Bound2) \forall\, l,t,s \\ 50\ tpd & \text{If } SDF_{t,s} \geq Bound2 \;\; \forall\, t,s \end{cases} \quad (1)$$

Equation 2 shows how the margin of selling one unit LNG is calculated. In this function escalation factor (*ESCF*) is used to consider the increasing trend of selling price (*SP*) and gas purchase (*GP*) during the entire study period.

$$Margin_t = ESCF \times (SP_t - GP_t) \tag{2}$$

The capacity expansion decision rule embedded at each demand site is presented in equation 3, where DRDEXP shows the capacity expansion decision rule for demand sites. The decision rule takes value 1 if the realized demand at demand site *l* in year *t* under demand scenario *s* is greater than or equal to the threshold value *TV* multiplied by the modular capacity *MDC*. Otherwise, the decision rule takes value zero.

$$DRDEXP_{l,t,s} = \begin{cases} 1 & \text{If}\left(RD_{l,t,s} \geq TV \times MDC\right) \quad \forall\, l,t,s \\ 0 & \text{Otherwise} \end{cases} \tag{3}$$

Equation 4 guarantees that sale quantity of LNG at demand site *l* is less than or equal to the capacity installed at demand site *l* in year *t* under demand scenario *s*.

$$SQ_{l,t,s} \leq CAP_{l,t,s} \quad \forall\, l,t,s \tag{4}$$

The objective function is NPV which is calculated based on discounted cash flow of costs and revenues without considering operational flexibility. General form of the objective function is demonstrated in equation 5, where $TR_{t,s}$ and $TC_{t,s}$ show the total revenue and total cost respectively in year t under scenarios s and $d_{t,s}$ is the sum of all noncash, or book, costs such as depreciation during year *t* under scenario *s*. Essentially in equation 5 an ATCFs analysis is used in place of a BTCFs approach by including expenses (or savings) to income taxes and then making equivalent worth calculations using the after-tax MARR (Sullivan, Wicks et al. 2009).

$$NPV_s = \sum_{t=1}^{T} \frac{(1 - Tax)\left(TR_{t,s} - TC_{t,s}\right) + Tax\, d_{t,s}}{(1+r)^t} \qquad \forall\, s \tag{5}$$

Equation 6 calculates the total revenue obtained by selling LNG in year *t* under scenarios *s*.

$$TR_{t,s} = \sum_{l=1}^{L} SQ_{l,t,s} \times Margin_t \quad \forall\, t, s \tag{6}$$

Equation 7 shows the components of the total cost including the CAPEX, OPEX and transportation cost in year *t* under scenario *s*, where $TRNC_{t,s}$ is the total transportation cost in year *t* under scenario *s*.

$$TC_{t,s} = CAPEX_{t,s} + OPEX_{t,s} \tag{7}$$

Equation 8 is considered to calculate the CAPEX of the project in year *t* under scenario *s*.

$$CAPEX_{t,s} = \sum_{l=1}^{L} \left\lceil \frac{InCap_{Initial_l}}{MDC} \right\rceil \times CAPEX_{MDC} + \sum_{l=1}^{L} \left(DRDEXP_{l,t,s} \right) \times CAPEX_{MDC} \quad \forall\, t, s \tag{8}$$

Equation 9 is considered to calculate the OPEX of the project in year *t* under scenario *s*.

$$OPEX_{t,s} = \sum_{l=1}^{L} \left\lceil \frac{CAP_{l,t,s}}{MDC} \right\rceil \times OPEX_{MDC} \quad \forall\, t, s \tag{9}$$

The objective of operational planning is to minimize the total transportation cost that leads to maximizing the added value of the system design, which is termed the added value of flexibility. Let m-plant equal the locations with unused capacity (supply) and the n-plant with unmet demand (demand). Let $USC_{i,t,s} \geq 0$, $i = 1, 2, \ldots, m$ be the amount of capacity idle at the i^{th} plant from a set of plants with unused capacity in year *t* under scenario *s*. Similarly, let $UMD_{j,t,s} \geq 0$, $j = 1, 2, \ldots, n$ be the amount of demand required at the j^{th} plant from a set of plants with unmet demand. Assume the cost of transporting one unit of LNG (i.e., one ton) from i^{th} supply to j^{th} demand site be $C_{i,j}$, in terms of i=1,2, …,m and j=1,2,….n. If $x_{i,j,t,s}$ is the amount of LNG to be transported from i^{th} supply to j^{th} demand point in year t under scenario s, then the problem is to determine $x_{i,j,t,s}$ so as to minimize the following function considering $x_{i,j,t,s} \geq 0$ for all values of i and j.

