MASTER THESIS

ASSET WIDE OPTIMIZATION IN SHELL'S LNG UPSTREAM VALUE CHAIN

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“Complexity comes free, it’s simplicity we have to work for”

Analysis Wisdom

Summary

Asset Wide Optimization (AWO)

Asset Wide Optimization (AWO), or Enterprise Wide Optimization (EWO) as it is also referred to, is a new and emerging research area that combines technical engineering disciplines such as chemical engineering with operations research techniques. It focuses on optimizing business operations on a global level, instead of optimizing assets to their individual objectives. Key feature of AWO is the integration of information and decision-making among the various assets that comprise the value chain of the company.

AWO provides several benefits from a business perspective, such as:

(1) Cost reduction and associated margin maximization from the integrated gas value chain
(2) Maximizing exploitation of (short term) market situations, related to spot opportunities
(3) Enabling a more efficient and faster response to upset situations by making optimal operational changes

In general, AWO involves optimizing the operations of supply, manufacturing and distribution activities of a company to maximize operational profits. It has become a major goal in the process industries due to the increasing pressures for remaining competitive on the global market. A major focus is the optimal operation of manufacturing facilities, which often requires the use of (non-)linear process models. Major operational items include planning, scheduling, real-time optimization and inventory control.

Liquefied Natural Gas (LNG)

In the petroleum industry, associated Natural Gas is often found in presence of crude oil. Historically, this ‘byproduct’ was released as a waste product by burning it off in gas flares. Both environmental issues and the increase in demand for alternative energy sources make processing and selling the gas commercially attractive. The Natural Gas (mainly methane) is cooled to -160°C and becomes a colorless, non-toxic liquid that occupies up to 600 times less space. This enables profitable shipment in special LNG carriers, each with a capacity of over 200,000 cubic meters.

At its destination the liquid LNG is then returned to gaseous state at regasification facilities and distributed to homes, businesses and industries through the existing gas network. The Liquefied Natural Gas (LNG) value chain is defined as all business activities from exploration at the on- or offshore wells, until the gas reaches its final customer.

The focus of this thesis is on the upstream activities, comprising production and inventory management to ensure shipments to customers. The main assets are (1) Wells, (2) Production facilities (3) Storage, (4) Contracting and (5) the relation with the Oil market. We set the scope of the project to short term decisions (operational), with a planning horizon of about 30 days taking into account risks (uncertainty) where possible. Besides definitions, historical facts and market and economic details, we describe the value of an Asset Wide Optimization (AWO) model for Shell's LNG supply chain.

Construction of a mathematical framework

This section might be rather technical due to mathematical terminology. In Chapter 3, references can be found for a comprehensive overview of mathematical models and definitions. Based on the detailed value chain description, we have constructed a mathematical framework to support integrated AWO decision making. An obvious starting point for decision making optimization is a Dynamic Programming (DP) framework, since it is of lower computational complexity than for example the Simplex method, in combination with branch and bound in case of Mixed Integer Linear Programs (MILPs)

Eventually, we propose a Mixed Integer Linear Programming (MILP) framework that is equivalent to the dynamic program. Although we lose the 'nice' structure of having smaller sub problems to solve the overall problem, this approach is not subject to the so called curse of dimensionality as we can use both continuous and integer variables in these models to get around the discretization step.

Two stage stochastic programming

To include uncertainty in the model, we proposed a two-stage stochastic program (with recourse costs) that is based on the deterministic MILP that was constructed previously. The first stage represents the decisions to be made today on contract delivery, production levels and flaring. We assume that the current (today's) state of the system is known with certainty and the associated transition function is deterministic. The decisions on production rates at the wells, as well as shipments affect the stock level at the start (tomorrow) of the remaining planning horizon (second stage). We maximize the sum of (deterministic) direct revenue in the first stage and expected future profits over all scenarios in the second stage.

The first stage decisions represent those decisions that are to be executed immediately. Second stage decisions represent future decisions, given the possible realization of scenarios from a pre-defined scenario set. If this pre-defined set is large, computational complexity of the increases drastically since all variables and constraints in the two stage stochastic MILP are duplicated for each scenario.

Results and conclusions

We have shown results on how our algorithm performs by comparing it with an average case alternative, in which the stochastic model parameters are replaced by their average case behavior. For this model, the risks associated with deviation from average case behavior are disregarded. We therefore expect the stochastic approach to perform better in an operational setting.

As expected, the two stage stochastic MILP outperforms its deterministic equivalent. However, the results show a significant increase in computational time for the two stage stochastic MILP. We have used Monte Carlo simulation to analyze the performance of both models. For large horizons, we divided them optimization problem in smaller sub problems and used of a rolling horizon approach. To do so, both the Two stage stochastic MILP and the so called average case behavior MILP were implemented in a software package called AIMMS. This package is used by ORTEC and Shell for many optimization purposes.

Discussion and Recommendations

We recommend to refine the proposed LNG upstream value chain model in terms of key parameters and level of detail, preferably in close cooperation with field experts and end-users. We recommend to start with a deterministic setting and a focus on capturing all important system characteristics. Here, a site-specific approach is recommended as it better captures the main factors and needs of the corresponding sites. It was not possible to compare our strategy to conventional decision rules within Shell, since these are confidential. We recommend to get a clear view on how decisions are being made traditionally, before modeling and constructing an AWO decision support tool.

Due to the low level of detail that was used in our analysis, computational time might become a major issue in extension of the model to an operational software tool. To illustrate this, it should be noted that we included only three production wells in our model, while at most production sites this number is multiple times higher (usually up to 10 to 100 times). It should be explored to what extend the model suits the level of detail that is necessary in AWO.

The introduction of uncertainty can be set up rather straightforward by means of a scenario based approach, such as the two-stage stochastic MILP, as long as computational complexity is kept limited. Alternative (heuristic) modeling approaches could also be considered. Expert opinion, historical data and a fair comparison of model performance in an operational setting should play a central role in future projects. If these constraints are met, Asset Wide Optimization is expected to add significant value to the business challenges faced by Shell, as well as other companies.

Preface

This thesis is the result of my graduation project in order to obtain the MSc degree in Applied Mathematics at Twente University. The project was performed at ORTEC, located in Zoetermeer, in close cooperation with Shell Global Solutions International B.V. It was my deliberate choice to work in a business environment, to gain experience with applied mathematics in a commercial setting and to get to know both ORTEC and Shell.

I really enjoyed the combination of theoretical and practical research in a relatively new environment with different stakeholders, all with their own interests. The enthusiasm of the people I have worked with made it a very pleasant time and helped me to deal with the ups and downs that come with a graduation project. I would like to express my gratitude toward the people who have helped me to make this project a success.

First, I would like to thank my ORTEC colleagues for the pleasant time, and for involving me in all company activities and meetings. In particular, I would like to thank Dave van den Hurck for giving me the opportunity to do my graduation internship at ORTEC, and for introducing me to the right people. It made me feel comfortable from the first day. Special thanks to Swapan Saha, for the opportunity to work on a challenging problem at Shell, for your enthusiasm and positive drive in all the meetings and for giving me the freedom I needed to set the scope of the project to graduation standards. I would like to thank my professor Richard Boucherie for our bi-weekly meetings. These were of great value for the project, through your honest and constructive comments. Thank you for the collaboration, not only during this project but in all years of my Master. I also want to thank Judith Timmer, for the textual and mathematical advices in the final stage of the thesis. Sometimes, you even apologized for the extreme level of detail in your comments, but that was exactly what I was looking for.

Finally, I am grateful to Alex Siem, my daily supervisor at ORTEC. You really helped me with all parts of the project. I think your composed, but constructive and critical attitude in our meetings was complementary to my way of doing things. Together we managed the expectations of all parties involved. Thank you for all the time you have put in helping me to make the project a success, not to forget the fun golf clinic you gave me on that Sunday afternoon.

Siebe Brinkhof

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Chapter 1

Introduction

This thesis focuses on the development of an asset wide optimization model in the upstream liquefied Natural Gas (LNG) value chain of Shell Global Solutions International B.V. The project was executed in close cooperation with them and ORTEC B.V. This chapter provides a brief introduction to Shell as a company and its business activities in Section 1.1. We start with a general overview of Asset Wide Optimization definitions and methods in Section 1.2. Physical and economical aspects of LNG are discussed in Section 1.3. The scope and goals of the project are defined in the last Section.

1.1 - Shell Global Solutions International B.V.

Shell is a global group of energy and petrochemical companies, with around 87,000 employees in more than 70 countries and territories. Traditionally, it is known as an oil production company and it produces over 3.3 million barrels of oil each day. However, over 50% of its production is natural gas with a yearly increase of approximately 12%. Some of the advantage of gas over oil is the cleanliness and availability. However, it is generally found on remote locations far away from the existing market so the infrastructure must take shape which requires major investments [1], as is the case for many upcoming technologies and markets.

The company is organized in four different departments: Upstream, Downstream, Upstream Americas and Projects & Technology. The Upstream department focuses on the exploration and extraction of oil and gas, often in joint ventures with other national and international oil companies. Besides oil and gas, Shell also produces Gas-to-Liquids (GTL), bitumen and bio-mass.

The downstream department comprises many different activities such as refining, supply and distribution and marketing. Key to these businesses is manufacturing end-products from the crudes and natural gas as provided by the upstream department and sell them at the right place, at the right time. Projects and Technology provides technical services and technology capability in upstream and downstream activities. It manages the delivery of major projects and helps to improve performance across the company as a whole [2].

1.2 - Asset Wide Optimization (AWO)

Asset wide optimization (AWO), or Enterprise Wide Optimization (EWO) as it is also referred to, is a new and emerging research area that combines technical engineering disciplines such as chemical engineering with operations research techniques. It focuses on optimizing business operations on a global level, instead of optimizing assets to their individual objectives. Key feature of AWO is the integration of information and the decision-making among the various assets that comprise the value chain of the company.

An asset wide approach bridges the gap between the individual, contradicting objectives in the value chain, comprising both technical and commercial assets such as production facilities and long term customer relations. The use of local optimization at individual assets results in possibly suboptimal strategies in terms of sustainable business goals.

AWO provides several benefits from a business perspective, such as:

(1) Cost reduction and associated margin maximization from the integrated gas value chain
(2) Maximizing exploitation of (short term) market situations, related to spot opportunities
(3) Enabling a more efficient and faster response to upset situations by making optimal operational changes

It is notable that the literature found on Asset Wide Optimization are either broad descriptions on the potential added value of this approach, such as [3,4,5,6,7], or show great detail on a specific part of a production process such as pipeline networks [8], processing plants [9,10] and storage [11]. To illustrate the added value in the LNG business, maximizing production rates at the wells (asset objectives) does not necessarily lead to higher profits (global or enterprise objective) since the resulting high LNG supply might exceed market demand. Instead, the market must be the driving factor in optimizing production. However, all intermediate business activities must be taken into account as well which may result in complex (computational) problems.

In general, AWO involves optimizing the operations of supply, manufacturing and distribution activities of a company to maximize operational profits. It has become a major goal in the process industries due to the increasing pressures for remaining competitive on the global market. A major focus in is the optimal operation of manufacturing facilities, which often requires the use of (non-)linear process models. Major operational items include planning, scheduling, real-time optimization and inventory control. The key differentiating factors of AWO applied to the LNG value chain are:

- Cost and pricing, as these are of primary interest in decision making
- Annual delivery plan (see Section 2.5) and spot sale opportunities, as these are the primary drivers for LNG production
- The integrated gas value chain, where oil and gas are two distinct products but are interlaced through their interlaced production at the associated wells.
- Operations advisory on how to act when the system is upset to make optimal choices for the system as a whole instead of locally.
- Finally, AWO provides a short term focus, but takes into account a long term view when it comes to optimization of costs and revenues.

Asset Wide Optimization can thus be interpreted as using a global optimization approach to a variety of different aspects of a system, which traditionally show conflicting interests which results in sub-optimal operation from an asset wide (usually economic) perspective. It does not necessarily mean that all business activities of a company are considered in a single optimization model, AWO can for example be applied to optimization of a chemical reactor process. In order to achieve AWO throughout the process industry, Grossman [3] states four major challenges involved with a new generation of computational tools, based on AWO:

- The modeling challenge: What type of production planning and scheduling models should be developed for the various components of a value chain, and how should they be linked properly?
- The multiscale optimization challenge: How to coordinate the proposed models to effectively manage decisions on different levels such as sourcing and investment (strategic), production planning (tactical) and control (operational)?
- The uncertainty challenge: How to handle stochastic variations in model parameters, as a result of the absence of realistic data and inevitable stochastic nature of system elements subject to delays (shipping) and breakdowns (production facilities)?
- The algorithmic and computational challenge: How to solve the models effectively in terms of computational time, and still maintain proper level of detail to provide correct decision support?

The interaction between these challenges is different in each environment. However, a higher level of detail in general leads to a more complex algorithmic and computational challenge. In this thesis, these four challenges will play a central role.

1.3 - Liquefied Natural Gas (LNG)

Liquefied Natural Gas (LNG) is a relatively clean fuel, and many sources are available. Technological progress and the emerging natural gas market increased the amount of potential buyers for natural gas. The world's first liquefaction plant was built at Arzew, Algeria in 1964. In the early 1990s global liquefaction capacity had increased to 100 MTPA (million tons per annum). Until then Global LNG supply was dominated by Algeria, Malaysia and Indonesia, accounting for more than 60% of the total volume [1].

Natural gas has a much lower environmental impact than other fossil fuels such as coal or oil. It emits less carbon dioxide, and produces less ash. Although LNG is burned in the form of natural gas it has a greater environmental impact than natural gas that has not been liquefied. This is because LNG requires energy to liquefy, transport and regasify. However, if one considers that the LNG might have been flared at the source as a waste product of oil production, the environmental impact is lowered.

The LNG value chain comprises all business activities from the time that Natural Gas (NG) is found in the reserves, until the moment that Liquefied Natural Gas (LNG) sold to the end-user. Two types of natural gas wells are distinguished: Non-Associated (NA) and Associated (A). Non-Associated Natural Gas is a stand-alone natural gas, where Associated Gas is found in presence of crude oil. Historically, this latter type was released as a waste product from the petroleum extraction industry by burning it off in gas flares. Both environmental issues and the increase in demand for alternative energy sources make processing and selling the gas commercially attractive.

After the production at onshore or offshore associated wells, the oil is separated from the gas and sold separately. The gas is transported to the liquefaction facility where it is pre-treated. All gaseous components that would freeze under cryogenic temperatures (below -150°C) are removed from the product stream to prevent them from freezing during the cooling process, thus blocking the pipeline flow. These components include propane, butane, ethane, carbon dioxide and water.

The remaining Natural Gas (mainly methane) is cooled to -160°C and becomes a colorless, non-toxic liquid that occupies up to 600 times less space. It is stored in specially constructed tanks, with complex cooling systems to keep the LNG in its liquid state. This enables profitable shipment in special LNG carriers, each with a capacity of over 200,000 cubic meters. At its destination the liquid LNG is returned to gaseous state at regasification facilities and distributed to homes, businesses and industries through the existing gas network.

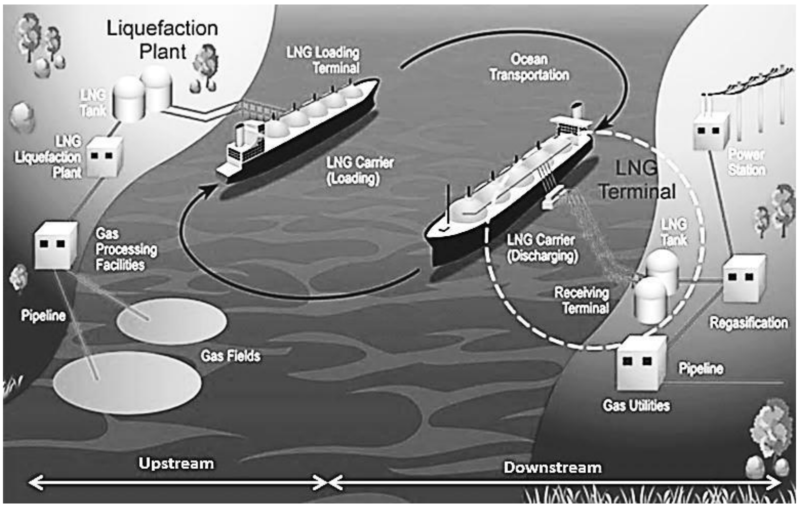


Figure 1.1 – Schematic overview of the LNG value chain, showing the distinction between Upstream (left) and Downstream (right) activities. Source: [12]

The LNG business can roughly be divided in two parts: Upstream and Downstream. The LNG value chain is defined as all business activities from exploration at the on- or offshore wells, until the gas reaches its final customer. The focus of this thesis is on the upstream activities, comprising production and inventory management to ensure shipments to customers. The distinction between up- and downstream is shown schematically in Figure 1.1. For a more detailed schematic overview of the assets involved with the upstream part of the value chain, we refer (forward) to Figure 3.2 and 3.3 on page 42.

Economic aspects

LNG offers increased flexibility with respect to pipeline transport, allowing cargoes of natural gas to be delivered where the need is greatest and the commercial opportunities are the most competitive. Figure 1.1 shows that as the distance over which natural gas must be transported increases, liquefaction of LNG has increased economic advantages over usage of pipelines. In general, shipping LNG becomes is more attractive than transporting natural gas in offshore pipelines if the distances is 700 miles or over. For onshore pipelines this breakeven point is found at a distance of 2,200 miles [13].

Both natural gas demand and LNG demand have grown strongly in the past century with 2,7% and 7,6% each year respectively. Between 2000 and 2013, global liquefaction capacity doubled, with main developments in Qatar and Australia. Approximately 25 other countries, which currently have little or no capacity, are expected to have entered the LNG market by 2020. However, the scale of investments and the ongoing economic uncertainty might postpone the final investment decisions of these projects. The fraction of total LNG capacity of importing and exporting countries in the year 2011 can be found in Figure 1.2.

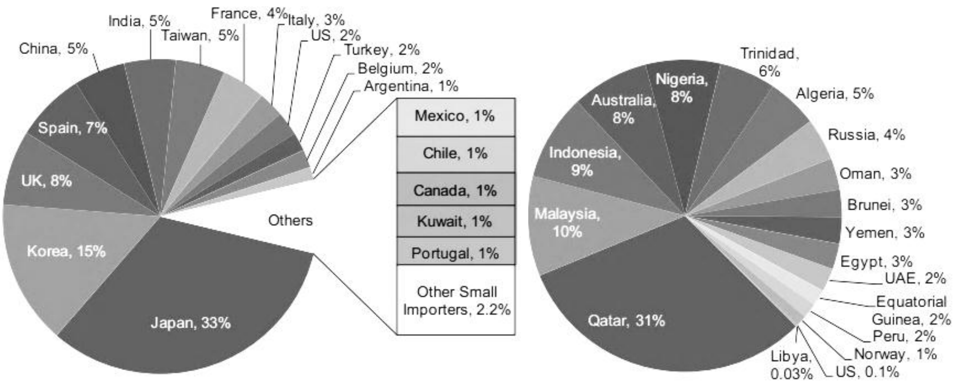


Figure 1.2 – LNG Importing (left) and exporting (right) countries in the year 2011. Source: [14]

The Annual World Energy Outlook, a forecast by the International Energy Agency (IEA), shows a growing role for natural gas in the world's energy mix, with the natural gas share growing from 21% in 2010 to 25% in 2035, with natural gas as the only fossil fuel whose share was growing [15]. This growth is illustrated in Figure 1.3.

It is also argued in [16] that the LNG market may become more like the oil market of today, with contracts having a shorter duration, more sales and purchases are made on the spot market, and switches between trading partners are more common. Long term LNG delivery contracts typically comprise a 25 year period and a present value of hundreds of millions of dollars. On the other hand, unscheduled and instantaneous LNG demand - the so called spot opportunities - is an upcoming and valuable feature of the LNG market, as illustrated by Figure 1.4. As an illustrating example, the Japanese earthquake disaster in 2011 forced the shutdown of multiple nuclear energy facilities. To keep up with the nationwide energy demand, LNG turned out to be the key source for short-term supply. As a result the demand for alternative energy sources such as LNG increased dramatically in a very short time period, pushing the spot market price significantly.

1.4 - Asset Wide Optimization in the LNG upstream value chain

The focus of this project is on the upstream part of the value chain, defined as all activities from reservoir exploration up to shipment. Roughly speaking, it consists of four technical assets that are directly related to LNG: (1) Exploration and Production, (2) Purification and Liquefaction facilities, (3) Storage, (4) Shipment. Furthermore, LNG production is highly interlaced with the oil value chain, since both products are recovered simultaneously from 'Associated' wells.

Therefore, (5) the oil market as well as the (6) LNG markets are considered non-physical assets. Chapter 2 describes all assets in more detail, and Chapter 3 constructs a mathematical framework to model the system as a whole.

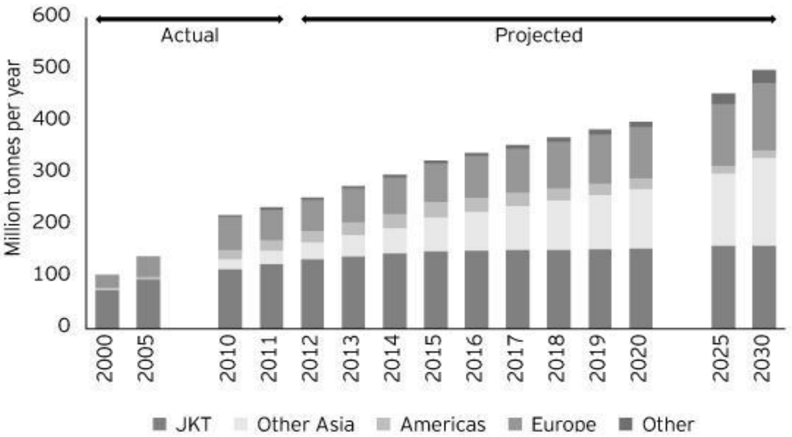


Figure 1.3 – Actual and projected global LNG liquefaction in Million tons per year, as forecasted in 2012. The abbreviation JKT refers to Japan, (Southern) Korea and Taiwan, the top 3 LNG consumers. Source: [1]

As an example, suppose that we just received the message that an LNG train has stopped working and needs maintenance. This means we could shut down the gas production at a sufficient number of wells to apply for the decreased liquefaction capacity. However, this would also decrease oil production. Another option is to maintain production levels at the wells, and to flare part of the produced natural gas. Furthermore, if the LNG stock is insufficient to load all LNG ships as planned for today we must reschedule some of them. However, how should we decide which one to reschedule? And is it possible to take for example future breakdown risks into account, such that costs associated with actual breakdowns are minimized? These are question that could be answered by application of AWO in the LNG value chain. Note that the coupling of both technical and commercial constraints and opportunities plays a central role in this application. In this thesis, we focus on optimizing commercial objectives, given the technical constraints in the system.

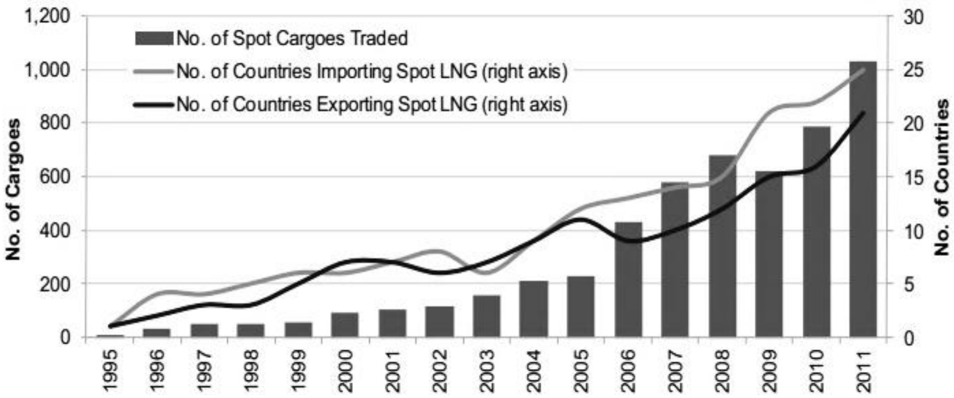


Figure 1.4 – Facts on spot cargoes, traded in the period 1995 to 2011. Source: [14]

1.5 - Project goals

The project started from scratch as a first attempt to apply Asset Wide Optimization methods to Shell's LNG upstream value chain. In the first meetings, it was emphasized that no data was available and the goal was to obtain an objective, mathematician's view on the process and business challenges faced within the LNG value chain instead of a data driven analysis.

