

Logistics and Cost Analysis at CORE Chemistry

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Preface

Dear Reader,

Before you lies the thesis that I have been working on in my final year of bachelor's degree in Industrial Engineering and Management at the University of Twente. The research was undertaken at CORE Chemistry from February till July 2021.

At CORE Chemistry I had the pleasure of working with a young and dynamic team, who were great of help during the execution of this thesis. I would like to thank to Dirk van Meer for this opportunity, and a special thanks to him and Niels Bongers for providing me with all necessary resources and support. I would like to thank my company supervisor, Sander Nagelkerken for his valuable feedbacks and guiding me at all times.

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I hope you enjoy reading my thesis.

Ekin Korkut

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Management summary

This research has been performed for CORE Chemistry, Eindhoven. CORE Chemistry is a newly built start-up with no operating factories yet, and there is a need to base investment decisions on a systematic approach. To solve this problem the research aimed to provide CORE Chemistry with land, machinery, and material requirements of building a factory. The focus was on optimizing the resource requirements and associated costs. Main research question is formulated as follows:

How can the land, machinery, and material requirements of building an installation for complex waste streams at CORE Chemistry be estimated?

CORE Chemistry is a start-up built from a student team, Team CORE, from Eindhoven University of Technology (TU/e) and focuses on recycling waste on an industrial scale with their unique recipes to produce useful raw materials. Recipes of CORE Chemistry include 7 different wastes: pyrolysis residual, dusty material, sludge, shredder waste, fly ash, soil, and oil. These can be classified as slag, fuel and support material.

A context analysis was executed to understand and visualize the process of CORE Chemistry and its specific requirements. This was achieved by in-depth interviews with the management team. A business process model (BPM), followed by a value stream map (VSM) were created for the process of CORE Chemistry. By analysing the process, special characteristics of CORE Chemistry as well as the raw materials of the process were identified. The presence of recipes i.e. products that result from different mixes of input materials, unknown compositions of input materials, fluctuating yield rates and formation of co- and by-products all characterize the process of CORE Chemistry. These characteristics also play a role in the specific material requirements in terms of storage and different phases of the process. With the current system analysis, the organization was analysed further, and the scope of the research were alternated accordingly.

To assist CORE Chemistry's strategic decisions, a Mixed-Integer Linear Programming (MILP) model was created and integrated into a decision support tool to enable ease of use by the management team. The MILP model maximized the profit of the first year of factory by considering the most significant cost parameters only. The high value found with the initial parameters promised a positive profit in the first year of the operation of the factory. The model also provided CORE Chemistry with optimal waste amounts to produce, which waste to focus on and what storage to invest in as well as how many machines are required for the process. The most influential cost parameters were included in the model as not much is known about the process yet. For storage this was the area costs and for machinery this was the investment costs. The investment cost was described in terms of a depreciation cost that considers the initial investment, present value of the salvage value, and useful life of the machinery.

The results of the MILP model were analysed by means of a sensitivity analysis. The model was converted to a Linear Programming (LP) model and solved. This did not cause any significant shift from the optimal value function and the optimal values largely remained the same. The validation of this was done by assessing the new profit and the slight change in the optimal values of the decision variables. Precisely, the difference was the change in one decision variable multiplied by its cost parameter.

By applying the model and analysing it through a sensitivity analysis the following conclusions were drawn:

- Pyrolysis residual is very valuable whereas with the current parameters slag is not profitable to be included in the business portfolio. If an increase of 64 € is achieved by increasing the processing price, storage height or decreasing the storage time of sludge, it can be included.

- If more cost parameters are included in the model, the waste amounts, machine numbers and storage decisions will remain optimal as shown by the very high allowable optimization coefficient increase for the mixer.
- CORE Chemistry can make 128 € more profit with each unit increase on the waste capacity of the whole factory.
- As the allowable right-hand side on the energy balance constraint is relatively high, this shows that more slag former waste can be added to the process with the current fuel waste amounts. As more slag will result in more products this can have a positive effect on the profit of CORE Chemistry.

Based on the research for CORE Chemistry, main recommendations were as follows:

- In order to calculate the optimal land, machinery, and material requirements of building a CORE Chemistry factory, it is recommended to make use of the user-friendly DST built upon the MILP model. It is essential that the data are kept updated to keep the model valid and useful.
- If CORE Chemistry desires to include sludge in their business portfolio, then work must be done in terms of increasing the value sludge brings. This can be achieved in several ways: by having different supplier arrangements and higher processing prices, increasing the height of the storage for sludge, acquiring cheaper drying installation, or lowering the storage time for sludge.
- As more is known, CORE Chemistry is encouraged to test the model with better data estimations to get results closer to reality. Including more cost parameters can also increase the validity of the model.