Equation 10 determines the total transportation cost incurred by enabling operational flexibility at time t under demand scenario s. Equation 11 ensures that the amount of LNG carried from site i at time t under demand scenario s is equal to the available unused capacity. In a similar fashion, equation 12 guarantees that the amount of LNG carried to site i at time t under demand scenario s is equal to the amount of unmet demand.

$$TRSC_{t,s} = \sum_{i=1}^{m} \sum_{j=1}^{n} x_{i,j,t,s} C_{i,j} \qquad \forall\, t = 1 \dots T,\;\; s = 1 \dots S \tag{10}$$

$$\sum_{j=1}^{n} x_{i,j} = USC_{i,t,s} \qquad \forall\, i = 1 \dots m, t = 1 \dots T,\;\; s = 1 \dots S \tag{11}$$

$$\sum_{i=1}^{m} x_{i,j} = UMD_{j,t,s} \qquad \forall\, j = 1 \dots n, t = 1 \dots T,\;\; s = 1 \dots S \tag{12}$$

Total revenue generated by enabling operational flexibility in year t under scenario s, shown as $TRO_{t,s}$, is calculated using equation 13.

$$TRO_{t,s} = \sum_{i=1}^{m} \sum_{j=1}^{n} (x_{i,j,t,s} \times SP_t) \quad \forall\, t, s \tag{13}$$

Total cost incurred by enabling operational flexibility, shown as $TCO_{t,s}$ that comprises gas purchase cost and transportation cost, in year t under scenario s is calculated using equation 14.

$$TCO_{t,s} = \sum_{i=1}^{m}\sum_{j=1}^{n}(x_{i,j,t,s} \times GP_t) + TRSC_{t,s} \quad \forall\, t,s \tag{14}$$

The value added by enabling operational flexibility in year *t* under demand scenario *s* is calculated using equation 15. It is assumed that operational flexibility is enabled in year *t* under scenario *s* when such flexibility is worthwhile.

$$\mathrm{VAO_{t,s}} = \max\left(0, TRO_{t,s} - TCO_{t,s}\right) \qquad \forall\, t,s \tag{15}$$

The NPV of the design under demand scenario s is calculated using equation 16. To generate the distribution of NPV outcomes, Monte Carlo simulation, which allows one to consider a large enough number of scenarios (e.g. 2000), is used.

$$NPV_s = \sum_{t=1}^{T} \frac{(1 - Tax)\left(VAO_{t,s} + TR_{t,s} - TC_{t,s}\right) + Tax\ d_{t,s}}{(1 + r)^t} \qquad \forall\, s \tag{16}$$

Appendix H: Sample VBA-MATLAB Programming Code

The following Visual Basic Application (VBA)-MATLAB programming code, with the help of "Spreadsheet Link EX" interface toolbox, is used to screen the flexible design solutions using the meta-model approach for the hypothetical capacity expansion problem demonstrated in section 3.4.1.