The goal of this thesis is to:

(1) Provide an overview of the LNG upstream value chain in terms of its assets, key parameters and potential conflicting objectives,

(2) Construct a mathematical framework to describe system behavior on an asset wide (global) level, to provide an operational (day-to-day) decision making model, preferably in a computer environment that is well-known to both ORTEC and Shell, and

(3) Examine to what extend uncertainty can be taken into account, to quantify and cope with the risks involved with the proposed decision model.

Based on these three sub-goals we set the overall project goal to

(4) Deliver a proof of concept method for day-to-day decision optimization in Shell's LNG upstream value chain from an Asset Wide Optimization perspective. Furthermore, we aim to provide recommendations on further research to investigate the potential of an AWO approach and future tool development.

Besides business oriented goals, we obtain some general mathematical results associated with Asset Wide Optimization models in a stochastic environment. Furthermore, we have chosen to present relevant literature throughout the chapters.

1.6 - Scope of the project

The project is mathematical of nature, applied to practical challenges from a business perspective. It applies mathematical models and ideas to Shell's LNG value chain challenges. Uncertainty in the integrated value chain plays an important role and has to be part of the project, since the project is the final stage of a Master studies in Stochastic Operations Research (SOR) at the University of Twente. We aimed at a model driven approach, instead of data driven as it is a first attempt to examine the potential of Asset Wide Optimization.

From a business point of view, Chapters 2 and 3 describe the parameters and optimization approach in a deterministic setting, which is most suitable for short term purposes. Chapters 4 and 5 describe the value of the extension to stochastic models, taking into account the risks involved with future uncertainties. Chapters 6 and 7 show implementation and results of the stochastic models, and should be considered from a proof-of-concept perspective. Furthermore, we do not use real business data due to confidentiality and the short time scope of the project. Application of the models to real business cases would be of great value for future research as described in Chapter 8.

Most of the information that is included in this thesis is a result of frequent meetings with Swapan Saha, Senior Smart Fields Engineer at Shell, in combination with the available literature on Asset Wide Optimization and the LNG upstream value chain. We decided to start from scratch with modeling the value chain, to gain a clear view of all important 'inputs' and 'outputs' that are to be considered. The work contained in this thesis should therefore be regarded as a first attempt to examine the potential of an Asset Wide Approach towards LNG value chain optimization to quantitatively support the AWO discussion involving chemical engineering experts and operation research specialists.

Chapter 2

The LNG value chain

As will become clear in the remainder of this thesis, a mathematical Asset Wide Optimization model cannot cope with all details concerned with the LNG upstream value chain. This chapter provides detailed background information on the LNG production process. The next chapter describes those details that are contained in the mathematical model as we use it for further analysis.

We focus on operation of existing production facilities, instead of strategic goals such as expansion of activities such as new reservoirs or plant investments. A schematic overview of the LNG upstream value chain was already presented in Figure 1.1. For a complete overview, we start our description of the LNG value chain with exploration details. In the next chapter, we construct a mathematical model of the LNG upstream value chain that is used for our Asset Wide Optimization purpose.

2.1 - Exploration

Once a team of exploration geophysicists and geologists has located a potential natural gas reserve, drilling experts dig into the ground to examine it. As these drilling activities are very expensive, many innovations and techniques have been developed over the last years that both decrease cost and increase efficiency of drilling. Despite this, the success rate of exploration is far from 100 percent, and the risk of no natural gas being found is an important factor in investment decisions.

The characteristics of the subsurface, depth and size of the target reservoir are key parameters to determine the exact placement of a drill site. Besides these technical considerations, it is necessary to obtain the mandatory documents for legal drilling. These usually involve securing permits for the drilling operations, a legal arrangement for extraction, priority of specific customers such as governmental power plants and a design of transportation infrastructure to connect a well to onshore or offshore pipelines.

Furthermore, if the exploration team was incorrect in its estimation of the existence of an economic attractive quantity of natural gas at a well site, the term 'dry well' is used, and production is stopped. Otherwise, the well is completed to facilitate its production of natural gas and is called a 'development' or a 'productive' well.

The well completion step determines properties such that it is suitable for gas and oil extraction, given its conditions. Different types of wells can be found, having their own prescribed completion such as (1) open hole, (2) sand exclusion or (3) multiple zone. Sand exclusion completion is used in wells with a large amount of loose sand to withhold the sand from mixing with the extracted products as this would increase production costs per product volume drastically. Multiple zone completion allows for simultaneous drilling in multiple parts of the well, and open hole completion consists of simply running a casing directly down into the reservoir, leaving the end of the pipe open without any protective filter.

2.2 - Well treatment

When the well is completed, the hydrocarbons (both natural gas and oil) start to flow from the reservoir up to the surface. In the first stage of a reservoir's production life, known as primary recovery, natural pressure from the reservoir forces the hydrocarbons in the reservoir to move to the well head. In absence of a natural drive, several artificial lifting techniques can be used, such as gas lift or rod pumps or downhole pumps, depending on well characteristics such as depth.

All of these methods involve an external energy source to the hydrocarbons to the surface, such as gas injection through a well that is drilled parallel to the extraction well. Natural gas is injected in the well to increase reservoir pressure. This gas is lost and cannot be used for LNG production. Therefore, if the gas quality coming from an associated well is low, this reinjection method may be economically favorable as oil flow is maintained. For any of the artificial methods, one should balance the cost of energy input and the economic potential of the oil and gas that is produced.

In this thesis, we assume that the maximum production rate of a well is known and constant over the full planning horizon. However, the so called Hubbert peak [17] theory states that for any given geographical area, from an individual oil and gas producing region to the planet as a whole, the production rate tends to follow a bell-shaped curve. Selecting a particular curve for a well, based on field experiments, determines a point of maximum production based on discovery rates, production rates and an expected well age.

The amount of oil and gas that is present in the product stream differs per well, and is determined by the well-specific Gas-to-Oil Ratio (GOR), also referred to as Gas-to-Liquid Ratio (GLR). It is a dimensionless volumetric ratio of gas that is present in the product stream of a well, to the volume of oil.

Another well specific parameter is the impurity ratio of the gas, referring to the fraction of the gaseous state components that have to be removed before liquefaction, such as water and sulfur. As these components have a higher (boiling and) freezing temperature than methane (the valuable element of natural gas), causing ice-forming in the liquefaction facilities if present. We speak of high-impurity wells if the gas coming from such a well has a high impurity fraction, and vice versa. We assume that, given the production rate, the Gas-to-Oil ratio and the impurity ratio, the composition of the product stream can be determined in terms of oil, natural gas and impurities.

At the wells, a surplus of gas can be flared. The amount of flared gas at a well and at a specific time cannot exceed the gaseous state products in the product stream at that time, as determined by the Gas-to-Oil ratio. According to [18], Approximately 150 billion cubic meters of natural gas are flared in the world each year, representing an enormous waste of natural resources and contributing 400 million metric tons of CO_2 equivalent emissions. This flared gas equals 30 percent the annual gas consumption in Europe.

Instead of flaring the natural gas, one could also decide to shut down production at the wells. However, well changeover costs are involved with such an operation. These costs represent the manpower that is needed to physically get to the wells to shut them down and the preference to maintain well settings instead of changing them regularly. The decision maker must decide whether he shuts down wells or preserve oil production by flaring the associated gas at the wells.

Another important decision from a business point of view is concerned with the choice in wells to produce from. As described, wells may vary in terms of gas impurities and Gas to Oil ratio. A decision maker must choose between producing more oil (open wells with low GOR) or more gas (wells with high GOR), based on knowledge about LNG and oil prices.

Maximizing LNG production is not always the best strategy here, since the associated oil production also plays a role in the obtained total revenues. This is where AWO can make a difference, as it focuses on commercial objectives such as total revenue for the value chain as a whole. For this example specifically, AWO focuses on balancing LNG and oil production, such that revenues are maximized and the technical constraints are respected.

2.3 - Purification and liquefaction

In order to process the associated dissolved natural gas, it is separated from the oil in which it is dissolved. The separation is generally performed at, or near to the well. The composition of raw natural gas varies between regions, so specific separation requirements apply. Therefore, the actual process that is used to separate gaseous state products from the oil, as well as the necessary equipment also varies. A widely used separator is known as a conventional separator. It consists of a closed tank, with the force of gravity separating the heavier oil from the gaseous state products.

The liquefaction plant may consist of several parallel units arranged in a sequential manner (which is why they are called LNG trains). By liquefying the gas, its volume is reduced by a factor of 600, which means that LNG at -161°C uses 1/600th of the space required for a comparable amount of gas at room temperature and atmospheric pressure.

The LNG cooling processes are generally patented by large engineering companies, or oil and gas companies such as Shell. It is a major business advantage if costs for cooling the natural gas can be decreased by even the smallest percentage. To illustrate this, a typical LNG train uses approximately 28 MW per million tons of LNG per annum (MTPA) (variable costs) and the liquefaction section generally accounts for 30% to 40% of the capital costs of the total plant (fixed costs). Therefore, companies act reservedly when it comes to sharing details on these processes.

LNG trains are subject to maintenance periods, both planned and unexpected (breakdowns). Based on an analysis in [19], the anonymous data from 8 LNG plants, with 3 to 8 trains per plant for a period of 1 year up to 10 years shows that approximately 75% of LNG train downtime is unexpected. The annual number of breakdowns per train, regardless of duration, differs between 0 and 41, with an average of 5.7. However, it is unknown which sites are included in this analysis.

In general, the cooling process is based on a two or three stage cooling process. The most critical component is the heat exchanger, which is designed for optimal cooling efficiency. Most of the exchangers use a mixed refrigerant (MR) design. Stability and efficiency of this process is mainly determined by the LNG Q/T (heat load to temperature ratio) curve, as depicted in Figure 2.1. The mixture of refrigerants is carefully selected, such that the Q/T curve of the LNG gas stream is matched as close as possible. It typically combines one or two main components and several smaller elements to meet location-specific LNG properties for the three cooling phases: (1) pre-cooling, (2) liquefaction and (3) sub-cooling.

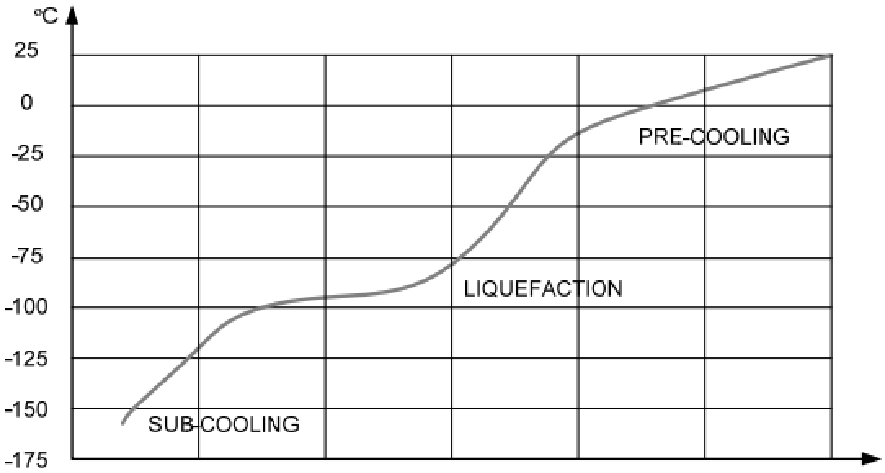


Figure 2.1 – Typical LNG cooling Q/T (heat load to temperature ratio) curve. Source: [16]

The pre-cooling stage cools the natural gas to approximately -40 degrees Celsius. The refrigerant is generally propane or a mixture of propane and ethane, with small supplements of other gasses. The liquefaction phase cools the gas to about -100 to -125 degrees Celsius with a mixture of methane and ethane. The final sub-cooling stage brings the LNG to a temperature of -162 degrees Celsius, using a mixture of methane and/or nitrogen. The details on refrigerant selection are not part of our analysis, but may influence the restrictions on production rates. We do take into account a maximum throughput parameter and a maximum impurity parameter.

2.4 - LNG Storage

The liquefied LNG is stored in heavily insulated storage tanks, specially designed to store cold-temperature (cryogenic) liquids. Most tanks have a double wall, with the outer wall made of thick concrete and an inner wall of high quality steel. Between them, a thick layer of highly efficient insulation is found. Many facilities have underground storage tanks for increased insulation. Albeit this insulation, some LNG will boil off and evaporate as natural gas. It is generally removed from the tank and exported as natural gas, reliquefied and returned to storage or used as power source for the liquefaction plant.

Sensitivity to temperature fluctuations can make LNG unstable, which may lead to a non-homogenous liquid inside the storage tank. The main causes of instability in LNG storage tanks are related to:

- Variable quality of the LNG flowing into the tank
- Pumping LNG in or out of the tank
- High nitrogen content (over 1%) in the tank composition

One of the main challenges associated with instability of LNG is the 'rollover' effect caused by the nitrogen component, if a sufficient quantity of nitrogen (greater than 1%), is present. Natural convection causes circulation of the LNG within the storage tank, such that a uniform liquid composition is maintained. The addition of new liquid from production, may result in the formation of different temperature and density layers within the tank. As the densities of two layers approach each other, the two layers mix rapidly, and the lower layer which has been superheated gives off large amounts of vapor and rises to the surface of the tank. This effect is known as 'rollover'.

The large amounts of vapor generated may cause a significant rise of internal tank pressure. In literature, extensive models are used to handle this rollover effect [20]. Furthermore, technical constraints restrict the in and outflow of the tanks. In our AWO approach, we only take into account the storage capacity and disregard other the restrictions on the input and release flow capacities.

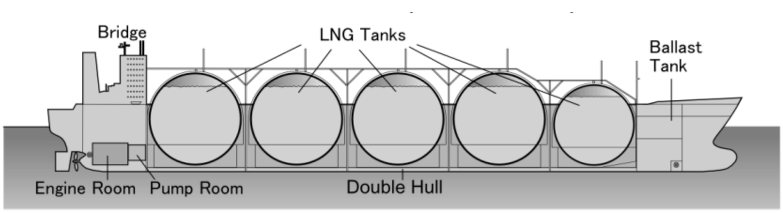
From an AWO perspective, the main risks associated with LNG storage is an overflow of LNG, known as 'tank top', or shortage, known as 'tank heel'. The latter risk is associated with LNG train breakdowns. When the storage level of LNG is low and suddenly an LNG train breaks down, we might need to cancel a ship due to insufficient LNG to (fully) load it. On the other hand, the tank top risk is associated with shipment delays. When a ship comes in late and we have an (almost) full LNG storage tank, we have to shut down production at the LNG trains, with flaring or well changeovers as a direct result.

2.5 – Shipment and terms of delivery

LNG is transported in large ships called LNG carriers. These specially designed ships are able to keep the liquid on its cryogenic temperature of -161 degrees Celsius by extreme insulation and cooling techniques. The tanks on the carriers are not much different from the LNG storage tanks, except for the floating feature and capacity. Shell is the world's largest LNG shipping operator. They operate 50 of the world's 370 LNG carriers. Their fleet is mainly based in Australia, Qatar, Nigeria and Brunei.

The LNG shipping sector has also been evolving quickly over the last decade in response to accelerated growth in the international gas markets and, as in other parts of the LNG supply chain, technological innovation is seen as the means of optimizing costs and increasing the number of shipped cargoes.

Furthermore, new companies have entered the LNG shipping business, and the LNG industry is increasingly looking for more flexible shipping arrangements. Larger ships, innovative ship designs and propulsion systems have been developed while safety and environmental factors remain the most important considerations in the construction and operation of the carriers. As new technologies evolve quickly, ship capacities fluctuate largely over the current worldwide LNG carrier fleet. In Figure 2.2, an intersection of the most common spherical LNG carrier is shown. Nowadays, 40 percent of the LNG carriers are of this type.



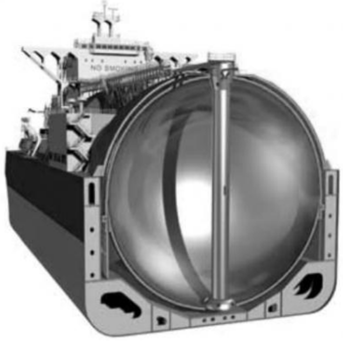


Figure 2.2 – (left) sideview of LNG carrier, having 5 spherical tank of approximately 40 meters in diameter. (right) intersection of spherical LNG storage tank.

LNG contracts can involve many types of delivery terms. The most common are:

- **Free-on-board (FOB) basis**, where the buyer takes ownership of LNG as it is loaded on ships at the export LNG facility. The buyer is responsible for LNG delivery, either on its own ships or ships chartered by the buyer. The contracted sales price does not include transportation costs.
- **Cost-insurance-freight (CIF) basis**, where the buyer takes legal ownership of the LNG at some point during the voyage from the loading port to the receiving port. The seller is responsible for the LNG delivery, and the contracted sales price includes insurance and transportation costs.
- **Delivered ex-ship (DES) basis**, where the buyer takes ownership of the LNG at the receiving port. The seller is responsible for LNG delivery, and the contracted sales price includes insurance and transportation costs.

Note that the responsibility for ship delivery can lie at both the seller and the buyer, so ship availability is not straightforward in the sense that an LNG production company is restricted to a fixed number of vessels it can use for its LNG transport. Besides the necessary arrangements, also the risks involved with shipment are different for the three terms of delivery mentioned above.

The Annual Delivery Program (ADP) is a schedule of gas volumes to be delivered on certain dates or within certain periods in a forthcoming contract year in a long term contract. For both the delivery side of the agreement as well as the customer, it is important to know on a reasonable term when to expect a new LNG cargo. As the name suggests, every year an ADP is constructed, and availability of loading berths, production rates, availability LNG carriers and a contractual delivery time slot are key factors in ADP construction. In practice this will often take the form of a detailed schedule covering the first few months, with looser numbers for the remainder of the year, which are then fixed at times as specified in the contract.

As discussed in the previous section, shipment delays may cause tank tops. These delays can have many causes, of which weather fluctuation are the most important. Since the journey of an LNG carrier generally takes many days or even weeks, bad weather conditions may cause ship delays of days.

Initially, the LNG market was very limited and regionally oriented. LNG was primarily sold by long-term arrangements through point-to-point deliveries to large, creditworthy customers (mainly gas and power companies). Furthermore, the pricing was highly segmented with LNG prices indexed to the Japan Customs-cleared (JCC) petroleum price in Asia, petroleum products in Europe and other indexes for other parts of the world.

Today, global LNG markets are significantly more inter-regional, and competition plays a more important role. The markets are more flexible, with a large number of suppliers and buyers, spread around the globe. In the past decade, the LNG market is more and more shifting from long term contracts to short term agreements and price negotiations. More cargoes are sold to the highest bidder on the so called spot opportunity or short term markets. Due to the short term character of spot arrivals, prices are generally much higher than those for cargoes associated with long term contracts.

If a company is able to deal with these sudden spot opportunity arrivals, it can make large revenues by taking on spot deliveries. From an AWO point of view, taking into account the possibility of commercially attractive spot opportunities, could lead to increased revenues. Due to seasonality and associated uncertainty in weather conditions, spot opportunities are most likely to emerge during winter months to overcome variability in LNG demand. However, as the winter period varies globally, spot opportunities differ largely per region and thus per production side.

2.6 – Key parameters for AWO

At the wells, the key parameters are the gas to oil ratio and the impurity ratio. These two parameters determine how much oil and associated natural gas can be extracted from the wells to meet the restrictions on gas and impurity throughput in the other assets of the production chain. Furthermore, the maximum production rate at a well and the change-over costs play an important role in the optimization. The latter represents the unwillingness of a decision maker to frequently change well settings. The oil price determines the willingness of producing oil over LNG. When oil prices are expected to rise, one could decide to postpone oil production in favor of a higher LNG production rate and vice versa. However, the LNG production should meet the demand as defined in the ADP, or rejection or rescheduling penalties might apply.

The (offshore) pipeline infrastructure restricts the LNG flow from the wells to the (onshore) production facilities. Pressure generators are used to 'push' the two-phase (gaseous natural gas and liquid oil) product stream away from the wells to the production facilities. We have not included this asset in our analysis as it introduces a high level of detail.

At the production facilities, roughly comprising a separation unit and a liquefaction plant, the key parameters are the maximum gas throughput and the maximum impurity throughput. Impurities are gaseous state elements such as water and sulfur, with a freezing temperature that is higher than for natural gas. If the ratio of impurities of the gas in the liquefaction plant is too high, the solid state impurities will accumulate in the pipes, blocking the gas flow. It is therefore important to meet the impurity restrictions of the LNG trains. Furthermore, each of the trains has a maximum throughput parameter. These parameters can be different per LNG train, as technologies have improved over the years.

The storage tank acts like a buffer for arriving ships to load the LNG. The most important parameter is the tank capacity. The Annual Delivery Plan is a key parameter in the shipment of LNG in the sense that it determines the demand side of the value chain, i.e. when the product can be sold to customers according to contractual agreements. We have assumed that the revenue of delivering a cargo on each of the periods involved in the optimization is known. In reality however, these revenues and costs involved with (re-)scheduling are difficult to determine or even to approximate. It was unknown to us to what extend the LNG delivery is flexible in terms of delivery periods and associated costs and revenues and to what extend our model is applicable to real data.

In many applications as well as the LNG case, it is well known to a system operator how to act as long as a system behaves according to plan. Asset Wide Optimization is expected to gain the greatest added value when a system is suddenly exposed to disruptions from its average case behavior. Sudden disruptions in a system's behavior behave like a stochastic process with its evolution is unknown prior to optimization. We therefore investigated the effect of adding uncertainty to the AWO optimization model from Chapter 4.

Chapter 3

Deterministic Dynamic Programming

In this chapter we elaborate on the LNG value chain description discussed in the previous chapter and construct a mathematical decision making framework. In many applications, such as in Shell's LNG value chain, decisions are made on a frequent basis having both immediate and long-term consequences. In such sequential decision problems a decision maker or agent observes the state of a system at specific points in time. He then selects an action resulting in a direct reward and the evolution of the system to a next state. At this subsequent point in time, he faces a similar problem. However, the system may be in a different state and the set of actions to choose from may be different.

One tries to optimize both direct and future rewards. If we do not take the impact of current decisions on those in the future into account, overall performance may be poor. Such a greedy approach to sequential decision problems in general results in less or at least worse possibilities at future decision moments. If this was not the case, one could simply isolate the individual decisions to obtain an overall optimal solution. An example of sequential decision making can be identified when running a marathon. Sprinting at the start may result in a good ranking for a while. However, due to rapid energy depletion the final result may be unsatisfying.

A widely used approach for solving sequential decision making problems is called Dynamic Programming. This chapter first defines the framework of Dynamic Programming (DP) in Section 3.1, along the same lines as found in many textbooks such as [21]. In Section 3.2 a widely used solution method known as backward induction by Bellman's equation of optimality is discussed. In Section 3.3 the framework is applied to Shell's LNG case.

3.1 - The dynamic programming framework

Dynamic Programming (DP) is an iterative method to solve sequential decision problems. It breaks down complex problem into smaller, easier to solve sub-problems. The key ingredients of a dynamic programming problem are the following:

- A set of decision periods N with elements denoted by t,
- A set of system states S with elements denoted by s and s',
- A set of (state dependent) available actions A_s with elements a,

- A state and action dependent direct reward function $r(s,a)$, and
- A state and action dependent transition function $g(s'|s,a)$.

Mathematically, a DP is defined by a five-tuple that is discussed in the following sections:

$$DP \coloneqq \{N, S, A_s, g(s'|s,a), r(s,a), \text{ with } s,s' \in S \text{ and } a \in A_s\} \tag{3.1}$$

We assume that the decision maker has complete information on the structure of the model. That is, he knows all system parameters (as discussed below) with certainty prior to the first decision that is to be made.

Periods

The most important feature of the Dynamic Programming method is the structure of an optimization problem containing multiple periods, which are solved iteratively one at a time. The periods often represent time intervals in the planning horizon of the problem, such as days, weeks or years and are denoted by an index $t \in N \subseteq [0,\infty)$. However, periods do not need to be time-related. The shortest path problem [22] is a well-known example in which time does not play a role.

Both a continuous and a discrete time DP variant exist that differ in the classification of the set N to be either discrete or continuous. In the latter case, decisions are made either constantly, or at predefined specific points in time. In this thesis we focus on the discrete variant, where time is discretized in periods or stages, and decisions can be made at the start of each period. If the set of periods is finite, so $N = \{1,2,\dots,T\}$ with $T < \infty$ the number of periods, the problem is defined as a finite (T-)horizon problem.

State Space definition

Associated with each period of the optimization problem is a set of states that can be attained by the process. The power set containing all states of the model is denoted by S. The definition and structure of a state space should respect the so-called memoryless property; it contains all the information that is necessary to select actions, regardless of how the process reached the current state. Furthermore, a state space definition should convey all information that is needed to assess the consequences of decisions upon future states. Decisions only depend on the current state and action set. These features considerably limit the applicability of the method to real-world problems in terms of complexity, but on the other hand it offers a rich variety in theory and literature.