It was advised to CORE Chemistry to validate the model by updating the input parameters as more is known. More realistic results can be achieved this way and enable CORE Chemistry to make profitable decisions

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Reader's guide

Along the seven chapters, the research performed at CORE Chemistry is described. Chapters are shortly introduced in this section.

Chapter 1: Introduction

An introduction to the research is given in the first chapter. Firstly a background on the company is provided, followed by a short description of the process. This is then followed by problem identification and problem cluster constructed for CORE Chemistry. The core problem of the research is mapped and related problem-solving approach with research questions are introduced.

Chapter 2: Context Analysis

The organization is studied more in depth by conducting interviews with the management team. The process and its requirements are described. The process is mapped by business process mapping (BPM) and value stream mapping (VSM). Specific characteristics of CORE Chemistry are identified.

Chapter 3: Theoretical Framework

Literature review is conducted on mathematical modelling on the process industry. Firstly, process industries are introduced, followed by operations research work and literature scope in this industry. Capacity planning problems are discussed, and batch process designs are introduced.

Chapter 4: Model Development

The resource problem of CORE Chemistry is described by a Mixed-Integer Linear Programming model that considers storage, capacity, and chemical requirements. The constraints are described in detail/

Chapter 5: Model Analysis

This chapter includes the case study on CORE Chemistry by using the developed MILP model. Initial parameter inputs are identified and validated. This is followed by a sensitivity analysis on the MILP model by converting it to a Linear Programming (LP) model.

Chapter 6: Design of Decision Support Tool

The decision support tool (DST) designed for CORE Chemistry is introduced in this chapter. The user interface, characteristics, and requirements of the tool are briefly discussed.

Chapter 7: Conclusions, Recommendations and Future Research

Conclusions with regards to the research are given. Recommendations to CORE Chemistry are provided by using the results of the research. Possible future research directions are also highlighted.

List of abbreviations

APICS American Production and Inventory Control Society

APEX Atmospheres Explosibles

BPM Business process modelling

CAPEX Capital Expenditure

CO Carbon monoxide

CO₂ Carbon dioxide

DDP Discretization Decoupling Point

DST Decision Support Tool

GDP Gross Domestic Product

LOI Letter of Intent

LP Linear Programming

NLP Non-Linear Programming

NO_x Nitrogen oxides

MILP Mixed-Integer Linear Programming

MINLP Mixed-Integer Non-Linear Programming

MPSM Managerial Problem Solving Method

OR Operations research

PoC Proof of concept

RHS Right hand side

SiO₂ Silicon dioxide

SSMBP Seven-Step Model-Building Process

TU/e Eindhoven University of Technology

VBA Visual Basics for Applications

VSM Value stream mapping

Glossary of terms

Compound The waste recycling factory, also referred to as chemical plant of CORE Chemistry. Used interchangeably with factory and plant.

Logistics flow Flow of materials from arrival to the factory, till the oven process.

1 Introduction

This section introduces the bachelor thesis conducted at CORE Chemistry. The research aims to assist the factory building process of CORE Chemistry by giving analytical insight to resource requirements through modelling cost and logistics. Section 1.1 introduces the company, Section 1.2 outlines the problem identification, Section 1.3 introduces the research question of this thesis, Section 1.4 provides an overview of the research design.

1.1 Company background

CORE Chemistry is a start-up built from a student team, Team CORE, from Eindhoven University of Technology (TU/e), and focuses on recycling waste within industrial production plants. They are aiming to create a circular solution for complex waste streams through the elementary retraction technique. With this technique, waste streams that are currently burned or dumped could be recycled and converted into useful raw materials achieved at lower prices. CORE Chemistry focuses primarily on three streams: contaminated soil, e-waste, and industrial residual flows.

In the national and global context, the need for processing options for waste streams is growing. With an estimated waste of 2.2 billion tons of contaminated soil (Hoornweg & Bhada-Tata, 2012), 50 million tons of e-waste (PACE, 2019), and 10 million tons of industrial residual flows per year worldwide, the demand for a sustainable and affordable alternative to process these residual flows is high. This waste currently ends up in landfills or needs to be burned. Companies within the market are required to transport their waste to the companies listed in the Full Load List (Vollast Lijst in Dutch) to be. If this is not, they are challenged to take care of significantly high exported costs for transporting it abroad.