*More computer programming codes related to the meta-model and computing budget allocation based screening approaches for case study I and case study II are available for interested readers upon written request.

```
'Sequential Kriging Method – Efficient Global Optimization
Sub SKM ()
'Define the variable used in Excel and MATLAB
Dim i As Integer; Dim j As Integer; Dim temp1 As Double; Dim temp2 As Double; Dim doe_no As Integer; Dim samples As Double; Dim stopping As Double; Dim rep As Integer; Dim iter As Integer; Dim maximp As Double; Dim untried As Double; Dim lastresponse As Double; Dim a, b, c As Variant; Dim LB, UB As Double
'Input data here or can be read from spreadsheet tab "SKM"
'Lower and upper bound of threshold value
LB = 0.5
UB = 0.95
'No of simulation replication
rep = Sheets("SKM").Cells(1, 5).Value
'Stopping criterion for sequential kriging method
stopping = Sheets("SKM").Cells(1, 2).Value
'No of samples chosen for initial space filling
doe_no = Sheets("SKM").Cells(2, 2).Value
'Sequential kriging counter
iter = 0
'Elapsed time of "SKM" process
a = Timer()
'Clear MATLAB environment
  MLevalstring "clear all"
  MLevalstring "clc"
  MLevalstring "clf"
'Put needed variable to MATLAB
Mlputvar "doe_no", doe_no
```

```
Mlputvar "LB", LB
Mlputvar "UB", UB
'Using Latin Hyper Cube sampling for initial space filling
MLevalstring "spacefill=LB+lhsdesign(doe_no,1)*(UB-LB)"
MLevalstring "samples=[1:doe_no]'"
MLgetmatrix "spacefill", Sheets("SKM").Cells(3 + 1, 2).Address
MLgetmatrix "samples", Sheets("SKM").Cells(3 + 1, 1).Address
matlabrequest
'Conducting simulation considering initial space filling and given replication no.
  For i = 1 To doe_no
     Sheets("demand data- 25 tpd - flex").Range("D6") =
     Sheets("SKM").Cells(3+ i, 2).Value
    temp1 = 0
    temp2 = 0
    For j = 1 To rep
      Calculate
      temp1 = temp1 + Sheets("Simulation - flex").Cells(4, 4).Value
      temp2 = temp2 + Sheets("Graph-Table").Range("N5").Value
    Next
    'ENPV
      Sheets("SKM").Cells(3 + i, 3) = temp1 / rep
    'Flexibility value
      Sheets("SKM").Cells(3 + i, 4) = temp2 / rep

  Next
  'Put the samples and response of simulation to MATLAB
  Mlputmatrix "S", Sheets("SKM").Range(Cells(3 + 1, 2), Cells(3 + doe_no, 2))
  Mlputmatrix "Y", Sheets("SKM").Range(Cells(3 + 1, 4), Cells(3 + doe_no, 4))

  MLevalstring "[untried maximp]=SKM(S,Y)"
  MLgetfigure 1, 0.75
  MLgetmatrix "untried", Sheets("SKM").Cells(2 + iter, 10).Address
  MLgetmatrix "maximp", Sheets("SKM").Cells(2 + iter, 11).Address
  matlabrequest
  untried = Sheets("SKM").Cells(2 + iter, 10).Value
  maximp = Sheets("SKM").Cells(2 + iter, 11).Value
  'Start sampling and sequential kriging method
  Do While maximp >= stopping
```

```
'This means next iteration is needed
iter = iter + 1
'Add to MATLAB variable Y
MLevalstring "S(end+1,:)=untried"
'Update values at sheet
Sheets("SKM").Cells(3 + doe_no + iter, 1).Value = doe_no + iter
Sheets("SKM").Cells(3 + doe_no + iter, 2).Value = untried
'Run simulation in a given untried point
Sheets("demand data- 25 tpd - flex").Range("D6") = untried
temp1 = 0
temp2 = 0
  For j = 1 To rep
    Calculate
    temp1 = temp1 + Sheets("Simulation - flex").Cells(4, 4).Value
    temp2 = temp2 + Sheets("Graph-Table").Range("N5").Value
  Next
    'ENPV
    Sheets("SKM").Cells(3 + doe_no + iter, 3) = temp1 / rep
    'Flexibility value
    Sheets("SKM").Cells(3 + doe_no + iter, 4) = temp2 / rep
    lastresponse = Sheets("SKM").Cells(6 + iter, 4)
'Update the response vector in MATLAB
MLevalstring "Y(end+1,:)=lastresponse"
'refresh matlab for next iteration and update the "S" and "Y"
MLevalstring "clear all"
MLevalstring "clc"
MLevalstring "clf"
Mlputmatrix "S", Sheets("SKM").Range(Cells(3 + 1, 2),
Cells(3 + doe_no + iter, 2))
Mlputmatrix "Y", Sheets("SKM").Range(Cells(3 + 1, 4),
Cells(3 + doe_no + iter, 4))
  'Refitting kriging method using the updated "S" and "Y"
  'MLevalstring "[untried maximp]=SKM(S,Y)"
  MLevalstring "[untried maximp X P MSE dmodel]=SKM(S,Y)"
  MLgetfigure 1, 0.75
  MLgetmatrix "untried", Sheets("SKM").Cells(2 + iter, 10).Address
  MLgetmatrix "maximp", Sheets("SKM").Cells(2 + iter, 11).Address
  matlabrequest
```

```
        untried = Sheets("SKM").Cells(2 + iter, 10).Value
        maximp = Sheets("SKM").Cells(2 + iter, 11).Value
        'Optimizing the finalized meta-model using "SKM_OPT"
          If maximp < stopping Then
            MLevalstring "[Thrld FV]=SKM_OPT(dmodel)"
            MLgetmatrix "Thrld", Sheets("SKM").Cells(2, 12).Address
            MLgetmatrix "FV", Sheets("SKM").Cells(2, 13).Address
            matlabrequest
          End If

    Loop
b = Timer()
c = b - a
Sheets("SKM").Cells(2, 8).Value = c
End Sub
```