The initial state of the system is defined as s_1 and is regarded as a starting point for optimization. We assume (without loss of generality) that every state $s \in S$ is assigned to exactly one period t, i.e. these pairwise disjoint subsets $S_t \subset S$ contain those states that can be assumed by the process in period t. If the state is described by more than one variable the problem is called a factored DP [23]. In such applications, a state space with elements x_i is usually presented in vector form:

$$s = (x_1, \dots, x_n), \quad x_i \in Dom_i \quad \text{for} \quad i = 1, \dots, n$$

with n defined as the dimension of the factored DP [24]. A 2-dimensional state space in our marathon example could have the elements (1) residual energy and (2) distance to finish. We need (at least) both to determine an optimal running pace to minimize finish time, regardless of our running history.

Actions and direct rewards definitions

At each period the decision maker selects an action a from the state dependent feasible action set $A_s \subseteq A$. Equivalent to the definition of a factored state space, an action space with multiple elements y_j is represented by a vector:

$$a = (y_1, \dots, y_m), \ \ y_i \in Dom_i \quad \text{for} \ \ i = n+1, \dots, n+m$$

A value is to be assigned to each of the elements y_j when selecting an action. The action set A_s can be characterized by a feasible region, as shown in Figure 3.1. As suggested by the figure, the constraints form a set of (linear) inequalities on the action vector a, as found in mathematical programming models. More on the equivalence between DPs and linear programming models is discussed in Section 5.1.

By selecting action $a \in A_s$ a direct reward $r(s, a)$ is obtained. In economic applications, this reward can be regarded as revenue (or cost if negative). It is assumed that the decision maker knows (or is able to calculate) the direct rewards that correspond to selecting each of the possible actions, so no uncertainty is involved here.

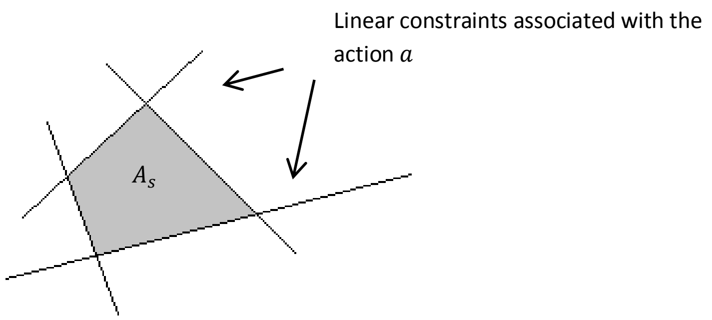


Figure 3.1 – The feasible action space A_s in state s is defined in terms of a set of linear inequalities

In the last period $t = T$, no action is to be selected and the direct reward $r_T(s_T)$ only depends on the final state s_T of the system. This function is often called the salvage value or terminal reward of the DP problem. In our marathon example, the terminal reward of residual energy at the finish line is zero since it has no 'value' regarding our objective of minimizing the finish time. A counter example is found in many inventory problems where the terminal reward usually represents the value of stock that is left at the end of the planning horizon.

Transition function definition

When an action is selected, the process evolves to the next period. The corresponding state of the process depends entirely on the current state of the process and the selected action. We define a deterministic transition function $g(s'|s, a)$, with $s \in S_t$ and $s' \in S_{t+1}$. It takes on the binary values 0 and 1 to indicate whether or not state s' is the next state if action a is selected in the current state s. This implies the important property that a DP is uniquely determined by the initial state and the successive actions at each period in the planning horizon.

In general, the transition function may depend on time. However, if every state can only be assumed at a unique time t, we can omit the time dependency and write $g(s'|\, s, a)$. By the same arguments we can write $r(s, a)$ instead of $r_t(s, a)$.

Strategies and value

The decision maker influences the system by selecting an action from a feasible action set A_s as described in the previous section. A strategy or policy α is defined as a prescribed sequence of successive actions to be selected in the $T-1$ periods of a DP:

$$\alpha = (a_1, \dots, a_{T-1}) \in A^{T-1}$$

When an action is selected, the process evolves to the next state according to a deterministic transition function. In other words, the next state is known with certainty if we know the current state and the action that is selected. Successive states that are assumed by the system, as a result of using strategy α in combination with initial state s_1 thus define a state sequence:

$$\delta_\alpha = (s_1, \dots, s_T) \in S^T$$

An action sequence is feasible if all actions are in the feasible action set of the system state at the corresponding period. That is,

$$a_t \in A_{s_t} \qquad \forall t$$

The set of all feasible strategies for a given initial state s_1 is denoted by Ω_{s_1}. The state sequence δ and a feasible action sequence α induce a reward sequence:

$$r_{\delta,\alpha} = (r_1, \dots, r_T) = (\, r(s_1, a_1), \dots ,\ r(s_{T-1}, a_{T-1}),\ r(s_T)\,)$$

Note that the reward sequence is uniquely defined by the initial state and a feasible action sequence α. We write $r_{\delta,\alpha}$ instead of $r_{s_1,\alpha}$ for clarity reasons. To be able to compare a given set of strategies, the value of a reward sequence is defined in terms of a utility function

$$R_{\delta,\alpha} : \ r_{\delta,\alpha} \to \mathbb{R}$$

An obvious choice in case of economic objectives is the sum of the reward sequence:

$$R_{\delta,\alpha} := \textstyle\sum_N r_t \tag{3.2}$$

This so-called total reward criterion presumes that the decision maker is indifferent to the timing of the rewards. A reward sequence in which a reward is received in each of the T periods is no more or less valuable than a reward sequence in which all rewards are received in the first (or the last) period. To account for preferences on the timing of rewards, we could introduce a discount factor λ:

$$R^{\lambda}_{\delta,\alpha} := \textstyle\sum_N \lambda^{t-1} \cdot r_t$$

The larger the discount factor the larger is the weight assigned to direct rewards with respect to future ones. In economic applications, the discount factor is usually related to the interest rate on capital, since it resembles the present value of future rewards. For short planning horizons, the discount factor is generally close to one. Therefore, we do not use a discount factor since it will play a minor role in our analysis. However, the model can be extended easily if needed in future applications.

Now that we are able to compare strategies in terms of their values, a strategy α^* is defined to be optimal for given initial state s_1 if it performs at least as good as any of its alternatives:

$$R_{\delta,\alpha^*} \geq R_{\delta,\alpha} \quad \forall \alpha \in \Omega_{s_1}$$

The value of a DP problem is defined as R_{δ,α^*}. The next section discusses how such an optimal strategy α^* can be found.

3.2 - Solution methods for finite horizon discrete time dynamic programming problems

Many dynamic programming problems are solved numerically, since the calculations required are generally lengthy and repetitive and are therefore more suitable for a computer. However, some DPs can be solved analytically. An important advantage of such an approach is that there need not be a restriction on the number of states and actions specified [25]. On the other hand, analytic solutions methods such as Lagrange methods or control theory might work for specific well-structured problems and thus cannot be applied to many real-world problems. In Section 4.3, the drawbacks are discussed in more detail. For now, we focus on a numerical solution method.

Given an initial state s_1 and a dynamic programming problem, the goal is to find an optimal strategy α^*. In theory, it is possible to find an optimal strategy by enumerating over all possible $\alpha^* \in \Omega_{s_1}$ if the action space A is finite. However, in practice this calculation may be intractable if A is 'large'. By using a recursive method known as backward induction, we break down the problem into sub problems.

We define the optimal value function $u_t(s)$ as the maximum (or optimal) return that is possible starting in period t and in state s. By starting at the end of the planning horizon we determine the value $u_T(s)$ for all $s \in S_T$. Since at the last period T no action is selected the value equals the terminal reward:

$$u_T(s) = r_T(s), \qquad \forall s \in S_T$$

Given these optimal values in the final period, we proceed to period $T-1$. The value function of a state $s \in S_{T-1}$ is now a combination of direct rewards and the reward that is obtained in the successive period T. If we extend this method by iteratively evaluating the value for states at all periods $t \in N$, we obtain:

$$u_t(s) = max_{a \in A_s} \left\{ r(s,a) + \textstyle\sum_{s' \in S_{t+1}} g(s'|s,a) \cdot u_{t+1}(s') \right\} \tag{3.3}$$

This equation is also known as Bellman's equation of optimality [26]. It states that, regardless of the action selected, all subsequent actions in successive periods must be optimal to obtain maximal (or optimal) possible revenue. Furthermore, the optimal action a_s^* in state s is defined by

$$a_s^* = arg\, max_{a \in A_s} \left\{ r(s,a) + \textstyle\sum_{s' \in S_{t+1}} g(s'|s,a) \cdot u_{t+1}(s') \right\} \tag{3.4}$$

The value of the initial state is obtained in the final step of the algorithm

$$u_1(s_1) = max_{a \in A_{s_1}} \left\{ r(s_1,a) + \textstyle\sum_{s' \in S_2} g(s'|s_1,a) \cdot u_2(s') \right\}$$

With the corresponding optimal action $a_{s_1}^*$ as found by equation 3.4. To evaluate the value of the initial state, only values of those states in the second period that can be reached have to be calculated. One could choose to first determine this set of reachable states before evaluation of the value function. However, one should take into account the computational effort to determine these reachable sets and compare it with direct application of equations 3.4 and 3.4.

Note that the optimization problem at each stage could be determined by application of a wide range of optimization techniques, such as linear programming or even another dynamic programming problem. If we can apply such techniques, enumerating over all options might not be necessary. However, this depends on the specific problem structure.

The recursive relation needs to be solved for all possible states of the system at each period. To directly apply the optimality equations, both the state and action space should be finite. However, uncountable state and action spaces play a central role in this thesis. The mathematical issues concerned with such problems are discussed in Section 4.2. Other technical considerations - i.e. with respect to non-discrete time problems - are not in the scope of this text. We refer to [27] for a comprehensive overview.

3.3 - Application of the DP framework to the LNG case

To apply the dynamic programming framework to the LNG case, we identify the decisions that are made on a daily basis. We focus on three types of decisions:

1. Well production levels
2. Flaring of gaseous state products
3. Contract delivery scheduling

In the following sections we apply the dynamic programming framework to the LNG case to find optimal strategies concerning the above decisions. We consider an instance with the sets W, K, C and N representing wells, LNG trains, cargoes and time periods respectively. The model is split in two parts: (1) well production and flaring of gaseous state products and (2) contract delivery scheduling, as illustrated by Figures 3.2 and 3.3.

Well production and flaring of gaseous state products

In each period t, the production rates $\pi_{t,w}$ (A1) for the wells w have to be selected. It is a positive and continuous variable that is limited by the maximum product flow out of well $w \in W$:

Production rate of well w in period t	$\pi_{t,w}$	(A1)

which is bounded by constraint (C1):

$$\pi_{t,w} \leq \Pi_w^{max} \qquad \forall t, w \qquad \text{(C1)}$$

With Π_w^{max} (P1) the maximal well flow of well w. If we decide to change well settings, a fixed cost c_w^{well} (P2) is involved, regardless of the amount of change. Besides some technical motives, a well engineer has to be paid to physically change the well settings on-site, so costs are associated with changing production flow.

Therefore, a constant well production rate is preferred such that costs are minimized. This system parameter represents the willingness (or unwillingness) to change well settings. The direct revenues associated with selecting a production rate are directly related to the amount of oil (liquid state products) that is produced. On the other hand, direct costs (negative direct rewards) are obtained by resetting wells. Furthermore, the production rate $\Pi_{t,w}$ (S1) at the start of a period is contained in the state description to be able to decide whether or not it is changed.

We need three dummy variables keep track of changes in well settings. The binary variable $\pi_{t,w}^{bin}$ (D1) equals one if the well settings of well w are changed in period t, and zero otherwise. It is completely determined by the value of the decision variables $\pi_{t,w}$ through set of big-M type constraints [28] as defined by (C2) and (C3). The dummy variables $\pi_{t,w}^{+}$ (D1) and $\pi_{t,w}^{-}$ (D2) are both positive and indicate increased or decreased production rates with respect to the previous period:

$$\pi_{t,w}^{+} - \pi_{t,w}^{-} = \pi_{t,w} - \Pi_{t,w} \qquad \forall t,w \qquad \text{(C2)}$$

$$\pi_{t,w}^{+} + \pi_{t,w}^{-} \leq \Pi_{w}^{max} \cdot \pi_{t,w}^{bin} \qquad \forall t,w \qquad \text{(C3)}$$

Note that we need the initial production rate $\Pi_{1,w}$ (P3) as input parameter. A second decision variable $f_{t,w}$ (A2) is the amount of natural gas that is flared at the wells. Due to environmental issues, a cost per flared unit volume of gas is paid so in the ideal scenario no gas is flared. However, in some cases it might be optimal to flare gas to maintain oil production.

Flared amount of gaseous state products at well w in period t $\qquad f_{t,w} \qquad$ (A2)

This decision variable cannot exceed the production rate at the corresponding well, since gas is flared immediately after production. The gaseous state production is determined by the well-specific parameter $GOR_w \in [0,1]$ (P3), representing the Gas-to-Oil ratio. We have the constraint:

$$f_{t,w} \leq \pi_{t,w} \cdot GOR_w \qquad \forall t \qquad \text{(C4)}$$

The product streams in terms of oil, gas and impurities as a result of selecting well production rates $\pi_{t,w}$ and the amount of gas that is flared at the wells $f_{t,w}$ are:

Oil production (feed to oil market) $\qquad \pi_t^{oil} = \sum_W \pi_{t,w} \cdot (1 - GOR_w)$

Gas production (feed to LNG trains) $\qquad \pi_t^{gas} = \sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot (1 - I_w)$

Impurity production (feed to LNG trains) $\qquad \pi_t^{imp} = \sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot I_w$

With I_w (P4) the fraction of impure gaseous state products. The oil production is assumed to generate immediate rewards at the oil market. Therefore, the direct oil reward R_t^{oil} is defined as:

Oil revenues in period t $\qquad R_t^{oil} = p_t^{oil} \cdot \pi_t^{oil}, \qquad$ (R1)

with p_t^{oil} (P5) the oil price in period t. On the other hand, the well changes are direct costs (or negative direct rewards):

Well change costs in period t $\qquad R_t^{well} = -\sum_W \pi_{t,w}^{bin} \cdot c_w^{well} \qquad$ (R2)

The product flow into the LNG trains equals the gaseous state product that is produced at the wells, minus the amount that is flared. The production capacity at the LNG trains restricts the production rate at the wells, as implied by constraint definition (C5). The maximal production rate of LNG train $k \in K$, with K the set of LNG trains that is considered in the model, is denoted by the parameter β_k (P6). Besides a limited production rate at the LNG trains, there is also a maximum on the amount of impurities that is fed to the LNG trains. This impurity maximum is implied by constraint (C6), with γ_k (P7) the maximum impurity parameter for LNG train k.

If maintenance of the LNG trains is planned, a factor $\mu_{t,k} \in [0,1]$ (P8) is used to indicate the fraction of the capacity of LNG train k that is available in period t. If this parameter equals 0, the capacity of the corresponding LNG train equals zero in that period. Equivalently, for a fully operating LNG train this parameter equals 1. We thus obtain the following constraints on LNG train inputs:

$$\sum_W \pi_{t,w} \cdot GOR_w - f_{t,w} \quad \leq \sum_K \beta_k \mu_{t,k} \qquad \forall t \tag{C5}$$

$$\sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w}\right) \cdot I_w \quad \leq \sum_K \gamma_k \, \mu_{t,k} \qquad \forall t \tag{C6}$$

The terminal rewards concerned with well production and flaring are 0. A schematic overview of product flows associated with well production and flaring is shown in Figure 3.1. What remains is the definition of the transition function $g(s_{t+1}|s_t, a_t)$ for the state space elements associated with well production and flaring. As the selected production rate of the wells at the current period equals the production rate at the start of the next period, the transition function is the following:

$$g(s_{t+1}|s_t, a_t) \quad = 1\,, \quad \text{if} \quad \Pi_{t+1,w} \quad = \pi_{t,w} \quad \forall w, \tag{T1}$$

and 0 otherwise. Where $\Pi_{t+1,w}$ are state space variables associated with s_{t+1}, and $\pi_{t,w}$ are action variables. To be more precise, the state space (so far) has the following elements:

$$s_t = \left(\Pi_{t,1}, \dots, \Pi_{t,w}\right)$$

And the action vector contains the elements

$$a_t = \left(\pi_{t,1}, \dots, \pi_{t,w}, f_{t,1}, \dots, f_{t,w}\right)$$

Note that this transition function is extended in the remainder of this section when other state space and action elements are added.

Decision/Action variable(s)

Production rate at well w in period t		$\pi_{t,w}$	(A1)
Flared amount of gaseous state products at well w in period t		$f_{t,w}$	(A2)

State variable(s)

Production rate at well w at the start of period t		$\Pi_{t,w}$	(S1)

Dummy variable(s)

Binary well change indicator		$\pi_{t,w}^{bin}$	(D1)
Positive well change w.r.t. previous period		$\pi_{t,w}^{+}$	(D2)
Negative well change w.r.t. previous period		$\pi_{t,w}^{-}$	(D3)

Constraint(s)

$\pi_{t,w}$	$\leq \Pi_{w}^{max}$	$\forall t, w$	(C1)
$\pi_{t,w}^{+} - \pi_{t,w}^{-}$	$= \pi_{t,w} - \Pi_{t,w}$	$\forall t, w$	(C2)
$\pi_{t,w}^{+} + \pi_{t,w}^{-}$	$\leq \Pi_{w}^{max} \cdot \pi_{t,w}^{bin}$	$\forall t, w$	(C3)
$f_{t,w}$	$\leq \pi_{t,w} \cdot GOR_{w}$	$\forall t, w$	(C4)
$\sum_{W} \pi_{t,w} \cdot GOR_{w} - f_{t,w}$	$\leq \sum_{K} \beta_{k} \mu_{t,k}$	$\forall t$	(C5)
$\sum_{W} (\pi_{t,w} \cdot GOR_{w} - f_{t,w}) \cdot I_{w}$	$\leq \sum_{K} \gamma_{k}\, \mu_{t,k}$	$\forall t$	(C6)

Parameter(s)

Maximum production rate of well w		Π_{w}^{max}	(P1)
Fixed cost of well w change		c_{w}^{well}	(P2)
Initial production rate at well w		$\Pi_{1,w}$	(P3)
Gas to oil ratio of well w		GOR_{w}	(P4)
Impure gaseous state fraction at well w		I_{w}	(P5)
Oil price at period t		p_{t}^{oil}	(P6)
Maximum throughput of LNG train k		β_{k}	(P7)
Maximum impurity throughput of train k		γ_{k}	(P8)
Break- or slowdown variable in period t for train k		$\mu_{t,k}$	(P9)

Direct reward(s)

Oil revenue in period t		$R_{t}^{oil} = p_{t}^{oil} \cdot \pi_{t}^{oil}$	(R1)
Well change costs (negative sign)		$R_{t}^{well} = -\sum_{W} \pi_{t,w}^{bin} \cdot c_{w}^{well}$	(R2)
Flaring costs at well w		$R_{t}^{flare} = -\sum_{W} c^{flare} \cdot f_{t,w}$	(R3)

Transition function

$g(s' \mid s, a) \quad = 1$, if			
$\Pi_{t+1,w} \quad = \pi_{t,w}$		$\forall w$	(T1)

Definitions 3.1 – DP elements concerned with well production and flaring of gaseous state products

Contract delivery scheduling

On a yearly basis, all long term contract deliveries are scheduled. Many parameters, such as expected LNG stock level, available ships and available loading docks are taken into account. We use this so-called Annual Delivery Plan (ADP) as an input for our model. In the ideal situation, we deliver LNG cargoes to customers exactly according to plan. However, many (production) variables are not taken into account:

- Unplanned maintenance of production facilities
- High oil prices
- Shipment of spot opportunities

Based on these three aspects, one could decide to differ from the initial ADP. If oil prices rise significantly, it might be profitable to produce a lot of oil, affecting LNG production as well. For example, wells with a low gas to oil ratio could be opened to increase oil production, resulting in a lower LNG production. Unplanned maintenance could lead to LNG stock shortage (called tank heel) since no LNG is produced during such periods. It might be preferable to postpone deliveries in such cases. This results in lower revenue, but it is still a good alternative to rejection of delivery implying even higher penalty costs.

Furthermore, spot opportunities are not taken into account when constructing ADPs (or not completely due to uncertainty). If a good (high revenue) opportunity is present, rescheduling ADP deliveries in favor of spot cargo deliveries could result in increased profit. The set of all cargoes considered (both long term contracts and spot) in the planning horizon of the DP problem is denoted by C.

Every day, a decision maker has the following decision options with respect to cargo deliveries:

1. Schedule a Spot delivery at a future time slot (i.e. add a cargo to the ADP)
2. Reschedule an ADP delivery from a future time slot to a different future time slot (change a cargo delivery in the ADP)
3. Cancel an ADP or spot delivery that was scheduled at a future time slot (i.e. delete a cargo from the ADP)

However, cargoes can only be delivered during specific time slots and have different revenues for different days of delivery. For example, a customer has the preference of receiving a cargo $c \in C$ of LNG exactly one week from now (period 7) at a revenue of $r_{7,c}$. If we schedule the shipment six days from now we obtain a revenue of $r_{6,c} \leq r_{7,c}$. For every contract that is considered in the planning problem, the revenues $r_{t,c}$ of delivery a cargo at time $t \leq T$ are assumed to be known and are set as a parameter (P10) in the DP model. From a customer point of view, if it is not possible (or preferred) to receive cargo c in period t, the revenue of the corresponding cargo and period is set to minus infinity. This way, all ADP delivery preferences are incorporated in the DP model as contract revenue parameters $r_{t,c}$.

The binary variables $\theta_{t,c}$ indicate the decision on whether or not cargo c is delivered in period t:

Indicator variable for delivery of cargo c in period t $\qquad \theta_{t,c} \qquad$ (A3)

If its value equals 1, cargo c is (to be) delivered in period t and is 0 otherwise. Cargoes can only be delivered if it has not been delivered in previous periods. Therefore, we need a state variable $\Theta_{t,c}$ to indicate whether or not a cargo is delivered prior to the current decision period t:

Indicator variable for delivery of cargo c prior to period t $\Theta_{t,c}$ (S2)

And the following constraint on cargo deliveries applies:

$$\theta_{t,c} \leq (1 - \Theta_{t,c}) \qquad \forall t, c \qquad \text{(C7)}$$

Furthermore, a cargo can only be shipped if a ship is available. We assume that all ships considered in the DP problem have equal size and are able to carry any of the cargoes considered. We thus restrict ourselves to the number of ships available in period t defined by the parameter σ_t (P11):

$$\sum_C \theta_{t,c} \leq \sigma_t \qquad \forall t \qquad \text{(C8)}$$

Shipment is only possible if the LNG stock level is sufficiently high. The available LNG equals the stock level at the beginning of period t plus the production rate π_t^{gas} as defined in the previous section. We define the following constraint on the LNG stock level:

$$\sum_C \theta_{t,c} d_c \leq L_t + \sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w}\right) \cdot (1 - I_w) \qquad \forall t \qquad \text{(C9)}$$

with d_c (P12) the size (the amount of LNG) parameter involved with cargo c. As becomes clear from (C9), the stock level L_t (S3) should be a state space element since it contains information that is necessary to decide on cargo deliveries.

The maximum stock level is defined by L^{max} (P13). Its limiting behavior on the stock level in each of the periods is implied by constraint (C9). The initial stock level L_1 is defined in the initial state s_1.

$$L_t \leq L^{max} \qquad \forall t \qquad \text{(C10)}$$

The direct rewards involved with contract deliveries are

Shipment revenues in period t: $R_t^{ship} = \sum_C \theta_{t,c} \cdot r_{t,c}$ (R4)

If a cargo is not delivered during the planning horizon, it is rejected. The costs involved with rejection of a cargo c are modeled in the terminal reward in period T:

Rejection costs at final period T $R_T^{reject} = -\sum_C (1 - \Theta_c) \cdot r_c^{reject}$ (R5)

In a deterministic setting, all spot cargo opportunities are known prior to optimization. However, these cargoes differ from standard ADP contracts in the sense that there is no contractual agreement yet. Therefore, the rejection costs r_c^{reject} (P13) equal 0, and revenues in case of delivery in general exceed those of standard ADP contracts. It implies that rejection does not imply costs, but delivery results in high revenues as is characteristic for spot cargo opportunities.