CORE believes in a world where problems of improperly treated waste streams are non-existent. With the CORE Chemistry technology based on elementary retraction, CORE offers its customers the option of disposing of this waste which in return is cheaper than the currently realized techniques. The process is based on the elementary retraction technique which draws its inspiration from the earth itself. Waste that drops to the ocean floor, sinks into the core of the earth where it is heated up and falls apart back into its pure elements. Eventually, it ends up on top again after millions of years through natural processes (*Vision CORE*, 2021). CORE is adapting this process on an industrial scale through their unique recipes to produce useful raw materials from waste streams.

1.1.1 The process

The uniqueness in the process comes from the combination and specific mixing of energy-containing waste flows with slag-forming flows in the oven installation. Melting takes place at a very high temperature, up to 1450°C. This causes metals to melt or vaporize and plastics to incinerate. As a result, three layers are formed, gas, slag, and metals. The gas layer consists of Carbon monoxide (CO), Carbon dioxide (CO₂), and Nitrogen oxides (NO_x) which are produced by organic contaminants falling apart into their constituent elements. The slag layer is formed through the addition of Silicon dioxide (SiO₂) to the mixture and once it cools down rapidly slag turns into obsidian. After melting, the metals form a third layer under the slag and can be separated using specific techniques. Output from this process, obsidian and basalt can be used within the infrastructure and garden market as the raw materials of end products.

Testing of this procedure is done through the pilot oven installation with residual flows supplied by HKS Steel, ATM, and Pouw Group, which are all committed to CORE by a Letter of Intent (LOI). Tests for the outputs have been carried out with initial buyers of CORE, NTP Groep using obsidian as a coating for roads, and ProRail using the process output as durable basalt.

CORE Chemistry is working towards building chemical compounds, which refers to the factory/plant of CORE Chemistry, that will realize the above-mentioned process on an industrial scale. As of right now, the whole process is accomplished and tested through pilot installations of the machinery and

laboratory experiments. Within project FENIX a pilot installation is built in the harbor of Delfzijl. Currently, this installation is non-operational and expected to process 30.000 tons of waste per year starting from the year 2022. According to the planning of two more compounds in the harbors of Moerdijk and Amsterdam, the pilot installation is expected to be taken on a larger scale with 100.000 and 120.000 tons of waste, respectively, being processed.

1.1.2 The team

CORE Chemistry works in collaboration with Team CORE and brings their innovative ideas into the real-world, where it is translated into factories and production. Team CORE takes part in the process of building a factory through assisting basic engineering¹ and detail engineering². The student team is also responsible for developing new technologies to the Proof of Concept (PoC) level and promoting CORE. The lead in basic engineering and detail engineering is taken by CORE Chemistry as well as the arrangement of financial plans, recruitment, and assisting the factories in the technical field. At the moment, Team CORE has 24 engineers working on 11 different sub-projects. These engineers are connected with the management team of CORE Chemistry which consists of 4 members.

1.2 The problem

This section outlines the problem identification at CORE Chemistry. Section 1.2.1 introduces the problem context with initially identified action problems, Section 1.2.2 provides more detailed problem identification. Section 1.2.3 introduces the core problem. Section 1.2.4 gives the norm and reality.

1.2.1 Problem context

Visits to the company in Eindhoven resulted in good insight into the process of CORE Chemistry. After the initial interviews with the management, three action problems within CORE are identified which provided a basis for further investigation. In this section the initial problems are discussed.

Non-operational compounds

CORE Chemistry is a newly built start-up with no operational compounds. The projects are mostly in the detailed engineering phase and not yet translated into factories. Not yet achieving the industrial production level is one of the reasons CORE is not in the market yet. This shift is crucial as it can only be done once CORE compounds start operating. This brings the first and the main action problem that is delivered by the management of CORE Chemistry.

Project delays

As discussed with the management, there have been significant project delays due to unforeseen reasons. This can be linked to non-operational compounds, as technical and management delays cause the shift to the industrial production level to be postponed. If everything goes according to plan, CORE aims to start production in its pilot-compound in the year 2022 after the constructions are finalized. However, up until now most of the planning is not followed and the management is concerned that project activities will not be executed within the planned time frame. Project delays follow from this.