The transition function as defined in (T1) is extended for the additional state space elements $\Theta_{t,c}$ and L_t. The contract delivery indicator for cargo c equals 1 if the cargo is delivered prior to, or in period t. In successive periods, this state variable evolves according to:

$$\Theta_{t+1,c} = \Theta_{t,c} + \theta_{t,c}$$

The LNG stock level at the start of the next period equals the value at the start of the current period, plus production during the current period and minus cargo deliveries:

$$L_{t+1} = L_t + \sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w}\right) \cdot (1 - I_w) - \sum_C \theta_{t,c} d_c$$

Therefore, we have the following transition function:

$$g(s'|s,a) \quad = 1\,, \tag{T2}$$

if $\quad \Theta_{t+1,c} \quad = \Theta_{t,c} + \theta_{t,c} \quad \forall c,$ and

$$L_{t+1} \quad = L_t + \sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w}\right) \cdot (1 - I_w) - \sum_C \theta_{t,c} d_c\,,$$

and 0 otherwise.

Note that we only stated the transition function for the variables that were introduced in this section. The objective function (O1) is to maximize the rewards associated with oil, flaring, shipping and well changes in periods $t = 1, \ldots, T - 1$, plus the terminal reward associated with contract rejections in period T:

$$max_A \quad \sum_N r_t^{oil} + r_t^{well} + r_t^{flare} + r_t^{ship} + r_T^{reject} \tag{O1}$$

Definition 3.2 states the DP formulation for the LNG case. In Figure 3.3 a schematic overview of the LNG flow associated with contract delivery scheduling is shown.

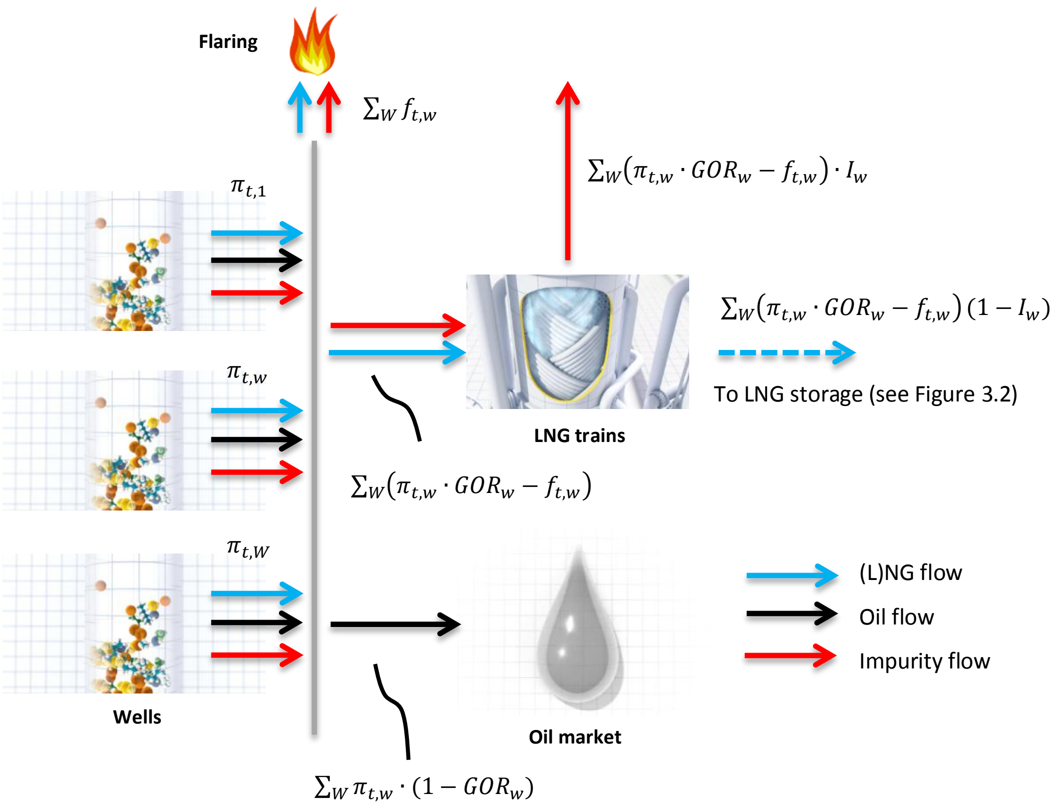


Figure 3.2 – Schematic overview of product flows associated with well production and flaring

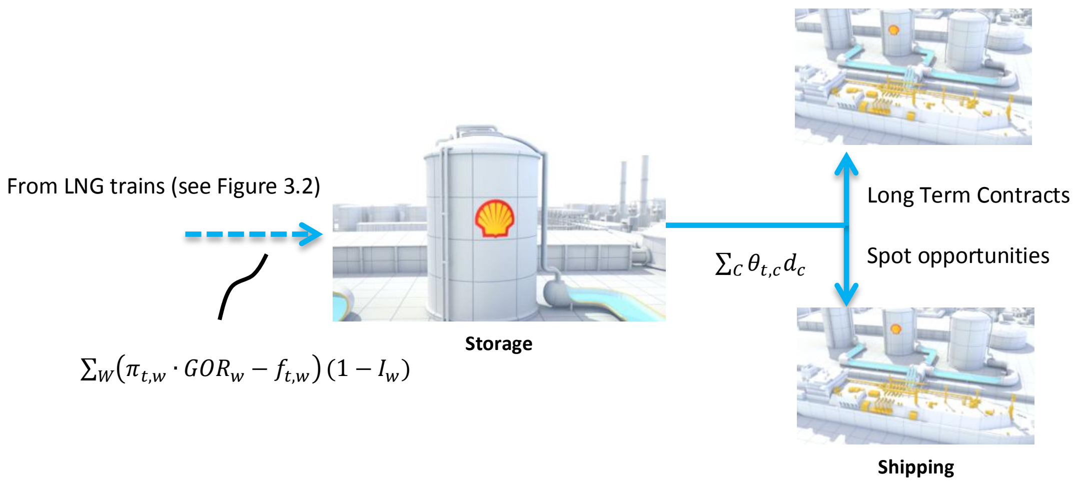


Figure 3.3 – Schematic overview of product flows associated with contract delivery scheduling

Set and index definitions			
Periods		$t \in N$	
Wells		$w \in W$	
LNG trains		$k \in K$	
Cargoes		$c \in C$	
Decision/Action variable(s)			
Production rate at well w in period t		$\pi_{t,w}$	(A1)
Flared amount of gaseous state products at well w in period t		$f_{t,w}$	(A2)
Indicator variable for delivery of cargo c in period t		$\theta_{t,c}$	(A3)
State variable(s)			
Production rate at well w at the start of period t		$\Pi_{t,w}$	(S1)
Indicator variable for delivery of cargo c prior to period t		$\Theta_{t,c}$	(S2)
Available LNG stock level at the start of period t		L_t	(S3)
Dummy variable(s)			
Binary well change indicator for well w in period t		$\pi_{t,w}^{bin}$	(D1)
Positive well change variable for well w in period t w.r.t. previous period		$\pi_{t,w}^{+}$	(D2)
Negative well change variable for well w in period t w.r.t. previous period		$\pi_{t,w}^{-}$	(D3)
Constraint(s)			
$\pi_{t,w}$	$\leq \Pi_w^{max}$	$\forall t, w$	(C1)
$\pi_{t,w}^{+} - \pi_{t,w}^{-}$	$= \pi_{t,w} - \Pi_{t,w}$	$\forall t, w$	(C2)
$\pi_{t,w}^{+} + \pi_{t,w}^{-}$	$\leq \Pi_w^{max} \cdot \pi_{t,w}^{bin}$	$\forall t, w$	(C3)
$f_{t,w}$	$\leq \pi_{t,w} \cdot GOR_w$	$\forall t, w$	(C4)
$\sum_W \pi_{t,w} \cdot GOR_w - f_{t,w}$	$\leq \sum_K \beta_k \mu_{t,k}$	$\forall t$	(C5)
$\sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot I_w$	$\leq \sum_K \gamma_k \, \mu_{t,k}$	$\forall t$	(C6)
$\theta_{t,c}$	$\leq 1 - \Theta_{t,c}$	$\forall t, c$	(C7)
$\sum_C \theta_{t,c}$	$\leq \sigma_t$	$\forall t$	(C8)
$\sum_c \theta_{t,c} \cdot d_c$	$\leq L_T + \sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot (1 - I_w)$	$\forall t$	(C9)
L_t	$\leq L^{max}$	$\forall t$	(C10)
Parameter(s)			
Maximum production rate of well w		Π_w^{max}	(P1)
Fixed cost of well w change		c_w^{well}	(P2)
Initial production rate at well w		$\Pi_{1,w}$	(P3)
Gas to oil ratio of well w		GOR_w	(P4)
Impure gaseous state fraction at well w		I_w	(P5)
Oil price at period t		p_t^{oil}	(P6)
Maximum throughput of LNG train k		β_k	(P7)
Maximum impurity throughput of train k		γ_k	(P8)
Breakdown indicator parameter in period t for train k		$\mu_{t,k}$	(P9)
Revenue if cargo c is delivered in period t		$r_{t,c}$	(P10)
Number of available ships in period t		σ_t	(P11)
Size of cargo c		d_c	(P12)
Maximum LNG stock level		L^{max}	(P13)

Definitions 3.2 (continued on next page) – DP formulation of LNG case

Direct reward(s)

Oil revenue in period t	$r_t^{oil} = p_t^{oil} \cdot \pi_t^{oil}$	(R1)
Well change costs (negative reward)	$r_t^{well} = -\sum_W \pi_{t,w}^{bin} \cdot c_w^{well}$	(R2)
Flaring costs at well w	$r_t^{flare} = -\sum_W c^{flare} \cdot f_{t,w}$	(R3)
Shipment revenues in period t(negative reward)	$r_t^{ship} = \sum_C \theta_{t,c} \cdot r_{t,c}$	(R4)
Rejection costs at final period T (negative reward)	$r_T^{reject} = -\sum_C (1 - \Theta_c) \cdot r_c^{reject}$	(R5)

Transition function

$g(s'|s,a) \quad = 1\,, \qquad$ if

$\Pi_{t+1,w} \quad = \pi_{t,w} \quad \forall w,$

$\Theta_{t+1,c} \quad = \Theta_{t,c} + \theta_{t,c} \quad \forall c,$ and

$L_{t+1} \quad = L_t + \sum_W \big(\pi_{t,w} \cdot GOR_w - f_{t,w}\big) \cdot (1 - I_w) - \sum_C \theta_{t,c} \cdot d_c\ ,$ (T1-2)

Objective function

$max_A \qquad \sum_N r_t^{oil} + r_t^{well} + r_t^{flare} + r_t^{ship} + r_T^{reject}$ (O1)

Definitions 3.2 (continued) – DP formulation of LNG case

Chapter 4

Markov Decision Problems

In many real world applications, model parameters are not (completely) known in advance. If such uncertainties are taken into account, a dynamic programming problem becomes a Stochastic Dynamic Program or more specific a Markov Decision Problem (MDP). In this chapter we extend the dynamic programming framework presented in the previous chapter to a MDP model.

Section 4.1 describes the fundamental theory on MDPs. In Section 4.2 the framework is applied to the LNG case, with stochastic model parameters and their corresponding probability distribution function. Two solution methods in case of continuous state problems are described in Section 4.3.

4.1 - The stochastic equivalent of the DP framework

Markov Decision problems offer a widely used optimization framework [29]. Its structure shows great similarity with the Dynamic Programming framework as presented in the previous chapter. An MDP is mathematically defined as:

$$MDP \coloneqq \{N, S, A_s, p(s'|s,a), r(s,a), \text{ with } s, s' \in S \text{ and } a \in A_s\}, \tag{4.1}$$

The important property of a DP that the process is uniquely determined by the definition of an initial state s_1 and a strategy α does not hold for MDPs. Instead, a probability transition function $p(s'|s,a)$ models uncertainties in the evolution of the process. The state sequence is a stochastic process that does not have a single fixed value. It can take on a variety of possible values, conditional on the initial state and the strategy α. In other words, a strategy α and an initial state s_1 induce a random state-action sequence:

$$\tilde{\delta}_{\alpha,T} = (s_1, a_1, \tilde{s}_2, \tilde{a}_2 \dots, \tilde{a}_{T-1}, \tilde{s}_T) \tag{4.2}$$

The tildes indicate the random variables that are subject to uncertainty prior to optimization. As the initial (current) state is known with certainty, it is not a random variable. The reward sequence associated with this state-action sequence (4.2) is also stochastic:

$$\tilde{r}_{\delta,\alpha} = (r(s_1, a_1), \tilde{r}(\tilde{s}_2, \tilde{a}_2), \dots, \tilde{r}(\tilde{s}_T))$$

Here, the action variables are stochastic as they depend on the stochastic state variable. In specific applications, the action realizations are stochastic variables themselves. That is, if an action is selected by the decision maker, the actual realization may differ according to some probability distribution. However, in this thesis we assume that the action selected by the decision maker is realized with certainty.

Expected total reward criterion

Due to the stochastic character of the reward sequence, the total reward utility function (Eq. 3.2) cannot be applied directly, since it involves a summation over stochastic variables. Therefore, an expected total reward utility function is used instead:

$$\mathbb{E}\tilde{R}_{\delta,\alpha} := \mathbb{E}\sum_N \tilde{r}_{\delta,\alpha} = \sum_N \mathbb{E}\tilde{r}_{\delta,\alpha} = r(s_1, a_1) + \sum_{t=2}^{T-1} \mathbb{E}\tilde{r}(\tilde{s}_t, a_t) + \mathbb{E}\,\tilde{r}(\tilde{s}_T) \tag{4.3}$$

Note that the expectation of a utility function as found in the second and third term does not equal the utility function of the expected state of the process in period t:

$$\mathbb{E}\tilde{r}(\tilde{s}_t, a_t) \neq r(\mathbb{E}\tilde{s}_t, a_t). \tag{4.4}$$

By definition [30], the expected value of the random reward sequence is a weighted average over the set S_t of states that can be assumed by the proces in period t:

$$\mathbb{E}\tilde{r}(\tilde{s}_t, a_t) = \sum_{S_t} p_\alpha(\tilde{s}_t = s_t | \tilde{\delta}_{\alpha,t-1}) \cdot r(s_t, a_t), \tag{4.5}$$

where $p(\tilde{s}_t = s_t | \tilde{\delta}_{\alpha,t-1})$ is the probability that the process is found in state s_t in period t, given the state-action history up to period $t-1$ and strategy α. A (conditional) probability distribution satisfies:

$$\sum_{S_t} p\left(\tilde{s}_t = s_t \middle| \tilde{\delta}_{\alpha,t-1}\right) = 1.$$

Equation (4.3) can be written as:

$$\mathbb{E}\tilde{R}_{\delta,\alpha} = r(s_1, a_1) + \sum_{t=2}^{T-1} \sum_{S_t} p\left(\tilde{s}_t = s_t \middle| \tilde{\delta}_{\alpha,t-1}\right) \cdot r(s_t, a_t) + \sum_{S_T} p(\tilde{s}_T = s_T | \tilde{\delta}_{\alpha,t-1}) \cdot r(s_T). \tag{4.6}$$

Each MDP satisfies the Markov property [27], which states that the current state only depends on its predecessor, instead if the complete history:

$$p\left(\tilde{s}_t = s_t \middle| \tilde{\delta}_{\alpha,t-1}\right) \sim p(\tilde{s}_t = s_t | s_{t-1})$$

Using this property, we can write for (4.5):

$$\mathbb{E}\tilde{R}_{\delta,\alpha} = r(s_1, a_1) + \sum_{t=2}^{T-1} \sum_{S_t} p(\tilde{s}_t = s_t | s_{t-1}) \cdot r(s_t, a_t) + \sum_{S_T} p(\tilde{s}_T = s_T | s_{T-1}) \cdot r(s_T).$$

If we define $u_t(s)$ to be the expected reward of using strategy α from period t onward, starting in state $s_t \in S_t$, we obtain the iterative relation:

$$u_t(s_t) = r(s_t, a_t) + \sum_{S_{t+1}} p(\tilde{s}_{t+1} = s_{t+1} | s_t) \cdot u_{t+1}(s_{t+1}) = r(s_t, a_t) + \mathbb{E}u_{t+1}(s_{t+1}) \tag{4.7}$$

As for the deterministic case, iterative application of (4.7) results in $u_1(s_1)$, which is defined as the value of the MDP. The expected total reward criterion (4.3) is used to compare a set of given strategies in terms of their MDP value. A strategy α^* is defined to be optimal for an MDP if it performs better than any of its feasible alternatives:

$$\mathbb{E}\tilde{R}_{\delta,\alpha^*} \geq \mathbb{E}\tilde{R}_{\delta,\alpha} \qquad \forall\alpha$$

To find an optimal strategy α^*, we use the following backward induction recursion using Bellman's principle of optimality, starting in period T:

$$u_T(s_t) = r(s_t) \qquad \forall s_t \in S_T,$$

$$u_t(s_t) := max_{a\in A_s}\{r(s_t, a) + \sum_{S_{t+1}} p_\alpha(\tilde{s}_{t+1} = s_{t+1}|s_t) \cdot u_{t+1}(s_{t+1})\}, \text{ and}$$

$$a^*_{s_t} := arg\,max_{a\in A_s}\{r(s_t, a) + \sum_{S_{t+1}} p_\alpha(\tilde{s}_{t+1} = s_{t+1}|s_t) \cdot u_{t+1}(s_{t+1})\}. \qquad (4.8)$$

To construct the optimal strategy α^*, we keep track of the optimal actions $a^*_{s_t}$ in each state as evaluated in equation (4.8). If we compare this recursive method with its deterministic counterpart 3.2, it only differs in the relaxation of the degenerate (distribution) function $g(s'|s, a)$.

4.2 - Extension of the LNG case DP to a MDP

As described in Section 2.3, several uncertainties in the LNG upstream value chain appear in real life. If we take this stochastic behavior of the process into account, the DP definition slightly changes. We distinguish (1) history dependent and (2) history independent uncertainties that differ in the need for information on the history of the process to determine the probability distribution for the current period.

As an example of the first category, suppose a LNG train breaks down and maintenance will take at least two days. The probability that the LNG train is broken tomorrow obviously depends on the fact that it broke down today. That is, we know with certainty that it will be down tomorrow. The information on the number of remaining days in maintenance must be part of the state space description.

We focus on three types of uncertainties and assume that the rest of the process behaves deterministically:

- Breakdown of LNG trains, related to the DP parameter $\mu_{t,k}$
- Spot opportunity arrivals, related to the number of cargoes available in period t
- The number of ships that is available for shipping, related to σ_t

These three parameters are described in more detail in the following sections.

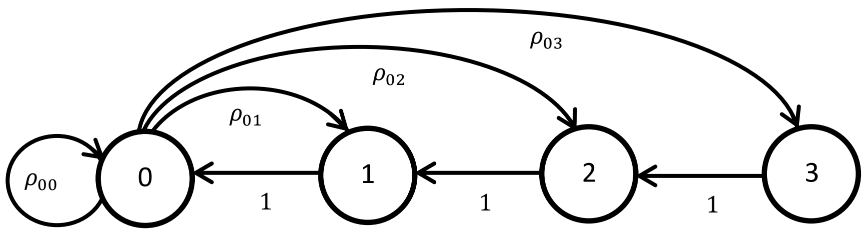


Figure 4.1 – Discrete time Markov Chain associated with LNG train breakdowns.

Breakdown of LNG trains

Whether or not LNG train k is working during period t, is modeled by a discrete random variable $\tilde{\mu}_{t,k}$ with sample space $\{0,1,2,3\}$ and associated discrete probability distribution. It represents the residual number of days that is needed to fix LNG train k at the start of period t. This stochastic breakdown process is independent of other processes in the LNG case and can be modeled as a discrete time Markov chain, as shown in Figure 4.1.

We have for the transition probability function associated with LNG train breakdowns:

$$\mathbb{P}(\tilde{\mu}_{t+1,k} = \mu_k | \tilde{\mu}_{t,k}) = \begin{cases} 1 & \text{if} \quad \mu_k = \tilde{\mu}_{t,k} - 1, \quad \tilde{\mu}_{t,k} \neq 0 \\ \rho_{00} & \text{if} \quad \mu_k = 0, \quad \tilde{\mu}_{t,k} = 0 \\ \rho_{01} & \text{if} \quad \mu_k = 1, \quad \tilde{\mu}_{t,k} = 0 \\ \rho_{02} & \text{if} \quad \mu_k = 2, \quad \tilde{\mu}_{t,k} = 0 \\ \rho_{03} & \text{if} \quad \mu_k = 3, \quad \tilde{\mu}_{t,k} = 0 \\ 0 & \text{otherwise} \end{cases}$$

With

$$\rho_{00} + \rho_{01} + \rho_{02} + \rho_{03} = 1 \quad \text{and} \quad \rho_{0i} \geq 0 \quad \text{for} \quad i = 0, \ldots, 3$$

The probabilities ρ_{00} to ρ_{03} are contained in the vector parameter ρ (P14) with elements ρ_m, indexed with $m = 1, \ldots, 4$. This parameter can easily be extended if more than three maintenance periods are necessary to model the system. However, such an extension has implications on the number of scenarios that is considered in the optimization, as discussed in the following.

The number of ships that is available for shipping LNG

Travel times for LNG carriers are affected by for example weather circumstances and other external factors. Therefore, the number of available ships for shipment of cargoes in each period is uncertain. If a ship is late, a storage overflow (tank top) might occur. This is a risk since we must shut down production in such as case. Therefore, uncertainty in ship arrivals with respect to the ADP must be taken into account.

The probability that a specific number of ships is available in a period can be calculated from associated probability distributions. The number of combinations becomes very large and since we present a different scenario based approach in chapter 5, we decided not to present a straightforward but tedious overview of probability theory associated with computation of these ship delay probabilities that we will not use anymore in this thesis.

Spot opportunity arrivals

In absence of historical data, we made some assumptions on the spot cargo arrival process and the potential revenues involved. During our meetings with Shell staff, it was mentioned that spot opportunity arrivals are known up to a certain degree of certainty. Therefore, we assume that the number of spot opportunities that will be present in the planning horizon is known, except for the exact arrival day with a known corresponding probability distribution. For example, suppose that we expect a spot opportunity $s \in S$ to arrive somewhere between period t and $t+3$, with corresponding probability distribution:

$\mathbb{P}(spot\ arrival\ s\ in\ period\ t) \quad = 0{,}1$
$\mathbb{P}(spot\ arrival\ s\ in\ period\ t+1) \quad = 0{,}1$
$\mathbb{P}(spot\ arrival\ s\ in\ period\ t+2) \quad = 0{,}7$
$\mathbb{P}(spot\ arrival\ s\ in\ period\ t+3) \quad = 0{,}1$

Here S is the set of spot opportunities that is to be considered. In this case, we expect the spot opportunity to arrive in period $t+2$. However, we are not sure about this and assign a probability of 10% to the other three options.

We assume that no two spot arrivals have overlap in arrival probabilities so that we cannot have two spot opportunities available on the same day. The probability that a spot opportunity is available in period t can be calculated using:

$$\mathbb{P}(\tilde{\varphi}_t = 1) = \sum_S \mathbb{P}(spot\ arrival\ s\ in\ period\ t)$$

The revenue of monetizing a spot opportunity if available is r_s^{spot} and the size of the spot opportunities is represented by the parameter d_s.

The transition probability function for the MDP model

As we have discussed the stochastic parameters of the MDP model, the probability transition function $p(s'|s,a)$ can be defined. To start, $|K|+5$ elements are added to the state space vector in period t, associated with:

- LNG train breakdown indicators $\tilde{\mu}_{t,k} \in \{0,1,2,3\}$, for all LNG trains $k \in K$, (S4)
- Shipment variable $\tilde{\sigma}_t \in \mathbb{Z}^+$, and (S5)
- Spot opportunity indicator $\tilde{\varphi}_t \in \{0,1\}$. (S6)

With $\mathbb{Z}^+$ the set of positive integers, including zero. Formally, the state space is now:

$$s_t = \big(\Pi_{t,1}, \dots, \Pi_{t,|W|}, \Theta_{t,1}, \dots, \Theta_{t,|C|}, L_t, \underbrace{\tilde{\mu}_{t,1}, \dots, \tilde{\mu}_{t,|K|}, \tilde{\sigma}_t, \dots, \tilde{\sigma}_{t+3}, \tilde{\varphi}_t}_{\text{Additional elements w.r.t. DP definition of Chapter 3}}\big)$$

The definition of the state elements is stated again for clarity reasons:

$\Pi_{t,w}$	Production level of well w up to period t,
$\Theta_{t,c}$	Indicator on whether or not cargo c is delivered prior to period t,
L_t	LNG stock level at the start of period t,
$\tilde{\mu}_{t,k}$	Stochastic variable, indicating whether or not LNG train k is broken during period t,
$\tilde{\sigma}_{t\prime}$	Stochastic variable, indicating the number of available ships in period t, and
$\tilde{\varphi}_t$	Stochastic variable, indicating whether or not a spot opportunity is available in period t.