High investment requirement

There are initial drawbacks to realizing a unique business idea and transforming this to industrial production level. Project IVER³ accounts for a Capital Expenditure⁴ (CAPEX) of 10 million euros with a processing rate of 30,000 tons of waste per year. Project Tambora⁵ accounts for a CAPEX of 25 million euros with a processing rate of 120,000 tons per year and Project Yellowstone⁶ with a CAPEX

¹ Basic engineering entitles the translation of ideation to a basic outline, with initial financial plans and visualization of the project.

² Detail engineering entitles system integration plan for all equipment as well as control system fully designed. In this phase, there should be arranged investors with contracts ready for building.

³ Factory operated by IVER BV in Delfzijl, detailed engineering phase.

⁴ Funds used by an organization to acquire physical assets. (Fernando, 2021)

⁵ Factory operated by Tambora BV in Amsterdam, concept development phase.

⁶ Factory operated by Yellowstone BV in Moerdijk, concept development phase

of 17.5 million euros with a processing rate of 100,000 tons per year. CORE Chemistry significantly relies on private investors, funding from banks, and funding from TU/E.

1.2.2 Problem identification

After getting introduced to the above problems communicated by the management of CORE, further investigation revealed more problems within the organization. A problem cluster is constructed to map the relationships between problems and eventually arrive at the core problem. Considering the three main action problems, high investment requirement, project delays and non-operational compounds, the problem cluster visualizes the causal links between identified relevant problems, depicted in Figure 1. These were decided by interviewing stakeholders and were confirmed with the management.

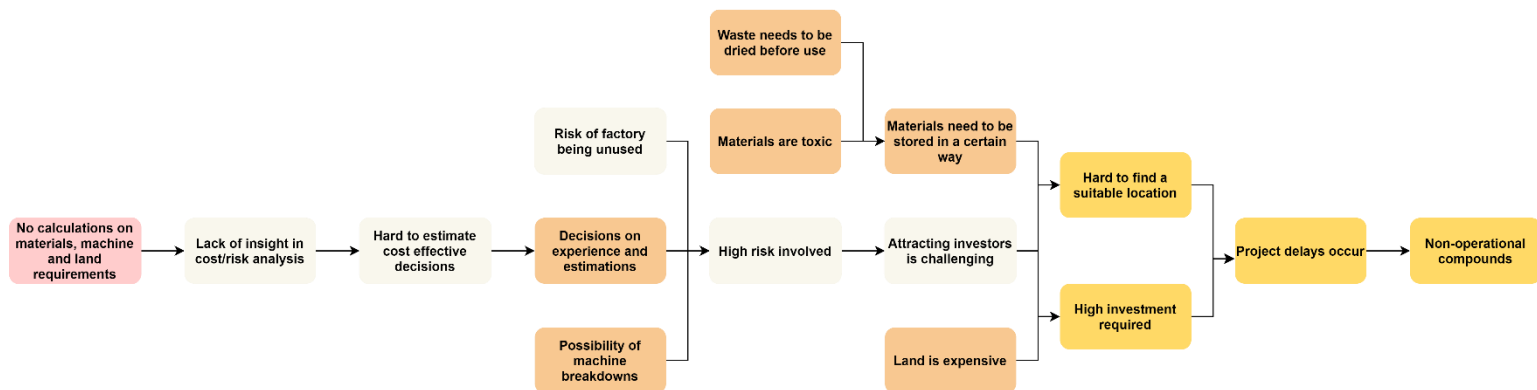


Figure 1: Problem Cluster for CORE Chemistry

With the required high investments to build and operate a compound, and what is available at the moment through private investors and funds, CORE is still in the process of attracting investors. Not reaching the CAPEX requirement of projects inevitably plays a role in the project delays. Before reaching this investment level, it is not possible for CORE to start production at an industrial level.

There are several reasons for the high investment requirement of realizing the CORE technology at an industrial level. Compounds must be located strategically, close to waste material suppliers, and within a good transport zone. Harbors within the industrial zones of the Netherlands are ideal in this case, as through the harbor goods can be transported and the compound is located close to the demanding market. Land prices and competition in these areas are high.

Some of the waste material is hazardous and some need to be dried before it can enter the process in the factory. Therefore, special storage compartments are required, and this waste needs to be stored separately for some time being. This also directly increases the investment required as it creates the need for extra measurements and extra storage.