The action vector a_t is also extended, with an indicator action variable θ_t^{spot} that is associated with the potential spot opportunity at period t:

θ_t^{spot} Indicator action variable on spot opportunity delivery in period t (A4)

It equals 1 if the spot opportunity is monetized (if present, i.e. $\tilde{\varphi}_t = 1$) and 0 otherwise. The action vector for the MDP case is:

$$a_t = \big(\pi_{t,1}, \dots, \pi_{t,|W|}, f_{t,1}, \dots, f_{t,|W|}, \theta_{t,1}, \dots, \theta_{t,|C|}, \underbrace{\theta_t^{spot}}_{\text{Additional element w.r.t. DP definition of Chapter 3}}\big)$$

Such that the set of constraints C1 to C10 (see Chapter 3) is respected, with the additional constraint associated with the spot opportunity in period t:

$$\theta_t^{spot} \leq \tilde{\varphi}_t \tag{C11}$$

And the extension of the stock constraint (C9) with the possible delivery of a spot cargo:

$$\textstyle\sum_C \theta_{t,c} d_c + \underbrace{\theta_t^{spot} \cdot d^{spot}}_{\text{Additional term w.r.t. DP definition of Chapter 3}} \leq L_t + \sum_W \big(\pi_{t,w} \cdot GOR_w - f_{t,w}\big) \cdot (1 - I_w) \qquad \forall t \tag{C9*}$$

With d^{spot} (P19) the spot cargo size parameter. Furthermore, the stochastic counterparts of the DP parameters $\mu_{t,k}$ and σ_t are used in constraints (C5*), (C6*) and (C8*) respectively, with the asterisk indicating the analogy with the DP constraint equivalent. Finally, the direct reward associated with spot delivery is added to the model:

$$R_t^{spot} = \theta_{t,s} \cdot r_t^{spot} \tag{R6}$$

The probability transition function $p(s'|s, a)$ is defined by:

$$p(s'|s,a) \quad = \textstyle\prod_K \mathbb{P}\big(\widetilde{\omega}_{t+1,k} = \omega_k \big| \widetilde{\omega}_{t,k}\big) \cdot \mathbb{P}(\tilde{\varphi}_{t+1} = \varphi) \cdot \mathbb{P}(\tilde{\sigma}_{t+1} = \sigma)\,, \tag{T3}$$

if

$$\begin{aligned}
\Pi_{t+1,w} &= \pi_{t,w} \\
\Theta_{t+1,c} &= \Theta_{t,c} + \theta_{t,c} \\
L_{t+1} &= L_t + \textstyle\sum_W \big(\pi_{t,w} \cdot GOR_w - f_{t,w}\big) \cdot (1 - I_w) - \sum_C \theta_{t,c} d_c - \theta_{t,s} d_s \\
\tilde{\mu}_{t+1,k} &= \mu_k \\
\tilde{\varphi}_{t+1} &= \varphi \\
\tilde{\sigma}_{t+1} &= \sigma
\end{aligned}$$

and 0 otherwise. Note that we have assumed that the stochastic processes associated with breakdowns, spot opportunity arrivals and shipment are independent of each other. An overview of the LNG MDP model can be found in definition 4.1.

4.3 - The curse of dimensionality

In many practical problems, the state variable is factored and thus described by a vector discussed in Section 3.1. Furthermore, as in the LNG case, (part of) the state space may be continuous. Therefore, an infinite sum is contained in equation 4.4 as the set S_{t+1} is uncountable and is thus replaced by an integral:

$$u_t(s_t) := max_{a \in A_s} \Big\{ r(s_t, a) + \textstyle\int_{s' \in S_{t+1}} p(\tilde{s}_{t+1} = s' | s_t, a) \cdot u_{t+1}(s') \Big\} \tag{4.9}$$

Since direct application of backward induction algorithm does not work in such cases, we could first discretize the state space. However, the size of the state space S grows exponentially with the state space dimension and corresponding fineness of discretization, producing what is widely referred to as the 'curse of dimensionality' in dynamic programming [29].

As an illustration, suppose we have a factored 5-dimensional state space and use a discretization grid having 10 levels per dimension. The discretized state space then contains 10^5 states. Thus, for a relatively small problem we already obtain a significant computational complexity if equation (4.8) is applied.

Furthermore, we did not take the necessary discretization of the action space and probability distribution (if continuous) into account. In general, the curse of dimensionality is associated with three elements of an MDP:

- The state space, if it appears in factored form,
- The action space as it may also be factored, complicating the search for the best action (maximum operator in equation 4.7),
- The probability space, in case of continuous or highly fractioned probability distribution functions

The desire to work with discrete representations for direct implementation in a programming environment is the main cause this increased complexity. As a rule of thumb, discretization only works well for 1d or 2d problems and rarely works for 6d-problems or higher [30].

If we apply this to the LNG DP model (see definition 3.3 for an overview), which contains continuous elements such as the well production rates and the stock level, resulting in a highly factored and continuous model description. Therefore, discretization does not work to obtain a good solution.

Control theory and Approximate Dynamic Programming

In contrast to MDP theory, optimal control theory focuses on problems with continuous state-and action spaces. The transition function in such models is defined as a set of linear equations:

$$s_{t+1} = As_t + Ba_t \ \ (+w_t)$$

With A and B the state and action specific transition matrices, and w_t a noise vector, in case of a stochastic model. In specific instances the reward function has a quadratic structure, such that it can be written as:

$$r(s,a) = a^T Ua$$

This type of reward functions refer to problems where deviations from a desired path incur costs that are to be minimized, such as helicopter hovering [31]. These Linear Quadratic Regulator (LQR) problems have a closed form solution since the linear-quadratic structure allows analytic minimization of the optimality equations [32]. For other cost structures, without a pre-defined 'desired path' or having both positive and negative rewards, an analytic solution cannot be obtained in general.

Another well-known approach is the Collocation method [33] or Approximate Linear Programming [34,35]. It uses a finite set of basic functions, i.e. polynomials up to a certain degree, to fit the value function in a given number of 'collocation states'. Continuous optimization methods such as Newton search are then applied to minimize (or maximize) the approximated value function.

The drawback of this approach is the sub-optimal solution due to the value function approximation. By increasing the number of collocation states, the solution quality increases. However, it also increases computational effort associated with fitting the set of basic functions. Furthermore, approximation of a highly discontinuous value function (as is the case for LNG due to binary contract variables) could result in strange and unreliable solutions at the discontinuities [33].

Set and index definitions		
Periods	$t \in N$	
Wells	$w \in W$	
LNG trains	$k \in K$	
Cargoes	$c \in C$	
Spot opportunities	$s \in S$	
Decision/Action space variable(s)		
Production rate at well w in period t	$\pi_{t,w}$	(A1)
Flared amount of gaseous state products at well w in period t	$f_{t,w}$	(A2)
Indicator variable for delivery of cargo c in period t	$\theta_{t,c}$	(A3)
Indicator variable for spot opportunity delivery in period t	θ_t^{spot}	(A4)
State space variable(s)		
Production rate at well w at the start of period t	$\Pi_{t,w}$	(S1)
Indicator variable for delivery of cargo c prior to period t	$\Theta_{t,c}$	(S2)
Available LNG stock level at the start of period t	L_t	(S3)
Stochastic variable, indicating if LNG train k is broken during period t	$\tilde{\mu}_{t,k}$	(S4)
Stochastic variable, indicating if a spot opportunity is available	$\tilde{\varphi}_t$	(S5)
Stochastic variable, indicating the number of available ships in period t	$\tilde{\sigma}_t$	(S6)
Dummy variable(s)		
Binary well change indicator for well w in period t	$\pi_{t,w}^{bin}$	(D1)
Positive well change variable for well w in period t w.r.t. previous period	$\pi_{t,w}^{+}$	(D2)
Negative well change variable for well w in period t w.r.t. previous period	$\pi_{t,w}^{-}$	(D3)

Constraint(s)

$\pi_{t,w}$	$\leq \Pi_w^{max}$	$\forall t, w$	(C1)
$f_{t,w}$	$\leq \pi_{t,w} \cdot GOR_w$	$\forall t, w$	(C2)
$\pi_{t,w}^{+} - \pi_{t,w}^{-}$	$= \pi_{t,w} - \Pi_{t,w}$	$\forall t, w$	(C3)
$\pi_{t,w}^{+} + \pi_{t,w}^{-}$	$\leq \Pi_w^{max} \cdot \pi_{t,w}^{bin}$	$\forall t, w$	(C4)
$\sum_W \pi_{t,w} \cdot GOR_w - f_{t,w}$	$\leq \sum_K \beta_k \cdot \tilde{\mu}_{t,k}$	$\forall t$	(C5*)
$\sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot I_w$	$\leq \sum_K \gamma_k \cdot \tilde{\mu}_{t,k}$	$\forall t$	(C6*)
$\theta_{t,c}$	$\leq 1 - \Theta_{t,c}$	$\forall t, c$	(C7)
$\sum_C \theta_{t,c} + \theta_t^{spot}$	$\leq \tilde{\sigma}_t$	$\forall t$	(C8*)
$\sum_C \theta_{t,c} \cdot d_c + \theta_t^{spot} \cdot d^{spot}$	$\leq L_T + \sum_W (\pi_{t,w} \cdot GOR_w - f_{t,w}) \cdot (1 - I_w)$	$\forall t$	(C9*)
L_t	$\leq L^{max}$	$\forall t$	(C10)
θ_t^{spot}	$\leq \tilde{\varphi}_t$	$\forall t$	(C11)

Parameter(s)		
Maximum production rate of well w	Π_w^{max}	(P1)
Fixed cost of well w change	c_w^{well}	(P2)
Initial production rate at well w	$\Pi_{1,w}$	(P3)
Gas to oil ratio of well w	GOR_w	(P4)
Impure gaseous state fraction at well w	I_w	(P5)
Oil price at period t	p_t^{oil}	(P6)
Maximum throughput of LNG train k	β_k	(P7)
Maximum impurity throughput of train k	γ_k	(P8)
Parameter (P9) is now a (stochastic) state space variable (S4)		
Revenue if cargo c is delivered in period t	$r_{t,c}$	(P10)
Parameter (P11) is now a (stochastic) state space variable (S6)		
Size of cargo c	d_c	(P12)

Definitions 4.1 (continued on next page) – MDP formulation of LNG case

Maximum LNG stock level	L^{max}	(P13)
LNG train breakdown probability vector	ρ	(P14)
Shipment delay probability vector	χ_s	(P15)
Spot cargo size	d^{spot}	(P16)
Spot price in period t	r_t^{spot}	(P17)

Direct reward(s)

Oil revenue in period t	$R_t^{oil} = p_t^{oil} \cdot \pi_t^{oil}$	(R1)
Well change costs (negative reward)	$R_t^{well} = -\sum_W \pi_{t,w}^{bin} \cdot c_w^{well}$	(R2)
Flaring costs at well w	$R_t^{flare} = -\sum_W c^{flare} \cdot f_{t,w}$	(R3)
Shipment revenues in period t (negative reward)	$R_t^{ship} = \sum_C \theta_{t,c} \cdot r_{t,c}$	(R4)
Rejection costs at final period T (negative reward)	$R_T^{reject} = -\sum_C (1-\Theta_c) \cdot r_c^{reject}$	(R5)
Spot revenues in period t	$R_t^{spot} = \theta_t^{spot} \cdot r_t^{spot}$	(R6)

Transition Probability function

$p(s'|s,a) \quad = \prod_K \mathbb{P}\left(\widetilde{\omega}_{t+1,k} = \omega_k \middle| \widetilde{\omega}_{t,k}\right) \cdot \mathbb{P}(\tilde{\varphi}_{t+1} = \varphi) \cdot \mathbb{P}(\tilde{\sigma}_{t+1} = \sigma)$, if (T3)

$\Pi_{t+1,w} \quad = \pi_{t,w}$

$\Theta_{t+1,c} \quad = \Theta_{t,c} + \theta_{t,c}$

$L_{t+1} \quad = L_t + \sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w}\right) \cdot (1 - I_w) - \sum_C \theta_{t,c} d_c - \theta_{t,spot} d_{spot}$

$\widetilde{\omega}_{t+1,k} \quad = \omega_k$

$\tilde{\varphi}_{t+1} \quad = \varphi$

$\tilde{\sigma}_{t+1} \quad = \sigma$

Objective function

$max_A \quad \sum_N R_t^{oil} + R_t^{well} + R_t^{flare} + R_t^{ship} + R_t^{spot} + R_T^{reject}$

Definitions 4.1 (continued) – MDP formulation of LNG case

Chapter 5

Two-Stage Stochastic Mixed Integer Linear Programming

This chapter discusses the equivalence between the DP framework and a Mixed Integer Linear Programming (MILP) approach. It provides a work-around for the necessary discretization of state and action spaces of DPs that was discussed in previous chapters. When uncertainty is introduced to a DP, we obtain an MDP as discussed in Chapter 4. For such models, the MILP equivalence does not hold since general solution methods, such as the simplex algorithm with branch-and-bound, do not apply directly [36]. In many applications, the uncertainty is therefore simply ignored and a single representative value of the data is used (expected values). However, we do want to take the risk associated with uncertainty into account instead of ignoring it.

Section 5.1 first describes the equivalence between a DP and a deterministic MILP model. We then introduce uncertainty in MILP parameters and discuss solution approaches from literature Section 5.2. Two-stage stochastic Mixed Integer Linear Programming approach is presented. General theory on such models is discussed in Sections 5.4. Application of this stochastic model to the LNG case is discussed in the last two sections, resulting in a stochastic counterpart to the average case MILP.

5.1 - The MILP equivalent of the DP framework

A DP model is equivalent to a Mixed Integer Linear Programming approach (MILP). However, the 'nice' structure of backward induction by dividing the planning horizon in smaller sub problems is lost. In the MILP solution method, the problem is solved as a whole at once. From a complexity point of view, it is less attractive since computational time increases exponentially in the number of variables and constraints, where backward induction is a linear solution method in terms of the planning horizon. However, a MILP is more suitable for discrete state and action spaces than backward induction in case of large models. We are thus able to solve the problem with MILP to optimality instead of approximating it by discretization, as discussed in the previous chapter.

The elements of the state and action space are modeled by continuous and binary decision variables. The feasible action space is modeled by a set of linear inequalities, as usual for linear programming definitions. The objective is to maximize the sum of all rewards over the planning horizon, as was the case for the backward induction algorithm. The (deterministic) transition function is modeled by a set of linear equalities. Formally, we obtain the following MILP equivalent of the DP framework:

$$\begin{aligned} &max_{a_t, t<T} \quad \textstyle\sum_{t<T} R(s_t, a_t) + R(s_T) \\ &\text{s.t.} \qquad a_t \in A_{s_t} \qquad\qquad\qquad\qquad\quad \forall t < T \qquad\qquad (*) \\ &\qquad\qquad s_{t+1} = \textstyle\sum_{s' \in S_{t+1}} g(s'|s_t, a_t) \cdot s_t \qquad \forall t < T \qquad\qquad (**) \qquad (5.1) \\ &s_1 \text{ (initial state) is an input parameter} \end{aligned}$$

For the LNG case, the set of constraints indicated with (*) in (5.1) equals the set of inequalities (C1) to (C10) as presented in the DP formulation at the end of section 3.3 (Definition 3.2). The constraints (or equalities) indicated by (**) refer to the deterministic transition function (T1) and (T2) of the DP formulation.

The model definition shows a one-to-one correspondence. However, differences are found in the solution methods that are used to solve the models. In the DP case, backward induction is used where a MILP is solved by first solving the relaxation by the Simplex method and then applying branch-and-bound or the cutting plane method [37]. However, If we introduce uncertainty in the DP formulation (making it an MDP), the one-to-one correspondence with an MILP formulation does not hold, as we obtain stochastic parameters. To be more specific, the equalities (**) in equation (5.1) do not hold, since they are not uniquely defined. In general, the simplex method cannot deal with stochastic model parameters. The next section discusses approximation methods for MILP models with uncertainty in parameters.

5.2 - Uncertainty in MILP parameters

For a general discussion on uncertainty in (Mixed Integer) Linear Programs (MILPs), we use its standard definition:

$$max_z \qquad \{\, r^T z \mid Az \leq b \text{, with } z \geq 0 \text{ and } z_i \in \{0,1\} \ \forall i \in I \,\}, \qquad (5.2)$$

instead of equation (5.1). The set I indicates which of the variables z_i are binary. If it is an empty set, the MILP is actually an LP, so the following holds for general LP definitions. In case of uncertainty in objective function coefficients c^T, constraint coefficient matrix A or right-hand-side b, solution methods for MILPs such as relaxation in combination with branch and bound do not apply directly.

A common way of solving MILP problems subjected to uncertainty in parameters is called scenario analysis [38]. A countable number of scenarios is considered, denoted by the index $q \in \Phi$. If continuous distributions are considered, these are discretized by sampling techniques or by manual selection [39,40]. In the literature, this discretization method is referred to as scenario tree construction. In general, computational time increases with the number of scenarios that is included. However, so does the solution quality.

If uncertainty is involved with any of the model parameters, we have a stochastic MILP. Such a model can be defined the following, with uncertainty denoted by the set of stochastic variables $(\tilde{r}, \tilde{A}, \tilde{b})$:

$$max_z \qquad \{\, \tilde{r}^T z \mid \tilde{A}z \leq \tilde{b} \text{, with } z \geq 0 \text{ and } z_i \in \{0,1\} \ \forall i \in I \,\}.$$

For each particular scenario realization $(r, A, b)_q$, the MILP can be solved to obtain an optimal strategy α^q:

$$max_z \qquad \{\, {r_q}^T z \mid A_q z \leq b_q \text{, with } z \geq 0 \text{ and } z_i \in \{0,1\} \ \forall i \in I \,\}.$$

Given the set of optimal solutions associated with each of the considered scenarios $q \in \Phi$, how should we combine them into a single optimal strategy? We present methods to consider all scenarios $q \in \Phi$, weighted by their probability of occurrence in a single optimization. An optimal strategy should be obtained that takes into account the 'risks' associated with each of the scenarios involved.

Scenario analysis in stochastic MILPs

In many applications such as [41], probability (or chance) constraints are used to ensure the feasibility of a MILP with a user-defined reliability parameter $\alpha \in [0,1]$. However, we are not interested in probability constraints to obtain strategies with such a reliability statement. We focus on uncertainty associated with hard constraints: those which must be satisfied, whatever the actual realization of the data will be. In line with [42], the following approaches for such problems are discussed: (1) worst case solution, (2) expected value approach, (3) absolute difference approach, all having significant drawbacks and are not further investigated in this thesis.

In Section 5.3 and 5.4 we present two methods: (4) the Average case behavior and (5) a two-stage stochastic programming (as discussed in the next section), which are implemented in a programming environment as discussed in chapter 6.

In the worst case solution approach (1), all scenario constraints are to be respected by the decision variables, resulting in a very conservative or even no solution (infeasibility). Formally, equation (5.2) is in this case:

$$max_z \qquad \{r_q^T z \mid A_q z \leq b_q, \quad \forall q \in \Phi, \text{ with } z \geq 0 \text{ and } z_i \in \{0,1\} \ \forall i \in I\},$$

Note that considering many scenarios at once results in 'large' problems, requiring a lot of computational effort (and time) to solve. Therefore, it is important to decide on a trade-off between the number of scenarios (i.e. the quality of the solution) and the available resources for solving the corresponding model.

A less restrictive and widely used solution method is (2) the expected value approach. It considers a single instance of the problem with the expected value of the model parameters as input:

$$max_z \qquad \{\mathbb{E}\tilde{r}z \mid \mathbb{E}\tilde{A}z \leq \mathbb{E}\tilde{b}, \text{ with } z \geq 0 \text{ and } z_i \in \{0,1\} \ \forall i \in I\}.$$

The expected value method is a very fast approach since only a single instance of the MILP is to be solved. However, it does not take the risks concerned with each of the individual scenarios into account. It may even perform as worse as the worst case scenario approach. Furthermore, the expectation of integer valued parameters can attain non-integer values. For example, the expectation of a uniform binary random variable is the non-integer value 0,5. This may lead to compatibility issues, i.e. we cannot deal with the arrival of half a ship in our models.

The absolute difference approach (3) minimizes the absolute differences between the scenario solutions and the resulting overall solution. It shows similarities with regression techniques for non-linear functions such as the least-squares method, as it minimizes 'distance' between a function that is to be fit (overall solution), and a given set of data points (scenario solutions). First, the MILP is solved for each of the individual scenarios to obtain the solutions $z_q, \forall q \in \Phi$. Secondly, we solve the following optimization problem:

$$min_{z^*} \qquad \{\mathbb{E}_{q\in\Phi}[r_q^T|z^* - z_q|] \ \mid \ Wz^* \leq h, \text{with } z^* \geq 0 \text{ and } z_i^* \in \{0,1\} \ \forall i \in I\}$$

The absolute value operator in the objective is evaluated element-wise. The expectation is taken with respect to the probability distribution on the set of scenarios Φ. This is also referred to as the probability of occurrence, i.e. the probability that scenario q is realized.

The set of constraints $Wz^* \leq h$ ensures that a feasible solution for z^* is found. If we would omit these inequalities, we could end up with a strategy that is not implementable. It resembles user preferences on implementability. For example, suppose we have two strategies that prescribe to not deliver a cargo on a particular day. If we then apply the absolute difference approach, cargo delivery on that specific day is disregarded, as it does not resemble the optimal actions as calculated for the two scenarios. Nonetheless, it could be optimal to do so from a risk point of view. This approach thus disregards potentially optimal strategies, that do not resemble the strategies z_q that are involved. Furthermore, due to the two evaluation steps, this approach performs rather slowly. In the next section we define the Average case behavior MILP, which is closely related to the expected value method, except for the integer valued stochastic parameters such as shipment delays and spot opportunity arrivals.

5.3 - Average case behavior of the LNG system

In the Average case behavior MILP, the stochastic parameters such as $\tilde{\mu}_{t,k}$ are replaced by their average case behavior $\hat{\mu}_k$, which is closely related to the expected value except for the compatibility issue with integer valued stochastic variables. The dash accent on a variable refers to its 'average case' behavior. This section describes for each of the stochastic variables (i.e. LNG train breakdowns, spot opportunity arrivals and shipment delays) how its average case behavior is defined.

We start with the breakdown process, for which the average case behavior is based on the Markov model as depicted in Figure 4.1. The probability that in an arbitrary period t the LNG train k is down, equals the probability $\mathbb{P}(\tilde{\mu}_{t,k} \neq 0) = \mathbb{P}(\tilde{\mu}_{t,k} \in \{1,2,3\})$. This probability is determined by solving the balance equations to obtain the stationary distribution [27,28]:

$$\begin{aligned}
&\mathbb{P}(\tilde{\mu}_{t,k} = 0) = \mathbb{P}(\tilde{\mu}_{t,k} = 0) \cdot \rho_{00} + \mathbb{P}(\tilde{\mu}_{t,k} = 1), \\
&\mathbb{P}(\tilde{\mu}_{t,k} = 1) = \mathbb{P}(\tilde{\mu}_{t,k} = 0) \cdot \rho_{01} + \mathbb{P}(\tilde{\mu}_{t,k} = 2), \\
&\mathbb{P}(\tilde{\mu}_{t,k} = 2) = \mathbb{P}(\tilde{\mu}_{t,k} = 0) \cdot \rho_{02} + \mathbb{P}(\tilde{\mu}_{t,k} = 3), \\
&\mathbb{P}(\tilde{\mu}_{t,k} = 3) = \mathbb{P}(\tilde{\mu}_{t,k} = 0) \cdot \rho_{03}, && \text{(redundant equation)} \\
&\mathbb{P}(\tilde{\mu}_{t,k} = 0) + \mathbb{P}(\tilde{\mu}_{t,k} = 1) + \mathbb{P}(\tilde{\mu}_{t,k} = 2) + \mathbb{P}(\tilde{\mu}_{t,k} = 3) = 1, && \text{(normalization equation)}
\end{aligned} \tag{5.3}$$

with ρ_{0j} the transition probabilities from state 0 to state j of the Markov chain, as defined in Section 4.2. To obtain $\mathbb{P}(\tilde{\mu}_{t,k} \neq 0)$, the set of equations (5.3) is simplified:

$$\mathbb{P}(\tilde{\mu}_{t,k} = 0) = \frac{1}{1+\rho_{01}+2\cdot\rho_{02}+3\cdot\rho_{03}}$$

In the deterministic first stage, the system state is known with certainty. The LNG breakdown status of train k in the first period $t = 1$ is denoted by μ_k^{curr}. We thus have for the average case breakdown parameter $\hat{\mu}_{t,k}$:

$$\hat{\mu}_{t,k} = \mu_k^{curr} \qquad \text{for} \qquad t = 1, \forall k \in K$$

$$\hat{\mu}_{t,k} = \mathbb{P}(\tilde{\mu}_{t,k} \neq 0) = 1 - \mathbb{P}(\tilde{\mu}_{t,k} = 0) = \frac{\rho_{01}+2\cdot\rho_{02}+3\cdot\rho_{03}}{1+\rho_{01}+2\cdot\rho_{02}+3\cdot\rho_{03}} \qquad \text{for} \qquad \forall t \geq 2,\ \forall k \in K \tag{5.4}$$

In the first period, the process is deterministic, so the state of breakdown is known with certainty to be either 1 (down) or 0 (up and running). Furthermore, note that the fraction in equation (5.4) can be interpreted from a renewal theory point of view. The denominator is the expected number of 'jumps' of the discrete time Markov process that is needed to re-enter state 0, defining a renewal cycle. The numerator represents the expected number of jumps from state 0 to any of the other states per renewal cycle, which is interpreted as the expected 'downtime' per cycle [43]. The average case breakdown parameter is plugged into the MILP definition of Chapter 3 (constraints C5* and C6*).