CORE works with existing technologies that have been used within a different market on an industrial scale, however, interfaces between different processes and mixing formulas of waste streams are newly developed. This is the main risk involved in the process, and consequently, it is hard to attract investors. Besides the pilot-installation in Delfzijl, other projects in CORE are still in search of investors and no agreements have been made yet. Therefore, the initial high investment requirement is a big obstacle and challenges CORE to find suitable investors willing to take the risks involved without witnessing concrete proof on an industrial level.

The high risk involved in the process is also closely related to the possibility of machine breakdowns, as once reached industrial level the complexity of the process will increase accounting for unexpected machine breakdowns. Once the pilot installation is operating, the management estimates that only 50%

of the time operation will go smoothly in the first year, causing half of the estimated waste to be processed.

As compounds are not yet operational and the process is not realized in an industrial level, handling of input and output flow of the process, as well as storage, is not dealt with yet. Consequently, there is also the risk of the factory being unused if more space than required is reserved. Reversely, the same case occurs if too little space is available. This also influences the overall high risk.

At the moment, the management bases most of their decisions on experience and estimations. As many complex cost decisions are involved in the process of realizing a compound, it is hard to estimate the most effective decisions. This challenge is an indication that the management does not hold any insight into the cost risk analysis of building an installation. It was found out that there were not any calculations about materials, machines, and land requirements of building an installation.

1.2.3 Core problem

By following the chain of problems that have no direct cause themselves, potential core problems are identified (Heerkens & van Winden, 2017). As it can be seen from Figure 1, there are four problems that have no direct cause. Three of these problems, namely, land is expensive, waste materials are toxic, and waste needs to be dried before use are non-influenceable within the context of this research.

Problems about the waste material cannot be influenced as CORE technology and unique recipes are revolving around these materials. Moreover, not much can be done about the nature of these materials, they were chosen by CORE after careful research and experiments, and there is a good market for them. Location is also non-influenceable as locating the compound in cheaper regions will attach extra costs in the long term such as transport because of being farther from the market.

In this regard and by consulting the company, no calculations on materials, machine and land requirements can be treated as the core problem. By solving this, the other problems in the chain can be solved as well. The following problem is selected as the core problem of this research:

There are no calculations on materials, machines, and land requirements.

1.2.4 Norm and reality

The core problem is used to arrive at the action problem, which according to definition occurs when the reality deviates from the norm (Heerkens & van Winden, 2017). Norm and reality are defined in this section.

As further investigation revealed, the management of CORE bases all their cost decisions with regards to materials, machines, and land requirements on educated guesses. However, the management would like to adopt a systematic approach, where these decisions can be based on logical calculations. This deviates from the norm, and brings the action problem as follows:

At CORE Chemistry, cost decisions are based on educated guesses whereas it should be based on a systematic approach.

1.3 Research question

Following research question is formulated which aims to solve the core problem of this research: *How can the land, machinery, and material requirements of building an installation for complex waste streams at CORE Chemistry be estimated?*

1.4 Research

In this section, the research design for the bachelor project is outlined. Section 1.4.1 focuses on problem approach with methodologies that are used and sub-research questions. Section 1.4.2 outlines the research design for each sub-research question, Section 1.4.3 highlights the related deliverables. A

discussion on validity and reliability in Section 1.4.4, followed by scope and limitation of research in Section 1.4.5 is given.

1.4.1 Problem approach

In this research Managerial Problem-Solving Method (MPSM) (Heerkens & van Winden, 2017) is used as the main methodology to solve the action problem and is complemented with the Seven-Step Model-Building Process (SSMBP) (Winston, 2004) to correctly formulate a suitable model. As MPSM is a general method which can be applied to various scenarios (Heerkens & van Winden, 2017), it gives the research a good structure, whereas the SSMBP tailors the approach to the problem-context of this research. There are overlaps between two methodologies, however SSMBP focuses on model development and has specific phases dedicated to this. The two methodologies are chosen to guide the research in a systematic and content-specific way.

To answer the main research question and consequently solve the identified core problem, for each step of MPSM except for step 1 which guided the research, sub-research questions are generated. These questions are formulated by following the seven-steps of MPSM and guided by the steps of SSMBP.

The first step of MPSM and SSMBP, defining the problem, has already taken place as the action problem within CORE is identified with the initial investigations, a problem cluster is constructed, and the core problem is chosen. The core problem is used to arrive at the action problem as stated above. All this information is achieved through interviews and approved by the organization.

The problem analysis step of MPSM firstly involves observing the system step of SSMBP. An analysis of the current system of CORE Chemistry is taken place. This is essential as the whole process within the factory including the requirements of the process and organization can be established. Following sub-research question is answered at this stage: *How can the logistics of building an installation be mapped for CORE Chemistry?*

To discover different methods that are used to support decision making, the current system analysis is followed by consulting literature to find related theory on the topic by answering the sub-question: *What methods/tools are there in literature to support organizations in decision making for resource allocation in the process industry?*

After analysing the problem, MPSM guides the research to formulating solutions phase, where based on literature findings a suitable method is chosen and developed. In this step of MPSM, formulating the mathematical modelling step of SSMBP will take place. Following sub-research question guides this phase of the research: *Based on the literature, how can a model be designed to be implemented in the process of CORE Chemistry?*

As CORE Chemistry is a newly launched start-up, not much data about the process is available and this might lead to data generation or estimations later in the project. Data investigation is tackled with the following research question: *What data is required for implementing the model and is available within the organization?*

As with the designed model, there is the possibility of evaluating different outcomes with respect to resource allocation and attached costs. As a continuation of the solution formulation and initiating choosing a solution step of MPSM, the following sub-research question is investigated: *Based on the developed method, what are the most profitable decisions for CORE in terms of resource allocation?* By answering this question, the model verification step of SSMBP is completed as well.

Solution implementation and evaluation is tackled together, to give recommendations on future implementation of the chosen alternative and draw conclusions. This is addressed with the following sub-research question: *What conclusions and recommendations can be drawn from this research conducted for CORE Chemistry?*

By answering this question, suitable alternatives and conclusions is also established.

1.4.2 Research design

In this section the research design of sub-research questions that are formed based on the problem approach is addressed. A schematic representation of the research design for each sub-research question can be found in Table 12 in Appendix A: Schematic overview of research design per research question.

1. *How can the logistics of building an installation be mapped for CORE Chemistry?*

This sub-research question is answered by conducting qualitative research and is descriptive in nature, where a current system analysis is conducted for CORE Chemistry. Consequently, the processes that are involved, required machinery and material flow in the future factory is mapped.

Firstly, logistics flow, defined in this research as the material flow starting from when waste materials enter the compound till, they reach the oven installation, is visualised using process mapping. First of all, a high level process map where processes are mapped at an aggregate level (Slack et al., 2016) is done. This is followed by business process mapping (BPM) and value stream mapping (VSM).

The research study is deep qualitative, and the data is collected through a series of individual in-depth interviews with the management team of CORE. Their responses are a valuable input to the research as the process is a unique creation of CORE. The interviews are organized either via Microsoft Teams or during compound visits. As specific information is required from the management team, the interviews is structured with predetermined questions. Grounded Theory is consulted for the interviews, in which analysis of data takes place simultaneously (Cooper & Schindler, 2014). Each subsequent interview is adjusted based on findings from the previous interviews.

When needed, primary sources, namely documentations of the company is consulted as the organization has permitted access to every document in their drive files.

2. *What methods/tools are there in the literature to support organizations in decision-making for resource planning in the process industry?*

A literature study is conducted to find out methods that support organizations in decisions revolving around resource management. The literature review focuses on mathematical modelling in the process industry. Following sub question will be answered by consulting literature.

a. *What mathematical modelling/optimization techniques are there in literature to guide organizations in the process industry for resource planning and cost estimation?*

The research is descriptive in nature and aims at identifying possible modelling techniques that could be relevant to the research. Collected data is qualitative and assessed with a systematic literature review. Academic databases such as Scopus, Web of Science and Business Source Elite is consulted to find papers. Search queries are constructed using key terms, synonyms and introduced concepts from relevant papers. The found literature is studied in-depth to provide an answer to the sub-research questions. The papers are chosen with regards to their relevancy and date of publication.

3. *Based on the literature, how can a model be designed to be implemented in the process of CORE?*

Based on the findings from previous research questions, a solution method for the core problem of CORE Chemistry is developed using an explanatory research. The relationships between variables is studied and objective function as well as constraints are established. This is done in incorporation with the management team, as they are the relevant stakeholders. A model is developed and programmed using Python, solved with Gurobi Optimization Solver. A clear and simple user interface is added.