Average case behavior for shipment delay and spot arrivals

For the shipment delays, we assume that no delays occur and ships arrive according to the ADP in the average case scenario. Formally, we define:

$$\hat{\sigma}_t = \sigma_t^{ADP}$$

For the spot opportunity arrivals, we assume that they arrive at their most-likely arrival time. In other words, suppose that for spot opportunity s the arrival probability is given by:

$$\begin{aligned}
&\mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ period\ 2\,) && = 0.1\\
&\mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ period\ 3\,) && = 0.1\\
&\mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ period\ 4\,) && = 0.7\\
&\mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ period\ 5) && = 0.1\\
&\mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ periods\ other\ than\ 2, \dots, 5) && = 0
\end{aligned}$$

The most likely period in which spot opportunity will arrive is 4, so in the average case scenario we define its period of arrival to be 4 with certainty. Formally:

$$\hat{\varphi}_{t,s} = 1 \qquad \text{if} \qquad argmax_{t'}\ \mathbb{P}(arrival\ of\ spot\ opportunity\ s\ in\ period\ t'\,) = t$$

and 0 otherwise.

Using the average case definitions for the stochastic parameters, we obtain the average case MILP presented in Definition 5.2. This model is used as a reference to compare the stochastic model that is discussed in the remainder of this chapter.

Average case constraints

$\pi_{t,w}$	$\leq \Pi_w^{max}$	$\forall t, w$	(AC1)
$f_{t,w}$	$\leq \pi_{t,w} \cdot GOR_w$	$\forall t, w$	(AC2)
$\pi_{t,w}^{+} - \pi_{t,w}^{-}$	$= \pi_{t,w} - \pi_{t-1,w}$	$\forall t, w$	(AC3)
$\pi_{t,w}^{+} + \pi_{t,w}^{-}$	$\leq \Pi_w^{max} \cdot \pi_{t,w}^{bin}$	$\forall t, w$	(AC4)
$\sum_W \pi_{t,w} \cdot GOR_w - f_{t,w}$	$\leq \sum_K \beta_k \cdot (1 - \hat{\mu}_{t,k})$	$\forall t, w$	(AC5)
$\sum_W \left(\pi_{t,w} \cdot GOR_w - f_{t,w,q}\right) \cdot I_w$	$\leq \sum_K \gamma_k \cdot (1 - \hat{\mu}_{t,k})$	$\forall t, w$	(AC6)
$\sum_N \theta_{t,c}$	≤ 1	$\forall c$	(AC7)
$\sum_c \theta_{t,c} + \theta_t^{spot}$	$\leq \hat{\sigma}_t$	$\forall t, c$	(AC8)
L_t	$= L_{t-1} + \sum_W \left(\pi_{t-1,w} \cdot GOR_w - f_{t-1,w}\right) \cdot (1 - I_w)$		
	$- \sum_C \theta_{t,c} \cdot d_c - \theta_t^{spot} \cdot d^{spot}$	$\forall t$	(AC9)
L_t	$\leq L^{max}$	$\forall t$	(AC10)
θ_t^{spot}	$\leq \hat{\varphi}_t$	$\forall t$	(AC11)

Initial variable values

$\pi_{0,w}$	$= \pi_w^{init}$	$\forall w$
L_0	$= L^{init}$	$\forall$

Reward in period *t*

$$R_t = p_t^{oil} \cdot \sum_W \pi_{t,w} \cdot (1 - GOR_w) - \sum_W \pi_{t,w}^{bin} \cdot c_w^{well} - \sum_W f_{t,w} \cdot c^{flare} + \sum_C \theta_{t,c} \cdot r_{t,c} - \left(1 - \sum_{\in N} \theta_{t,c}\right) \cdot c_c^{rej} + \theta_t^{spot} \cdot r_t^{spot}$$

Objective function

$$max_A \quad \sum_N R_t \qquad A = \{\, \pi_{t,w}, f_{t,w}, \theta_{t,c}, \theta_{t,q}^{SPOT}, \forall t \in N, \forall w \in W, \forall c \in C \,\}$$

Definitions 5.2 – Average case scenario MILP

5.4 – Two stage Stochastic Mixed Integer Linear Programming

The methods presented previously to cope with uncertainty in MILPs result in a single strategy for the full planning horizon, as demanded. Since the decision model for the LNG case is intended for operational use, decisions are made on a daily basis with a focus on here-and-now. In other words, we are mainly interested in how to act today, taking into account possible future scenarios and their probability of occurrence. How we should act tomorrow is of later issue, since in practice we will re-evaluate our strategy by then with additional information. The output of the model should at least provide the optimal actions for today. I wide variety of models based on two stage stochastic programming can be found in literature [44,45,46, among many others]

Conceptually, one could think of the decision process having two stages. In the first, values for the first stage variables – contained in the vector z - are selected by the decision maker. The first stage objective is to maximize direct rewards obtained by selecting today's actions:

First stage rewards: $$r_1^T \cdot z \tag{5.5}$$

In the second stage, for each scenario realization $(r, A, b)_q \in \Phi$ of the random parameters, a so called recourse action vector z_q is selected, which represents costs associated with corrective actions to prevent infeasibility or sub-optimality in a particular scenario.

Expected second stage recourse rewards/costs: $$\mathbb{E}_{q\in\Phi}\left[r_q^T z_q\right] := \sum_{\Phi} p_q \cdot r_q^T z_q \tag{5.6}$$

Suppose for example, that we have scheduled a delivery in the first stage in period t, but in a particular scenario the stock level in period t is insufficient to actually do so. The recourse action is to reschedule or to cancel the cargo, and results in recourse costs. On the other hand, in a different scenario we could decide to plan an extra cargo to prevent stock overflow. In the latter case we obtain recourse revenue, where in the first case costs are incurred. Both recourse costs (negative sign) and recourse revenues (positive sign) in scenario q are denoted by r_q^T.

We assume that the set Φ of possible scenarios is known by the decision maker prior to optimization, and we are able to calculate the recourse costs r_q^T for each scenario q. The expected cost of the second stage is the weighted average of recourse costs for all scenarios. The objective is to find the optimal balance between first stage rewards (5.5) and expected second stage recourse costs (5.6):

Expected total reward (objective function) $$max_{x,z_q} \quad r_1^T z + \mathbb{E}_{q\in\Phi}\left[r_q^T z_q\right] \tag{5.7}$$

Note that this SMILP approach is actually a large-scale deterministic equivalent problem, which can be solved by general deterministic MILP solution methods. The two stage stochastic programming framework is shown schematically in Figure 5.1. The formal two-stage stochastic (MI)LP model is defined in Definition 5.1. Note that periods represent days in our model, but any time interval such as minutes, hours or day sessions can be used. One should carefully pick an appropriate setting, that fits the goals of the optimization problem in terms of a given business question.

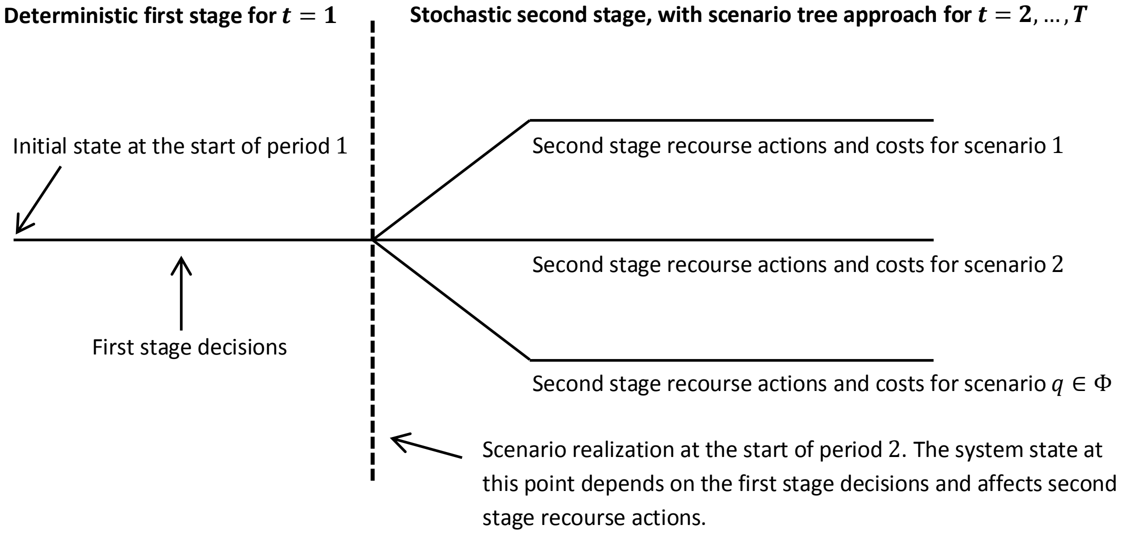


Figure 5.1 – Schematic illustration of the two-stage stochastic programming approach. Note that 'stages' refer to the two-stage stochastic MILP and 'periods' refer to decision moments (days in the LNG case), as presented in the sequential optimization models of this and previous chapters.

max_{x,z_q}	$r_1^T z + \mathbb{E}_{q\in\Phi}\left[r_q^T z_q\right]$	(Expected first and second stage revenues)	
s.t.	$A_1 z \leq b_1$	(First stage constraints)	(*)
	$A_q z_q \leq b_q - Vz \quad \forall q \in \Phi$	(Second stage constraints)	(**)

with

z	First stage decision vector,
z_q	Second stage recourse action vector, associated with scenario $q \in \Phi$,
$\mathbb{E}_{q\in\Phi}[\cdot]$	Expected value with respect to the probability distribution on Φ,
r_1^T	First stage reward vector,
r_q^T	Second stage recourse revenue (or cost) vector, associated with scenario q,
A_1	First stage constraint parameter matrix,
A_q	Second stage constraint parameter matrix, associated with scenario q
b_1	First stage Right-Hand-Side (RHS) vector,
b_q	Second stage RHS vector, associated with scenario q, and
V	Matrix to model dependency of second stage RHS vector b_q on first stage decisions z.

Definition 5.1 – The two-stage stochastic (MI)LP framework

5.5 - Scenario set construction

Given a set of scenarios Φ, the two stage stochastic MILP can be applied to solve the first stage decisions to optimality, as discussed in previous sections. It takes into account the 'risks' associated with each of the scenarios $q \in \Phi$. In this section we discuss how we construct such a scenario set for the LNG case.

The stochastic processes associated with LNG train breakdowns, shipment delays and spot opportunity arrivals are independent, so we can discuss them separately. Given the scenarios sets for each of these three stochastic processes, we construct the overall scenario set as all combinations that can be constructed from them. To illustrate this procedure, suppose we flip a coin and roll a dice having the usual two and six possible outcomes (scenarios) respectively. These outcomes can be regarded as individual scenario sets:

Scenario set of a coin: $\{H, T\}$
Scenario set of a dice: $\{1,2,3,4,5,6\}$

If we combine these sets to obtain an overall scenario set, the number of scenarios contained in it is the Cartesian product of the individual sets:

Overall scenario set: $\{ (H,1), \dots, (H,6), (T,1), \dots, (T,6) \}$

For the LNG case, we first define the individual sets (1) B for the LNG breakdown stochastic process, (2) D for Shipment delay stochastic process and end this section with the construction of the overall scenario set Φ as the Cartesian product of these sets. In this thesis, we do not implement the set SP for the stochastic process associated with spot opportunity arrivals to avoid lengthy definitions and arithmetic. However, it could be implemented along the same lines as for the other sets B and D.

LNG train breakdown scenarios

Given the current breakdown state μ_k^{curr} of the LNG trains $k \in K$ in period 1, we distinguish between four scenarios per LNG train k. If the train is down for μ_k remaining days, we face a single scenario that represents the remaining number of days that is needed to fix the train is decreased by one day:

$$\mu_{2,k,b} = \mu_k^{curr} - 1,$$

where $\mu_{t,k,b}, t \in N, k \in K, b \in B$ denotes whether or not LNG train k is operative in period t for breakdown scenario b. On the other hand, if LNG train k is operational, we consider the following four different breakdown scenarios, denoted by the index $b = 1, \dots, 4$:

1. LNG train k is up in period 2,
2. LNG train k is down in period 2, and is operational again in period 3,
3. LNG train k is down in periods 2 and 3, and is operational again in period 4,
4. LNG train k is down in period 2 to 4, and is operational again in period 5,

If (case 1) LNG train k is operational in the first period, we consider the following scenarios:

Deterministic behavior for first period

$\mu_{1,k,b} = \min(1, \mu_k^{curr})$ $\qquad b = 1, \dots, 4$

Stochastic behavior for periods 2 to 5

Scenario $b = 1$	**Scenario $b = 2$**	**Scenario $b = 3$**	**Scenario $b = 4$**
$\mu_{2,k,1} = 0$	$\mu_{2,k,2} = 1$	$\mu_{2,k,3} = 1$	$\mu_{2,k,4} = 1$
$\mu_{3,k,1} = \hat{\mu}_{3,k}$	$\mu_{3,k,2} = 0$	$\mu_{3,k,3} = 1$	$\mu_{3,k,4} = 1$
$\mu_{4,k,1} = \hat{\mu}_{4,k}$	$\mu_{4,k,2} = \hat{\mu}_{4,k}$	$\mu_{4,k,3} = 0$	$\mu_{4,k,4} = 1$
$\mu_{5,k,1} = \hat{\mu}_{5,k}$	$\mu_{5,k,2} = \hat{\mu}_{5,k}$	$\mu_{5,k,3} = \hat{\mu}_{5,k}$	$\mu_{5,k,4} = 0$

Average case behavior for remaining periods ($t \geq 6$)

$\mu_{t,k,b} = \hat{\mu}_{t,k}$ $\qquad t \in \{6, \dots, T\}$ $\qquad b = 1, \dots, 4.$

Otherwise (case 2), if the LNG train k is broken in the first period (so $\mu_k^{curr} \neq 0$), we consider the scenario in which LNG train k is under maintenance for the residual μ_k^{curr} days. When it is fixed, it behaves like it is in its average case behavior for the remainder of the planning horizon. To summarize, if LNG train k is broken in period t, we have to consider a single scenario that represents the residual number of maintenance days being decreased by one day. On the other hand, if the train is working in the first period, we consider the four different scenarios as stated above.

Note that the number of <u>distinct</u> breakdown scenarios is either 1 (if $\mu_k^{curr} \neq 0$) or 4 (if $\mu_k^{curr} = 0$) per LNG train. However, we always define four scenarios per LNG train for convenience in later definitions. In case of a single scenario, we therefore duplicate it four times.

The total number of breakdown scenarios in the set B is thus $4^{|K|}$, as we have the four scenarios for each of the LNG trains. Suppose the model contains two LNG trains, so $|K| = 2$, we have $|B| = 4^2$ scenarios in each period t. Note that the number of scenarios increases dramatically if additional LNG trains are added to the model.

Shipment delay scenarios

The parameter $\tilde{\sigma}_t$ denotes the stochastic number of available ships in period t. Based on the Annual Delivery Plan (ADP), we know the expected number of ships, defined by σ_t^{ADP}, as if the model was deterministic. However, uncertainties are not taken into account when constructing this schedule. To model stochastic behavior, we start with the assumption that at most a single ship is delayed in each time period t. In each period t, we distinguish between four different shipment scenarios $d = 1, \dots, 4$:

1. No ships are delayed in any of the periods
2. A single ship is delayed by one day in period 2, no ships are delayed in other periods
3. A single ship is delayed in period 3 by one day, no ships are delayed in other periods
4. In both periods 2 and 3 a single ship is delayed by one day, no ships are delayed in other periods

Given the initial number of ships σ_t^{ADP} that is available in period t according to the ADP, we calculate the number of ships $\sigma_{t,d}$ in case of the four shipment scenarios denoted by index $d = 1, \dots, 4$:

Deterministic behavior for first period

$\sigma_{1,n} = \sigma_1^{ADP}$ $\qquad d = 1, \dots, 4$

Stochastic behavior for periods 2 to 4

Scenario $\boldsymbol{n = 1}$	Scenario $\boldsymbol{n = 2}$	Scenario $\boldsymbol{n = 3}$	Scenario $\boldsymbol{n = 4}$
$\sigma_{2,1} = \sigma_2^{ADP}$	$\sigma_{2,2} = \sigma_2^{ADP} - 1$	$\sigma_{2,3} = \sigma_2^{ADP}$	$\sigma_{2,4} = \sigma_2^{ADP} - 1$
$\sigma_{3,1} = \sigma_3^{ADP}$	$\sigma_{3,2} = \sigma_3^{ADP} + 1$	$\sigma_{3,3} = \sigma_3^{ADP} - 1$	$\sigma_{3,4} = \sigma_3^{ADP}$
$\sigma_{4,1} = \sigma_4^{ADP}$	$\sigma_{4,2} = \sigma_4^{ADP}$	$\sigma_{4,3} = \sigma_4^{ADP} + 1$	$\sigma_{4,4} = \sigma_4^{ADP} + 1$

Average case behavior for remaining periods $(\boldsymbol{t \geq 5})$

$\sigma_{t,n} = \sigma_t^{ADP}$ $\qquad t \in \{5, \dots, T\} \qquad d = 1, \dots, 4$

We assume that at least one ship arrives each day in the ADP, so no maximum operator is necessary to ensure non-negativity of the $\sigma_{t,n}$. The probability vector containing the delay probabilities associated with each of the scenarios is defined as $\chi \in [0,1]^4$, such that the summation over its elements, denoted by χ_d, equals 1.

If we combine the $|D| = 4$ delay scenarios with the $|B|$ breakdown scenarios of the previous section by means of their Cartesian product, we obtain the scenario set Φ that contains $|B| \cdot |D|$ scenarios. Its elements are $q = (b, d)$, for $\forall b \in B$ and $\forall d \in D$. The probability of occurrence p_q associated with scenario $q = (b, d)$ is the element-wise multiplication (known as Hadamard product) of the breakdown and delay probability vectors ρ and χ:

$$p_{q \in \Phi} = p_{(b,d) \in B \times D} = \mathbb{P}(breakdown\ scenario\ is\ b\ and\ delay\ scenario\ is\ d) = \rho_b \cdot \chi_d$$

The summation of these probabilities of occurrence over all scenarios $q \in \Phi$ adds up to 1, as is necessary for $p_q$to be a probability distribution.

5.6 - The LNG two stage stochastic MILP

Now that we have defined the scenario set Φ, the definition of the two stage stochastic MILP for the LNG case is presented. As discussed, the optimization model divides the problem in two stages. The first stage models the deterministic first period, comprising a single period $t = 1$. The second stage comprises all of the remaining periods $t = 2, \dots T$. Since the process is stochastic in the second stage, we use the scenario set Φ to model it.

The decision variables (actions) are defined for each of the scenarios $q \in \Phi$:

Flow out of well w in period t in case of scenario q	$\pi_{t,w,q}$	$\forall t, w, q$
Flare at well w in period t in case of scenario q	$f_{t,w,q}$	$\forall t, w, q$
Indicator whether contract c is shipped in period t for scenario t	$\theta_{t,c,q}$	$\forall t, w, q$
Indicator whether spot opportunity in period t is monetized, if present	$\theta_{t,q}^{SPOT}$	$\forall t, q$

The number of decision variables has increased by a factor $|\Phi|$ with respect to the deterministic (and average case) MILP definition, and therefore affects computational time significantly, as illustrated in Chapter 6. The first stage decision variables must attain the same value in each of the scenario, as we need a single decision for the first period (which is to be executed immediately today). This property is modeled by the following set of first stage constraints:

$\pi_{1,w,q}$	$= \pi_{1,w}$	$\forall w, q$	(SC12)
$\pi_{1,w}^{bin}$	$= \pi_{1,w,q}^{bin}$	$\forall w, q$	(SC13)
$f_{1,w,q}$	$= f_{1,w}$	$\forall w, q$	(SC14)
$\theta_{1,c,q}$	$= \theta_{1,c}$	$\forall c, q$	(SC15)
$\theta_{1,q}^{SPOT}$	$= \theta_{1}^{SPOT}$	$\forall c$	(SC16)

The corresponding first stage revenue is:

$$R_1 \ = p_1^{oil} \cdot \sum_W \pi_{1,w} \cdot (1 - GOR_w) - \sum_W \pi_{1,w}^{bin} \cdot c_w^{well} - \sum_W f_{1,w} \cdot c^{flare} + \sum_C \theta_{1,c} \cdot r_{1,c}^{ADP} + \theta_1^{SPOT} \cdot r_1^{SPOT} \tag{5.8}$$

In contrast to first stage decision variables, the second stage decision variables can be different for each scenario, with likewise different associated second stage rewards per scenario:

$$R_{t,q} = p_t^{oil} \cdot \sum_W \pi_{t,w,q} \cdot (1 - GOR_w) - \sum_W \pi_{t,w,q}^{bin} \cdot c_w^{well} - \sum_W f_{t,w,q} \cdot c^{flare} + \sum_C \theta_{t,c,q} \cdot r_{t,c}^{ADP} + \theta_{t,q}^{spot} \cdot r_1^{spot} \tag{5.9}$$

These rewards are corrected by the rejection costs associated with non-delivered cargoes in each of the scenarios. We subtract these costs from the second stage reward equation (5.10), to obtain the scenario rewards R_q:

$$R_q \ = \sum_{t>2 \in N} R_{t,q} - \sum_{c \in C} (1 - \sum_{\in N} \theta_{t,c,q}) \cdot c_c^{rej}$$

Each scenario has a known probability of occurrence that is defined by the parameter $p_q, \forall q \in \Phi$ as defined in Section 5.4. Using this parameter, the expected total reward is:

$$R_{tot} = R_1 + \sum_{q \in \Phi} p_q \cdot R_q \tag{5.10}$$

Equation (5.10) is used as the objective function of the two stage stochastic MILP. We thus optimize both the first and second decision stages simultaneously. If we would not do so, we lose the effects of first stage decisions on those in the second stage. Therefore, we cannot optimize each of the scenarios individually and then calculate expected rewards by means of a weighted average. For example, shipping many cargoes in the first stage results in a low stock level at the start of the second stage. In certain scenarios, this may lead to significant risks due to for example LNG train breakdowns in the third or fourth period.

Note that the second stage decision variables do not have operational implications, since only first stage decisions are executed today. However, second stage variables are used to determine the expected recourse costs (or revenues) as result of our choice for the value of first stage variables.