4. *What data is required and available for implementing the methods?*

Due to little documentation and being a new organisation, there is not a lot of data available and necessary data needs to be extracted from what is available and when missing, from literature. In this exploratory research, the first step is highlighting required data as identified with the literature review. Then quantitative data about waste quantities and breakdown of costs is collected by consulting primary sources, such as company documents. When data is missing, the management team is contacted. If no conclusions can be reached, data generation techniques are considered. In later stages, sensitivity analysis is conducted to test the validity of data that are not taken into consideration.

5. *What are the most profitable decisions for CORE in terms of resource allocation?*

With the developed model an exploratory research takes place where experiments are conducted to test different scenarios. What-if analysis are done to identify the changes in the outcome if certain assumptions are changed (Hillier & Lieberman, 2010). Sensitivity analysis is conducted to determine the sensitive parameters of the model and an overall validity analysis is made (Hillier & Lieberman, 2010, Winston, 2004).

6. *What conclusions and recommendations can be drawn from this research conducted for CORE Chemistry?*

With this final sub-research question, a descriptive research design is established. Conclusions are drawn, and recommendations are given to CORE with regards to answering the main research question. A brief discussion on relevance of the model and reliability of the research are done.

1.4.3 Deliverables

This section highlights the deliverables of the bachelor project. Following are delivered at the end of this research, linked to the sub-research questions discussed previously.

- 1 Process map of the logistics flow
- 2 Theoretical framework regarding decision making, mathematical modelling and resource/cost allocation
- 3 Solution method that determines the land, machinery, and material requirements as well as costs associated with building a compound as well as a decision support tool
- 4 Results of data analysis within the organization
- 5 Results of sensitivity analysis
- 6 Recommendations and conclusions of research

1.4.4 Validity and reliability

In this section the validity and reliability of the proposed research design are discussed. According to Saunders et al. (2019), validity and reliability are two aspects to consider when assessing the quality of research design. Firstly, validity of the research design is discussed, followed by the reliability.

Validity refers to the rightness of the measures in research design as well as accurate analysis of results and generalizability of research findings (Saunders et al., 2019). There are three types of validity: measurement, internal and external. Within measurement validity, the major threat arises from high dependence on interviews. As the research is done with an organization that is newly entering the market with their unique solution to industrial residual flows not a lot of previous research is available within the field. As a result, the organization itself is the main information source. Therefore, questions should be constructed very carefully and on to the point.

The main deliverable of the bachelor project is a model that gives analytical insight into the material, land, machinery, and cost calculations and is based on estimations and not on a real factory. There is also the possibility of missing data and data generation might be required during the research. These can threaten the internal validity, as it is difficult to assess whether the model can be applicable to the real world. This threat can be found in many modelling studies and can be mitigated by sensitivity

analysis. Different scenarios are assessed with this technique, and suggestions on the different cost solutions is provided to the organization. Sensitive parameters are also discovered using sensitivity analysis, to inspect if missing data has any effect on the overall performance.

The research is not intended for the creation of a general model that could be used in other cases. Therefore, external validity is not as important. As the process is unique and not practiced before, the model and relationships in the model as well as data available might be unique to the process of CORE Chemistry. Therefore, it is challenging to generalize it as it is very case sensitive.

Reliability refers to the consistency of research design (Cooper & Schindler, 2014). A possible threat to reliability comes from relying on interviews for collecting information. Interviews are always conducted with the management team, and different members of the team have different perspectives or wishes. Therefore, when the same questions are asked, different answers are received. Also, throughout the project, available information as well as answers of management are prone to change depending on the phase their projects are at. To ensure that reliability is maintained, interview questions are structured and confirmation after findings of the interview are done with the management.

1.4.5 Scope and limitations

The research is restricted to the logistics of compound building at CORE Chemistry. Chemical processes involved, waste material compositions and the activities that take place after the oven process are not in the scope of this project. In Chapter 2, schematic representation of this is given in Figure 2. The research involves only the operations within the plant. The supply network as well as transportation of goods are not a point of consideration. The research is bounded to design and logistics of a single plant and can be used for different locations as desired by the organization. The developed model aims to be a general decision tool for resource planning and cost requirements when CORE Chemistry would like to open factories in various locations.

CORE Chemistry holds different waste recipes, however due to confidentiality issues dummy recipes are provided by the organization to be used in the model. These dummy recipes are used to test different scenarios and in the future the organization can use the model with their real recipes.