First and Second stage constraints

$\pi_{t,w,q}$	$\leq \Pi_w^{max}$	$\forall t,w,q$	(SC1)
$f_{t,w,q}$	$\leq \pi_{t,w} \cdot GOR_w$	$\forall t,w,q$	(SC2)
$\pi_{t,w,q}^{+} - \pi_{t,w,q}^{-}$	$= \pi_{t,w,q} - \pi_{t-1,w,q}$	$\forall t,w,q$	(SC3)
$\pi_{t,w,q}^{+} + \pi_{t,w,q}^{-}$	$\leq \Pi_w^{max} \cdot \pi_{t,w,q}^{bin}$	$\forall t,w,q$	(SC4)
$\sum_W \pi_{t,w,q} \cdot GOR_w - f_{t,w,q}$	$\leq \sum_K \beta_k \cdot (1-\mu_{t,k,q})$	$\forall t,w,q$	(SC5)
$\sum_W \left(\pi_{t,w,q} \cdot GOR_w - f_{t,w,q}\right) \cdot I_w$	$\leq \sum_K \gamma_k \cdot (1-\mu_{t,k,q})$	$\forall t,w,q$	(SC6)
$\sum_N \theta_{t,c,q}$	≤ 1	$\forall c,q$	(SC7)
$\sum_C \theta_{t,c,q} + \theta_{t,q}^{spot}$	$\leq \sigma_{t,q}$	$\forall t,c,q$	(SC8)
$L_{t,q}$	$= L_{t-1,q} + \sum_W \left(\pi_{t-1,w,q} \cdot GOR_w - f_{t-1,w,q}\right) \cdot (1-I_w)$ $- \sum_C \theta_{t,c} \cdot d_c - \theta_{t,q}^{spot} \cdot d^{spot}$	$\forall t,q$	(SC9)
$L_{t,q}$	$\leq L^{max}$	$\forall t,q$	(SC10)
$\theta_{t,q}^{spot}$	$\leq \varphi_{t,q}$	$\forall t,q$	(SC11)

First stage constraints

$\pi_{1,w,q}$	$= \pi_{1,w}$	$\forall w,q$	(SC12)
$\pi_{1,w}^{bin}$	$= \pi_{1,w,q}^{bin}$	$\forall w,q$	(SC13)
$f_{1,w,q}$	$= f_{1,w}$	$\forall w,q$	(SC14)
$\theta_{1,c,q}$	$= \theta_{1,c}$	$\forall c,q$	(SC15)
$\theta_{1,q}^{SPOT}$	$= \theta_1^{SPOT}$	$\forall c$	(SC16)

Initial variable values

$\pi_{0,w,q}$	$= \pi_w^{init}$	$\forall w,q$
$L_{0,q}$	$= L^{init}$	$\forall q$

First and second stage rewards

$$R_1 = p_1^{oil} \cdot \sum_W \pi_{1,w} \cdot (1 - GOR_w) - \sum_W \pi_{1,w}^{bin} \cdot c_w^{well} - \sum_W f_{1,w} \cdot c^{flare} + \sum_C \theta_{1,c} \cdot r_{1,c} + \theta_1^{spot} \cdot \tau_1^{spot}$$

$$R_{t,q} = p_t^{oil} \cdot \sum_W \pi_{t,w,q} \cdot (1 - GOR_w) - \sum_W \pi_{t,w,q}^{bin} \cdot c_w^{well} - \sum_W f_{t,w,q} \cdot c^{flare} + \sum_C \theta_{t,c,q} \cdot r_{t,c} - \left(1 - \sum_N \theta_{t,c,q}\right) \cdot c_c^{rej} + \theta_{t,q}^{spot} \cdot r_t^{spot}$$

Objective function

$$max_A \quad R_1 + \mathbb{E}_{q\in\Phi} \sum_N R_{t,q} \qquad A = \{\pi_{t,w,q}, f_{t,w,q}, \theta_{t,c,q}, \theta_{t,q}^{SPOT}, \forall t \in N, \forall w \in W, \forall c \in C, \forall q \in \Phi\}$$

Definitions 5.3 – Two stage stochastic MILP for the LNG case

Chapter 6

Strategy evaluation in an operational setting

In this chapter we discuss the two models presented in Definition 5.2 and Definition 5.3 in an operational setting: (1) Average case behavior MILP and (2) two-stage stochastic MILP respectively. If we do not mean one of both in specific, we refer to them as 'strategy models'. Since the goal of this thesis (among others) is to construct an operational model that is used on a day-to-day basis, we introduce a rolling horizon approach in Section 6.2 that simulates behavior of the system. We used Monte Carlo simulation, which is discussed in Section 6.1, to obtain the average total rewards of the strategy models to compare performance of the proposed models.

The formulations of this chapter are suitable for any software package that is capable of solving MILPs and evaluation of basic logical expressions, including random number generation from the standard Uniform distribution. We decided to use the software package AIMMS for our analysis, as it is a frequently used modeling environment within ORTEC and Shell.

6.1 - Monte Carlo simulation

Monte Carlo simulation is a broad class of evaluation methods that use repeated random sampling to obtain numerical results. In general, it simulates a large number of realizations of a stochastic process to approximate performance metrics, for example mean revenue. It is based on the strong law of large numbers, that is $\tilde{X}_n \to X$ if $n \to \infty$ with $\tilde{X}_n$ a realization n of the stochastic variable $\tilde{X}$. It is a widely used method to analyze a systems' behavior if an analytic solution is unavailable [47].

Sampling a stochastic process

A sampler is a procedure that produces an independent sample of the random variable X each time it is called. A sampler turns a uniform sample $U \in [0,1]$ into a sample of another random variable X, using the corresponding cumulative distribution function. Suppose X can take on J different values X_j with $j = 1, \dots, J$ and having cumulative distribution function p_j^{cum}:

$$p_j^{cum} = \mathbb{P}(X \leq X_j)$$

Given a uniform sample U, we calculate the sample value of X by:

$$X = \min\{ X_j \mid p_j^{cum} \geq U \} \tag{6.1}$$

To illustrate this sampling procedure, suppose we have the discrete distribution of a random variable X, which can take values from the set $\{1,2,3\}$, with the following density and distribution function:

$X =$	1	with probability	$0.1,$	so $p_1^{cum} = 0.1$
	2	with probability	$0.6,$	so $p_2^{cum} = 0.7$
	3	with probability	$0.3,$	so $p_3^{cum} = 1.0$

For a given uniform sample $U = 0.4$ we find:

$$X = \min\{ X_j \mid p_j^C \geq 0.4 \} = \min\{2,3\} = 2$$

This method also holds for continuous random variables, such as the Normal distribution. Even though the number of values that can be attained is infinite, the cumulative distribution function is defined such that equation (6.1) can be applied directly. However, in the LNG case as we present it, only discrete distributions are used.

A large Monte Carlo simulation may spend most of its time in the sampler and it often is possible to improve the performance by paying attention to the details of the concerned algorithm and coding. Detailed information on this topic is not in the scope of this text, more information can be found in [47].

The stochastic model parameters such as the LNG train breakdown, spot opportunity arrivals and shipping delays were sampled from their associated probability distribution. This way, we create a single realization (or scenario) of the stochastic process over the planning horizon. Given a scenario, we use the two-stage MILP and the Average case behavior models to obtain total revenues for both methods. In the next section, we often use the term 'sample of the stochastic LNG process', which is defined as follows:

> **A sample of the stochastic LNG process** is a single realization of all stochastic variables in the LNG model, as defined in Section 4.2, using the sampling method. That is, a sample of the stochastic process assigns a sampled value to each of the variables $\tilde{\mu}_{t,k}$, $\tilde{\varphi}_t$ and $\tilde{\sigma}_t$ for all $t \in N$ and $k \in K$, according to their cumulative probability distribution.

A sample of the stochastic LNG process is different from a scenario in the sense that scenarios are predictions on how the stochastic process might behave in the future. A sample of the stochastic process does not have this predictive character, but is unknown to the decision maker until the end of the planning horizon. However, for implementation simplicity it is also possible to sample the complete stochastic process prior to optimization, as is the case in the algorithm presented in Figure 6.2.

Furthermore, note that the number of different samples for a stochastic process with finite support is also finite. Therefore, one could argue that exact analysis of the process (instead of Monte Carlo simulation) is possible by enumerating over all possible scenarios. However, since the number of possible samples of the stochastic process is large, such analysis is computationally intractable. Therefore, we choose to use a Monte Carlo simulation approach.

6.2 - Rolling horizon approach

To compare the performance of both strategy models, (1) two-stage stochastic MILP and (2) the average case behavior MILP, we use a rolling horizon approach in combination with Monte Carlo simulation. The planning horizon, containing $|Z|$ periods, is divided in smaller sub-horizons containing $Y \subseteq Z$ periods. This subdivision is illustrated in Figure 6.1. For example, we could analyze approximately one month ($|Z| = 30$ days) with a rolling horizon of $|Y| = 10$ days. If we would include all periods of Z in a single optimization run, the problem could become computationally complex. However, this generalized definition allows $Y = Z$.

The algorithm starts at $t = 1$ and takes into account all periods up to $t = |Y|$. The remaining periods $t \notin Y$ are disregarded. The optimal first stage decisions and the direct rewards associated with them are calculated using the two strategy models. The optimal actions calculated by these models might differ. The direct rewards associated with the two stage stochastic MILP and the average case behavior MILP are indicated by R_1^S and R_1^A respectively for $t = 1$ (superscripts indicate Stochastic and Average).

We then start the optimization at $t = 2$ and include all periods up to $t = |Y| + 1$. Again, we calculate the optimal first stage actions to obtain R_2^S and R_2^A. However, the initial parameters such as stock level and production rates are updated according to the decisions of the previous step ($t = 1$). The second period optimization is directly affected by decisions made in the first period. The direct reward in step t for either of the models (indicated by the S/A superscript) is defined the following:

$$R_t^{S/A} = p_1^{oil} \cdot \sum_W \pi_{1,w} \cdot (1 - GOR_w) - \sum_W \pi_{1,w}^{bin} \cdot c_w^{well} - \sum_W f_{1,w} \cdot c^{flare} + \sum_C \theta_{1,c} \cdot r_1^C \quad (6.2)$$

where the subscript 1 refers to the first period that is taken into account in the optimization, starting at time t. Note that the input parameters must be shifted by one period before every subsequent rolling horizon step. The rolling horizon procedure is repeated until $t = |Z|$, as illustrated in Figure 6.1. However, if

$$|Z| - t < |Y|, \quad \text{then} \quad |Y| = |Z| - t, \quad (6.3)$$

so at the end of a Monte Carlo cycle, the number of periods involved in the optimization decreases. The total rewards associated with a single iteration i of the Monte Carlo simulation are calculated by summation over revenues for all $t \in M$:

$$\bar{R}_i^S = \sum_M R_t^S, \quad \text{and} \quad \bar{R}_i^A = \sum_M R_t^A. \quad (6.4)$$

In the final rolling horizon step, at $t = |Z|$, we substract a penalty from the total rewards as calculated in (6.4) for every contract that is rejected (delivered). Therefore, we need to keep track of the contracts that are shipped during every Monte Carlo cycle. One such iteration (a full rolling horizon iteration) is indicated by the grey box on the left of Figure 6.2. However, a single iteration is not suitable for comparison of the two methods, since it only takes into account an arbitrary instance of the stochastic LNG process out of many possible realization. Therefore, we iterate the rolling horizon procedure to obtain a large number of scenario samples, with corresponding total revenues $\bar{R}_i^S$ and $\bar{R}_i^A$ for all $i \in I$, with I the index set of Monte Carlo iterations. These Monte Carlo iterations are indicated by the grey box on the right in Figure 6.2.

Note that scenarios with higher probability of occurrence are sampled more often than those with small probability of occurrence. This is a key feature of Monte Carlo simulation to obtain a good representation of the LNG process in reality. After finishing all iterations, the average total reward was calculated, using:

$$\bar{R}^S = \frac{1}{|I|}\sum_I \bar{R}_i^S, \text{ and } \quad \bar{R}^A = \frac{1}{|I|}\sum_I \bar{R}_i^A. \tag{6.5}$$

These average total rewards enable us to compare the performance of the strategy models in an operational setting. Note that, an increasing number of Monte Carlo iterations results in more reliable comparison, but also increases computational time. In general, several methods are known to determine a suitable 'stopping rule', as can be found in [47].

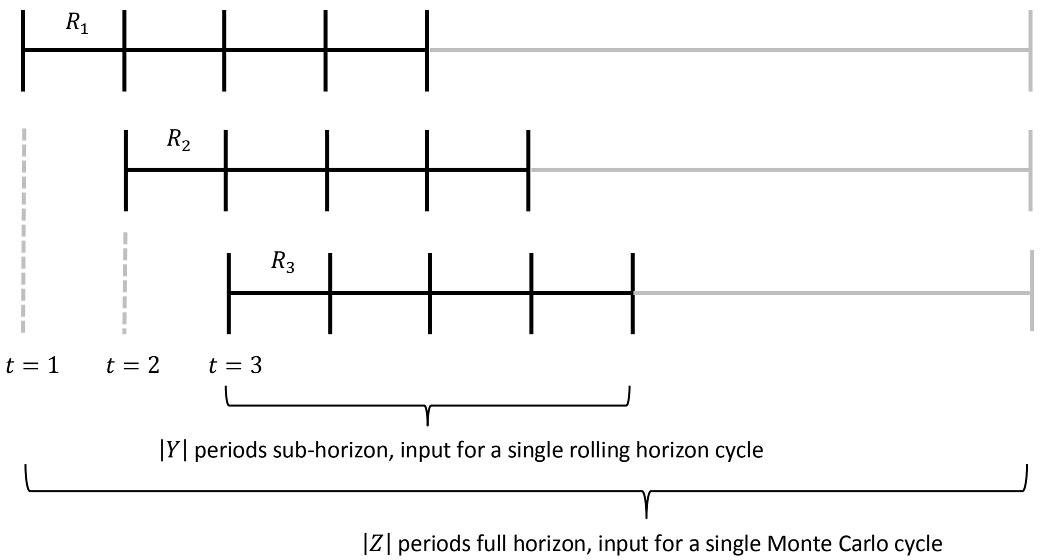


Figure 6.1 – Rolling horizon approach to evaluate $|Z|$ periods (i.e. 1 month) in smaller sub-problems containing $|Y|$ periods (i.e. 1 week)

Figure 6.2 shows the algorithm to compare the two proposed strategy models schematically, including the rolling horizon method (grey box) and Monte Carlo simulation (dotted box). The parallel section indicates the strategy models to be evaluated simultaneously:

(1) Average case behavior MILP (See section 5.4), also referred to as the A-model in Figure 6.2
(2) Two-stage stochastic MILP (See section 5.5), also referred to as the S-model in Figure 6.2

In the next chapter we present some examples of the algorithm applied to (imaginary) business cases. Note that the output of the comparison depends heavily on the input parameters such as contract revenues and costs. The goal of the comparison is to show that a stochastic approach results in better results in terms of rewards, and performs worse in terms of computational time if a large number of scenarios are to be included in the optimization.

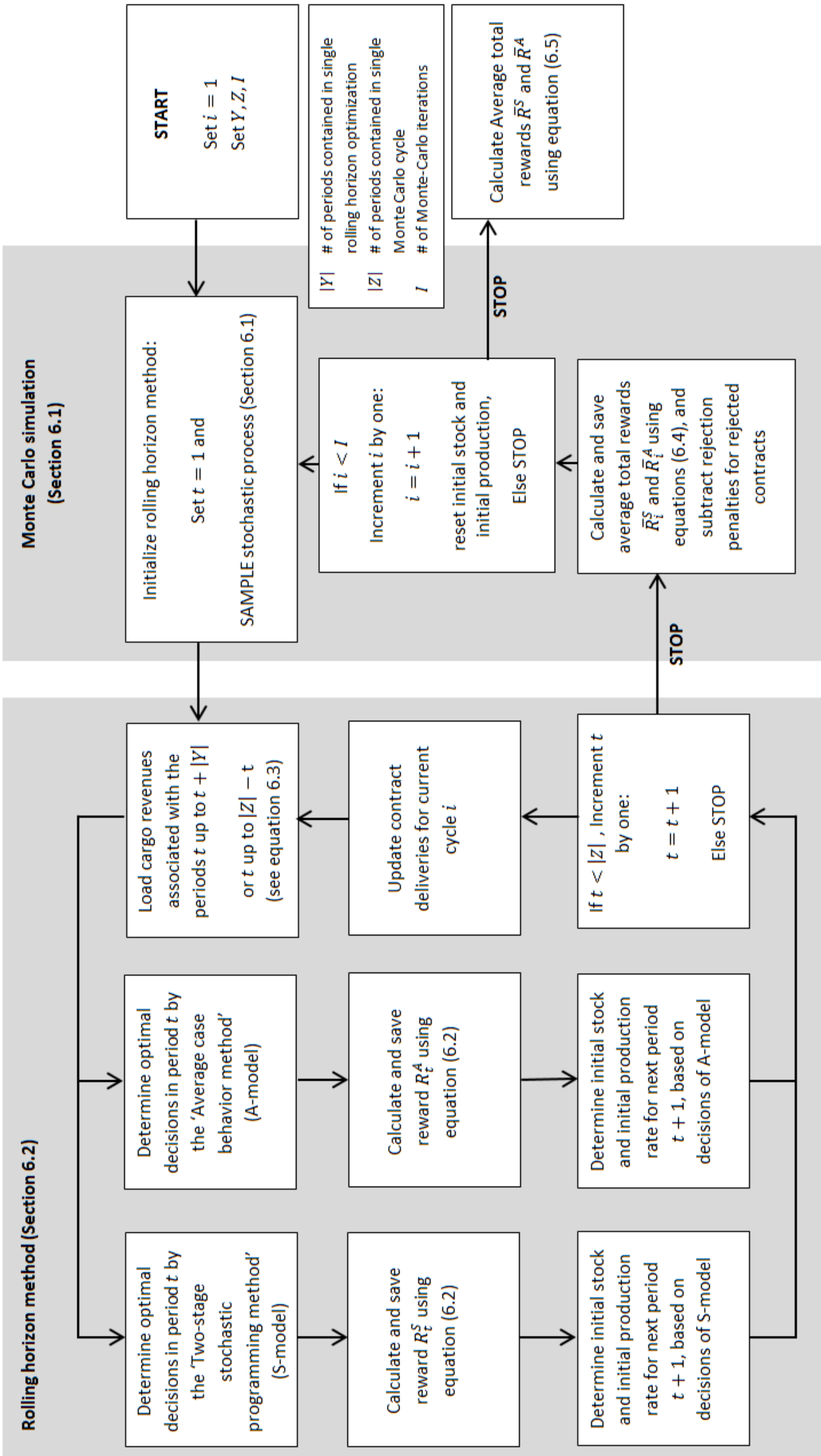


Figure 6.2 –Evaluation algorithm with rolling horizon method and Monte Carlo simulation

Chapter 7

Numerical results

In this chapter we show results of the evaluation algorithm presented in the previous chapter (see Figure 6.2 for an overview) as it was implemented in AIMMS. As discussed, it is unknown how decision making in the LNG value chain is executed in reality. Furthermore, no data was available on costs and revenues involved. Therefore, we stress the fact that the presented results focus on the difference between a stochastic and a deterministic approach to AWO. The business case that is used to facilitate this comparison is purely imaginary.

The output of the program consists of five KPIs for both two models that were presented in the previous chapters: (1) Average case behavior MILP and (2) Two-stage stochastic MILP:

(1) Mean total revenue, in dollars [$]
(2) Mean percentage of cargoes shipped, without unit [-]
(3) Mean LNG production, in volumetric units [V]
(4) Mean oil production, in volumetric units [V]
(5) Mean computational time, in seconds [s]

All of these KPIs are calculated over I Monte Carlo simulations. Each of these simulations comprises $|Z| = 30$ rolling horizon optimization runs that all include $|Y| = 10$ periods (or less in some cases, see equation 6.3). Before we present the comparison of the models with the above mentioned KPIs, we first show the differences between the stochastic two stage stochastic MILP and the deterministic Average case behavior MILP for a single optimization run. We use a visualization of the stock levels associated with their optimal solutions to the same business case, to point out the variability in scenarios.

7.1 - Evaluation of a single optimization run

For a single optimization run of the rolling horizon process, we visualize the effect of uncertainty in model parameters by plotting the stock levels associated with the 64 different scenarios. We use a horizon of five days, so $Y = \{1, \ldots, 10\}$ (see previous chapter for definition of the set Y), and the following scenario probabilities:

$$\mathbb{P}(breakdown\ scenario\ is\ b) = \begin{cases} 0.80 & \text{for} \quad b = 1 \\ 0.10 & \text{for} \quad b = 2 \\ 0.06 & \text{for} \quad b = 3 \\ 0.04 & \text{for} \quad b = 4 \end{cases}$$

$$\mathbb{P}(ship\ delay\ scenario\ is\ d) = \begin{cases} 0.60 & \text{for} \quad d = 1 \\ 0.15 & \text{for} \quad d = 2 \\ 0.15 & \text{for} \quad d = 3 \\ 0.10 & \text{for} \quad d = 4 \end{cases} \tag{7.1}$$

As discussed in the previous chapter, no spot opportunity arrivals are included in the business case, so we focus on the effect of LNG train breakdowns and ship delays. For the definitions associated with $b \in B$ and $d \in D$, we refer to Section 5.5. For definition of the other input parameters, such as initial stock and Gas-to-Oil ratios (GOR) at the wells, and so on, the reader is referred to Appendix A.1.

Figure 7.1 shows the stock level for each of the 64 scenarios of the two-stage stochastic MILP, for all periods $t \in Y$. Figure 7.2 shows the stock level as determined by the average case behavior MILP. We use this visual approach because it incorporates all decision variables of the models, captured in a graph instead of a large table of numbers, as it better exposes the variability in decision variables between scenarios.

Note that multiple scenarios in Figure 7.1 use the same color indication. This is because AIMMS cannot easily deal with multiple graphs in a single figure, and uses only a small set of (basic) colors. However, the goal of the figure is to points out that the 64 scenarios lead to different solutions for decision variables, resulting in different stock levels. The first five periods show significant differences per scenario, as a result of the uncertainty in breakdown and ship delay in these periods (see Section 5.5).

Furthermore, since the first stage decisions are the same for all scenarios, the stock level at the start of period 2 is equal for all scenarios, as should be since decision variable values are the same for all scenarios in the first stage. For the presented business case, the first stage decisions of the two stage stochastic MILP are different from those in the average case behavior (Figure 7.2), as indicated by the difference in stock level at the start of period 2. This is a result of the optimization of expected rewards over all scenarios, instead of using a single scenario as is the case for the average case behavior MILP.

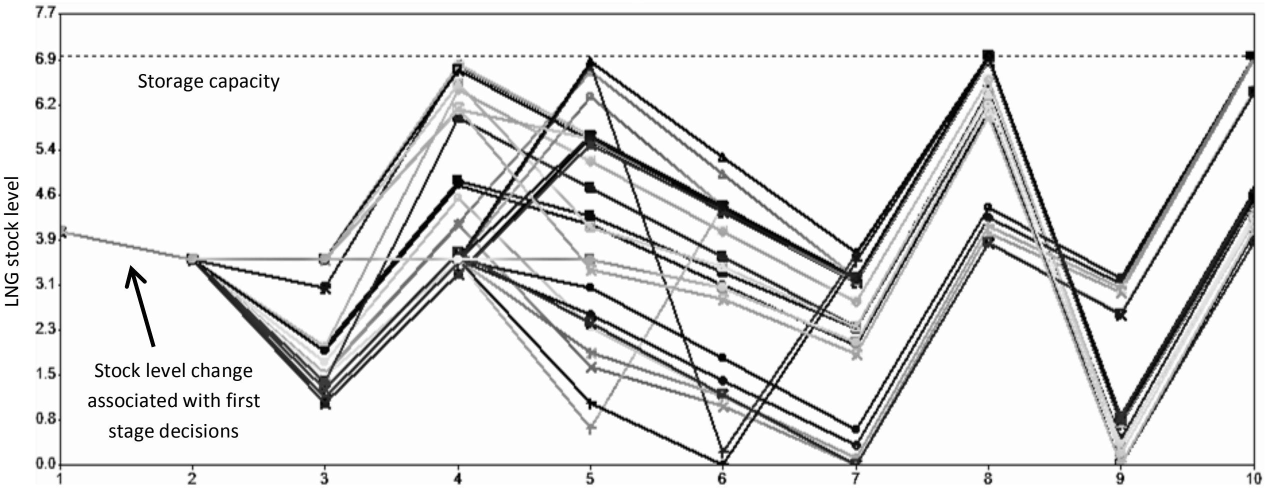


Figure 7.1 – Stock levels for all 64 scenarios of the two-stage stochastic MILP, to demonstrate the effect of using the two stage stochastic MILP (for definition of the business case, see Appendix A.1). The graph lacks a legend, since the figure is intended for qualitative instead of quantitative comparison with Figure 7.2

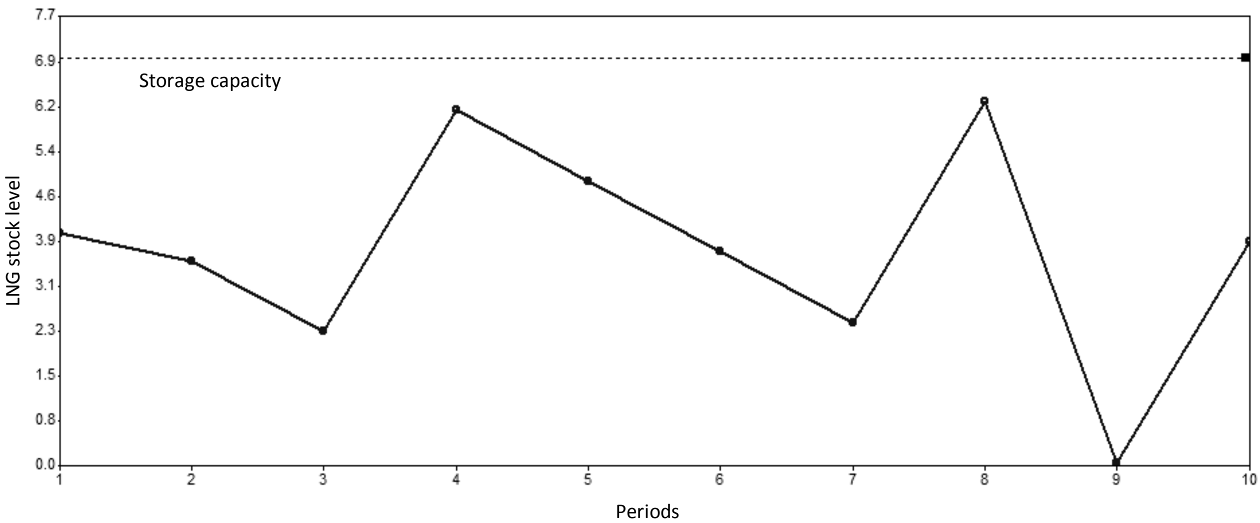


Figure 7.2 – Stock level for the average case behavior MILP optimization, applied to the same business case as was used for the results in Figure 7.2 (see Appendix A.1)

7.2 – Results in an operational setting

Unfortunately, we do not have data on the revenues and costs involved with the LNG business. Therefore, the business case we use for comparison of the models is based on arbitrarily chosen numbers. The absolute total revenues do not have any value, and no conclusions can be made upon them. However, the relative difference in results between the two models indicates that the Two stage stochastic MILP performs better in terms of mean total revenue than the Average case behavior MILP, as we would expect.

We now turn to results obtained by the evaluation algorithm that was presented in Figure 6.2, including multiple Monte Carlo cycles and a rolling horizon approach. We first present a validation of the model by means of extreme example with expected results that are known beforehand. If we omit uncertainty in the models, they should both obtain the same results (except for computational time). We use the input parameters as defined in Appendix A.2, and the following scenario probabilities:

$$\mathbb{P}(breakdown\ scenario\ is\ b) \qquad = 1 \quad \text{for } b = 1, \quad \text{and 0 otherwise,}$$
$$\mathbb{P}(ship\ delay\ scenario\ is\ d) \qquad = 1 \quad \text{for } d = 1, \quad \text{and 0 otherwise.}$$

In other words, no LNG train breakdowns occur and all ships arrive according to the ADP. We use a smaller sub horizon of $Y = \{1, \ldots, 5\}$. Table 7.3 shows the four KPIs for the two models in Figure 6.2. Since no uncertainties are involved, we can use a single Monte Carlo cycle ($I = 1$) since every sample of the stochastic process would be the same.

KPI	Two stage stochastic MILP	Average case behavior MILP
1. Mean total revenue	13,722 [$] (+0.0%)	13,722 [$]
2. Mean percentage of cargoes shipped	83.3 [-]	83.3 [-]
3. Mean LNG production	122.040 [V]	122.040 [V]
4. Mean Oil production	305.886 [V]	305.886 [V]
5. Mean computational time	12.23 [s]	0,44 [s]

Table 7.1 – KPIs for Two stage stochastic MILP and Average case behavior MILP applied to the same business, without uncertainties. A single Monte Carlo cycle ($I = 1$) suffices, since no uncertainties are involved.

If we now introduce uncertainty in LNG train breakdowns and ship delays, the models perform significantly different from each other. To show this, we again use the probabilities as defined in (7.1). The results of 500 Monte Carlo cycles are presented in Table 7.2. As we would expect, the stochastic model performs better than the average case behavior MILP. Both the mean total revenue as well as the mean percentage of cargoes that are shipped are higher for the two stage stochastic MILP. However, computational time increases drastically for the scenario based two stage MILP, due to the large number of variables and constraints that are involved with such a model.

KPI	Two stage stochastic MILP	Average case behavior MILP
1. Mean total revenue	10.039 [$] (+12.93%)	8,889 [$]
2. Mean percentage of cargoes shipped	70.0 [-]	65.7 [-]
3. Mean LNG production	103.22 [V]	97,03 [V]
4. Mean Oil production	300.74 [V]	294.85 [V]
5. Mean computational time	64.48 [s]	0,51 [s]

Table 7.2 – KPIs for Two stage stochastic MILP and Average case behavior MILP applied to the same business case, with uncertainties involved (see Appendix A.1). We used $I = 1000$ *Monte Carlo iterations.*

Mean total revenues have decreased for both models, since uncertainties in LNG train breakdowns and shipment delays are now present. The most important result is the difference of 12.93% in revenue between the models, partially due to a larger number of cargoes that were shipped on average. Note the increase in computational time for both models, and in particular the significant increase for the two stage stochastic MILP due to the inclusion of 64 scenarios.

As mentioned, Monte Carlo simulation is based on the strong law of large numbers. Therefore, we must be sure to use enough simulation cycles to capture system characteristics. We therefore visualized the mean total reward versus the number of cycles, as depicted in Figure 7.3. The figure clearly shows that the value is stabilized around its mean for the included 1000 cycles. If this was not the case, a larger number of cycles should have been used.

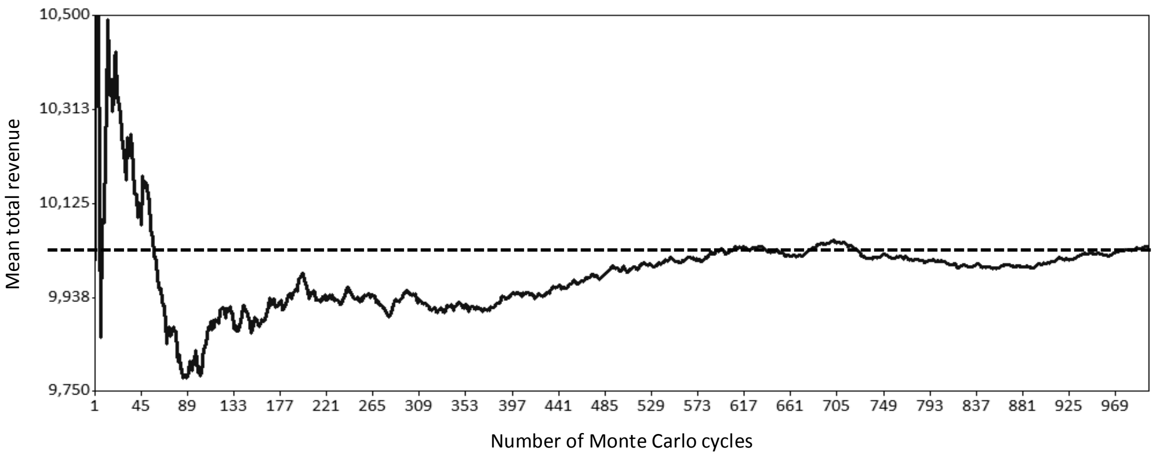


Figure 7.3 – Mean total revenue versus the number of Monte Carlo cycles to illustrate convergence of the KPIs

Generally, a storage tank can be seen as a buffer in a production system subject to uncertainties in production and demand [48]. Therefore, we would expect a decrease in difference between the two models if we increase the storage capacity, since the effect of uncertainties decreases. In the previous case the storage tank capacity ($L^{max} = 7$) was slightly more than the size of a cargo ($d_c = 5, \forall c$). If we increase (double) the storage capacity to ($L^{max} = 14$) and evaluate model performances by the evaluation algorithm to obtain the results as shown in Table 7.3. As expected, the mean total revenue has increased for both models due to the extra storage capacity, and the difference between them has decreased form 12.93% to 4.64%.

KPI	Two stage stochastic MILP	Average case behavior MILP
1. Mean total revenue	12,315 [$] (+4.64%)	11,769 [$]
2. Mean percentage of cargoes shipped	78.3 [-]	76.2 [-]
3. Mean LNG production	111.92 [V]	108.65 [V]
4. Mean Oil production	311.73 [V]	306.50 [V]
5. Mean computational time	48.72 [s]	0,41 [s]

Table 7.3 – KPIs for Two stage stochastic MILP and Average case behavior MILP applied to the same business case, with uncertainties involved (see Appendix A.1), and increased storage capacity ($L^{max} = 14$). We used $I = 1000$ Monte Carlo iterations

Chapter 8

Discussion, Conclusion and recommendations

In this thesis we have presented a proof of concept model for Asset Wide Optimization in Shell's LNG upstream value chain. We have shown that significant business value can be gained by integration of decision making in different assets of a value chain. Initially, a deterministic decision model was presented in Chapter 3. In the remainder we have focused on the added value of a stochastic approach that includes the risk associated with uncertainty in the model The three uncertainty factors we have addressed are LNG train breakdowns, shipment delays and spot opportunity arrivals. In the first chapter of this thesis, we presented three sub goals as well as an overall project goal. We now present our conclusion on these topics, based on our analysis. For every sub goal, we discuss our methods and present recommendations for future research.

(1) **Provide an overview of the LNG upstream value chain in terms of its assets, key parameters and potential conflicting objectives**

Chapter 2 provides a detailed overview of the assets of the LNG upstream value chain. It is important to note that an asset does not need to be a physical object such as a production facility, but can also for example refer to the set of long term contractual agreements that are contained in the Annual Delivery Plan. Therefore, besides wells, separation and liquefaction facilities and storage tanks, we also define the long term contract market, spot opportunity (or short term) LNG market and the oil market to be assets of the LNG upstream value chain.

The key parameters can be sorted in four different categories: (1) System properties, such as Gas to Oil ratio and impurity ratios of the wells. These are given and cannot be changed. (2) Technical restrictions, such as maximum production rates, and maximum (impurity) throughput at the LNG trains. These parameters could be changed, but involve major investments. (3) Contractual parameters such delivery windows, revenues and rejection costs, these parameters involve third parties. (4) Disruptive parameters, such as breakdown probabilities, shipment delays and spot opportunity arrivals. These parameters describe the uncertainties to cope with.

(2) **Examine to what extend uncertainty can be taken into account, to quantify and cope with the risks involved with the proposed decision model.**

We identified three main uncertainties in the LNG upstream value chain: (1) LNG train breakdowns, (2) Shipment delays and (3) spot opportunity arrivals. By adding these uncertainties to the model, we obtain a so called stochastic sequential decision making problem. In such stochastic controlling applications, Markov Decision Problem (MDP) theory is often an obvious starting point for optimization purposes, with its wide variety in theory and applications. However, finite horizon MDPs are generally solved by (discretization and) backward induction. This method has the nice property of having smaller sub problems that are solved iteratively. However, if large and/or continuous action and state spaces are considered, this method may lead to computationally intractable models if a fine discretization grid is applied, as discussed in Section 4.3.

For the DP counterpart of an MDP, so without the uncertainty in transition of a system, we proposed an equivalent MILP model that can be solved exactly. For such models, no discretization is necessary in case of continuous state spaces as these are replaced by continuous decision variables. We explored how we could extend this equivalence to models where uncertainty is involved. This is not straightforward, since for this type of problems the standard MILP solution methods such as simplex and branch and bound do not work in general. We discussed a set of different approaches to MILPs with uncertainty in model parameters in Chapter 5. The majority of the models in literature, such as the expected value method, does not take risks associated with stochastic parameters into account, but simply ignores it.

Our approach was to solve the MDP by approximation through a two stage stochastic MILP, which takes into account uncertainty in model parameters by means of a scenario tree. Instead of maximizing the total reward of a single deterministic instance of the problem, the objective function was defined as the expected total reward over all possible scenarios. Monte Carlo simulation showed the operational performance with respect to a deterministic model, defined as Average case behavior MILP. A schematic overview is shown in Figure 8.1 that summarizes our solution method.

Compared to backward induction, our method does not have the nice structure of smaller sub-problems being solved iteratively. For such methods, the computational complexity scales linearly with the planning horizon. Our MILP approach solves the problem for the full horizon at once, with the number of constraints and variables scaling linearly with the planning horizon such that computational complexity scales exponentially. Although the search for the 'complexity bound' between both models is an interesting topic for further research, we tackled the problem by introducing a rolling horizon approach that essentially only regards a small part of the full horizon to determine an optimal solution.

As expected, the two stage stochastic MILP outperformed its deterministic equivalent. However, the results show a significant increase in computational time for the two stage stochastic MILP. Given the low level of detail that was used in our analysis, computational time might become a major issue in extension of the model to an operational software tool. For example, we included only three wells in our model. At many production sites this number is multiple times higher (usually up to 10 to 100 times).

Our solution method can be generalized to finite horizon MDPs having large and/or continuous state and action spaces, it is not restricted to the LNG case. The set of constraints on the state transition and action variables of the MDP determines the type of equivalent mathematical programming problem that can be used to solve the problem. For example, suppose the set of constraints that defines the feasible actions in the MDP is linear. In other words, it contains only linear (in-)equalities and continuous unbounded variables. Such an MDP can be written as a pure Linear Program (LP) as no integer variables or quadratic constraints are required. If integer or binary action variables are involved with the MDP definition, the equivalent mathematical programming model is a Mixed Integer Linear Program (MILP) and if quadratic (in-) equalities are involved, we obtain a Mixed Integer Quadratic Program (MIQP).

(3) **Construct a mathematical framework to describe system behavior on an asset wide (global) level, to provide an operational (day-to-day) decision making model, preferably in a computer environment that is well-known to both ORTEC and Shell**

The Two stage stochastic MILP was implemented in a software package called AIMMS. This package is used by ORTEC and Shell for many optimization purposes. We also implemented the Monte Carlo simulation and rolling horizon approach that were presented in Chapter 6, to compare the performance of the models in a day-to-day operational setting. Numerical results showed that the stochastic model outperforms its deterministic counterpart, as we would expect.

The mathematical modeling framework fits well with the software knowledge at ORTEC, and enables future expansion of the model to an implementable software tool that is well known to all parties involved.

(4) **Deliver a proof of concept method for day-to-day decision optimization in Shell's LNG upstream value chain from an Asset Wide Optimization perspective. Furthermore, we aim to provide recommendations on further research to investigate the potential of an AWO approach and future tool development.**

Asset Wide Optimization is a promising field of research for application in Shell's LNG value chain. However, the presented level of detail in our model might not be sufficient for application to Shell's LNG production sites. We therefore strongly recommend additional research on the necessary level of detail and the associated computational feasibility, given the present-day computational possibilities.

Secondly, no real world data was available for this project and we strongly recommend the use of such data in future research on this topic. It would be most valuable to map the current decision making protocols to enable a fair comparison of proposed AWO models. Currently, we have no reason to believe that our approach outperforms the current decision making methods, as these are unknown to us due to confidentiality. Therefore, our AWO model should be considered no more than a proof of concept, showing the feasibility of an integrated decision making tool and the added value of including stochastic parameters to model uncertainties.

Furthermore, a site-specific model instead of a generalized approach could lead to better performance as each site possesses site-specific characteristics. For example, at one site the wells may show great differences in Gas-to-Oil and impurity ratios. In such a case, a detailed model on well characteristics is recommended. At a different site, the wells could all be very similar such that a detailed model is unnecessary. Aggregation of the wells might even be possible to lower the model complexity. Additionally, this latter production site might have a highly complex Annual Delivery Plan, with lots of different customers.

Site-specific models are recommended to be constructed in close cooperation with field experts and potential end-users, to ensure the practicability of the resulting software tool. Last but not least, heuristic methods could be identified to obtain sub-optimal but computationally fast decision making. Finally, we recommend additional research on complexity issues concerned with Asset Wide Optimization.

To summarize, we recommend to refine the proposed LNG upstream value chain model in terms of key parameters and level of detail, preferably in close cooperation with field experts and end-users. We recommend to start with a deterministic setting and a focus on capturing all important system characteristics. Here, A site-specific approach is recommended as it better captures the main factors and needs of the corresponding sites. The introduction of uncertainty is then rather straightforward by means of a scenario based approach, such as the two-stage stochastic MILP, as long as computational complexity is kept limited. Alternative (heuristic) modeling approaches could also be considered. Expert opinion, historical data and a fair comparison of model performance in an operational setting should play a central role in future projects.

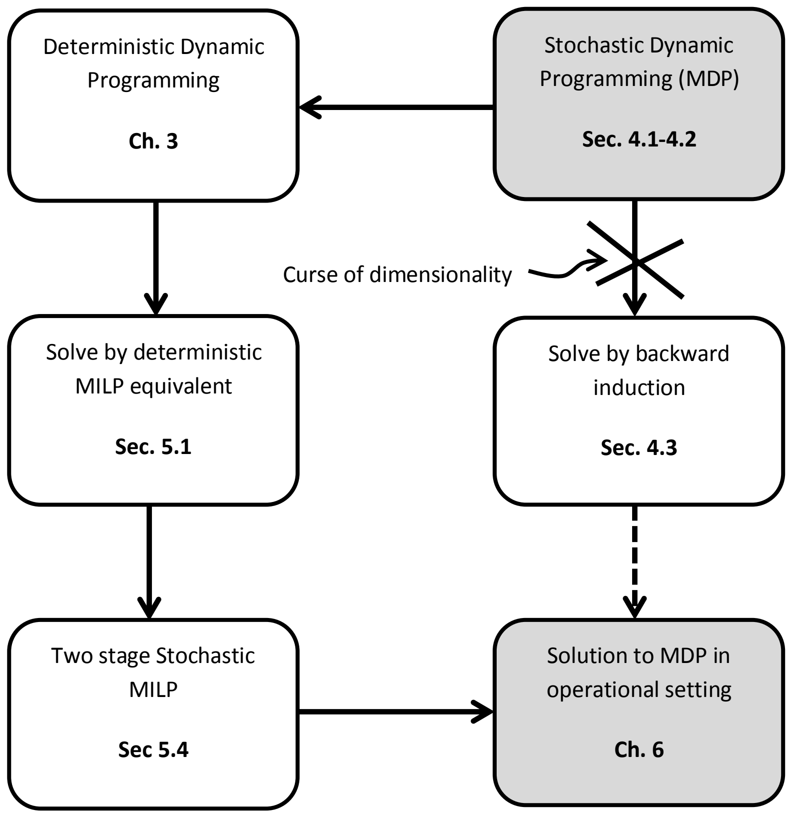


Figure 8.1 – Schematic overview of the solution route that was presented in this thesis. Starting in the right top corner, we were unable to solve the presented MDP by backward induction due to the curse of dimensionality. We then disregarded the uncertainties, to obtain a deterministic dynamic programming model that was solved by an equivalent MILP representation. This MILP was turned into a two stage stochastic MILP to cope with uncertainties. This model was used to obtain solutions to the MDP in an operational setting. The corresponding sections of the thesis are mentioned in bold font.

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Appendix

In this appendix, we provide the model parameters that make up the business case as used for the analysis presented in Chapter 7. We stress that the business case is purely imaginary. However, we have tried to set up a business case that captures most of the important system characteristics, such as differences in well properties, variability in ship arrivals and so on. Due to the absence of real data, we have no guarantee that the parameters represent real world behavior of the model. This should be validated in future research in Asset Wide Optimization.

Monte Carlo and Running Horizon parameters				
Number of Monte Carlo cycles	I		**1000**	[-]
Number of periods in a single Rolling Horizon optimization	$\|Y\|$		**5**	[-]
Total number of periods	$\|Z\|$		**30**	[-]
MILP parameters				
Number of wells	$\|W\|$		**3**	[-]
Number of LNG trains	$\|K\|$		**2**	[-]
Number of cargoes	$\|C\|$		**30**	[-]
Maximum production rate at well w	Π_w^{max}	$w = 1$	**8**	[V/period]
		$w = 2$	**5**	[V/period]
		$w = 3$	**4**	[V/period]
Fixed cost of well w change	c_w^{well}	$w = 1$	**25**	[$]
		$w = 2$	**30**	[$]
		$w = 3$	**20**	[$]
Initial production at well w	$\pi_{0,w}$	$w = 1$	**6**	[V/period]
		$w = 2$	**2**	[V/period]
		$w = 3$	**1**	[V/period]
Gas to Oil ratio (GOR) of well w	GOR_w	$w = 1$	**0.3**	[-]
		$w = 2$	**0.4**	[-]
		$w = 3$	**0.5**	[-]

Impurity ratio of well w	I_w	$w = 1$	**0.2**	[-]
		$w = 2$	**0.4**	[-]
		$w = 3$	**0.3**	[-]
Cost of flaring	c^{flare}		**15**	[$/V]
Oil price in period t	p_t^{oil}	$t \in \{1 \dots 9\}$	**25**	[$/V]
		$t \in \{10 \dots 20\}$	**50**	[$/V]
		$t \in \{21 \dots 30\}$	**25**	[$/V]
Maximum throughput of LNG train k	β_k	$k = 1$	**4**	[V/period]
		$k = 2$	**5**	[V/period]
Maximum Impurity throughput of LNG train k	γ_k	$k = 1$	**0.9**	[V/period]
		$k = 2$	**1.2**	[V/period]
LNG train breakdown probabilities	ρ_i	$i = 0$	**0.8**	[-]
		$i = 1$	**0.1**	[-]
		$i = 2$	**0.06**	[-]
		$i = 3$	**0.04**	[-]
Size of cargo c	d_c	$\forall c$	**5**	[V]
Maximum LNG stock level	L^{max}		**9**	[V]
Initial LNG stock level	L^{init}		**4**	[V]
Rejection costs of cargo c	r_c^{reject}	$\forall c$	**500**	[$]
Shipment delay probabilities	χ_i	$i = 0$	**0.6**	[-]
		$i = 1$	**0.15**	[-]
		$i = 2$	**0.15**	[-]
		$i = 3$	**0.1**	[-]
Cargo shipment revenues	$r_{t,c}$	See table A.1 on page 91		[$]

t/c	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	100	50	-	-	-	-	-	-	-	-	-	-	-	-	-
2	50	110	-	-	-	-	-	-	-	-	-	-	-	-	-
3	-	50	50	-	-	-	-	-	-	-	-	-	-	-	-
4	-	-	120	50	50	-	-	-	-	-	-	-	-	-	-
5	-	-	50	130	140	50	-	-	-	-	-	-	-	-	-
6	-	-	-	50	50	150	-	-	-	-	-	-	-	-	-
7	-	-	-	-	-	50	50	50	-	-	-	-	-	-	-
8	-	-	-	-	-	-	160	170	-	-	-	-	-	-	-
9	-	-	-	-	-	-	50	50	50	-	-	-	-	-	-
10	-	-	-	-	-	-	-	-	180	50	-	-	-	-	-
11	-	-	-	-	-	-	-	-	50	190	-	-	-	-	-
12	-	-	-	-	-	-	-	-	-	50	50	50	-	-	-
13	-	-	-	-	-	-	-	-	-	-	200	210	50	-	-
14	-	-	-	-	-	-	-	-	-	-	50	50	220	50	-
15	-	-	-	-	-	-	-	-	-	-	-	-	50	230	50

t/c	15	16	17	18	19	20	21	22	23	24	25	26	27	28	39	30
16	240	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
17	50	50	50	-	-	-	-	-	-	-	-	-	-	-	-	-
18	-	250	260	-	-	-	-	-	-	-	-	-	-	-	-	-
19	-	50	50	50	-	-	-	-	-	-	-	-	-	-	-	-
20	-	-	-	270	50	-	-	-	-	-	-	-	-	-	-	-
21	-	-	-	50	280	50	-	-	-	-	-	-	-	-	-	-
22	-	-	-	-	50	290	50	50	-	-	-	-	-	-	-	-
23	-	-	-	-	-	-	300	310	50	50	-	-	-	-	-	-
24	-	-	-	-	-	-	50	50	320	330	-	-	-	-	-	-
25	-	-	-	-	-	-	-	-	50	50	50	50	-	-	-	-
26	-	-	-	-	-	-	-	-	-	-	340	350	-	-	-	-
27	-	-	-	-	-	-	-	-	-	-	50	50	-	-	-	-
28	-	-	-	-	-	-	-	-	-	-	-	-	50	-	-	-
29	-	-	-	-	-	-	-	-	-	-	-	-	360	50	50	-
30	-	-	-	-	-	-	-	-	-	-	-	-	50	370	380	50

Table A.1 – Cargo shipment revenues. Columns denote cargoes and rows denote periods. All unlisted entries denote non-available delivery period, and so does the '-' sign.