There are certain limitations to the problem solving and research approach. First of all, the research is bounded to a time frame of 10 weeks and due to this a good planning is required. The lack of documentation and data is a limitation to the research as well and arise validity issues as discussed previously. This is minimized by conducting sensitivity analysis and data generation when necessary.

Currently, the unique waste management process by CORE Chemistry is only practiced in a pilot level. As there are no compounds yet, once the process is taken on an industrial level there can be problems not accounted for. This needs to be taken into consideration as it is a limitation to the research design which is based on the pilot installation. There is also not much research with regards to operations research in this specific industry. Validation of the model is possible through consulting experts and comparison to real world is not possible as the first compound of CORE Chemistry is not finished before the end of this project.

2 Context analysis

In this section, context analysis at CORE Chemistry is presented by answering the first sub-research question:

How can the logistics of building an installation be mapped for CORE Chemistry?

The information in this chapter is primarily obtained via in-depth interviews with the management team.

Section 2.1 describes the process in a hypothetical CORE factory in detail as well as the materials and their specific requirements. In Section 2.2 the process is mapped using business process modelling, followed by value stream mapping in Section 2.3.

2.1 The process in detail

The CORE process is uniquely established by CORE Chemistry and combines energy-containing waste with slag-forming flows and metals. The industrial residual flows supplied by different suppliers, are combined together in a special oven, and heated up to 14.500 degrees Celsius. The mixture is heated up electrically or with burners, and once a certain temperature is reached the waste that is added to the mixture reacts and produces additional heat. The chemistry process is based on elementary retraction, the earth system of recycling its residues. The CORE process is achieved by miniaturization and acceleration of this system.

Slag former, fuel and support material with oxygen is combined in the oven installation. At the end of the process, three layers are formed. First layer consists of gases. At the relevant temperatures, the organic contaminants fall apart back into their constituent elements, which are oxidized. Various gases are produced due to this, such as CO, CO₂, Oxygen (O₂), Methane (CH₄) and Hydrogen (H₂). According to the recipe different combinations of these gases arise during the process. These gases are treated in a separate gas washing installation. These installations are located in the factory but not developed by CORE.

The second layer is the slag layer which is formed by the addition of SiO₂. Contaminants such as silicon and oxides are absorbed through the slag layer. The viscosity is crucial for easy transportation of the slag layer and achieved by balancing acidic and basic components. The acidic materials contribute to having a more structural slack and are capable of forming large bonds. The basic materials on the other hand do not allow the formation of large bonds by destroying them, hence contributing to the viscosity of the slag. After the slag is cooled down rapidly, the slag becomes amorphous and forms the obsidian output of the process.

After melting, a third layer below slag is formed: metals. Various alloys are formed. After melting, the metal layer can be separated. The metal is very small in quantities that it can be considered negligible, and no extra action needs to be taken.

After the waste is transported with trucks from several suppliers to the compound, they are stored either in a silo, shed or tank. Silo storage is done by large tubes and enable longitudinal storage requiring less surface space. They are approximately 1,5 times more expensive than shed storage and suitable for materials that do not require drying because there is no air-circulation in a silo. Certain residual flows require pre-treatment before they can be used in the oven installation, namely mixing, and drying.

There are seven types of industrial residual flows CORE Chemistry currently focuses on in their recipes. These are fly-ash, shredder waste, pyrolysis residual, polluted oil, dusty materials, sludge, and polluted soil. This waste can be distinguished as slag former, fuel and support material. The slag former is used to form the slag, and these with the fuel are the waste streams that need to be treated. As a certain level of viscosity is essential, support materials help with balancing this.

Fly ash - fuel

Fly ash which is supplied by AEB Amsterdam, Eneco Golden Raand and HV Alkmaar, is generated when coal is combusted for energy production (Ahmaruzzaman, 2010). It is an industrial by-product generated by power, and incineration plants that operate with coal (Zacco et al., 2014). The supplier plants of fly ash focus on producing heat and electricity from biomass and municipal waste. CORE uses biomass fly-ash that is produced as a result of thermal conversion of biomass, this is supplied by Eneco Bio Golden Raand and HVC Alkmaar. The fly ash supplied by AEB Amsterdam is a product of recycling of municipal residual waste and classified as municipal solid waste fly ash.

Fly ash contains high amounts of SiO_2 and CO_2 , which are essential substances in the CORE process. It is very dusty, basic and also contains toxic materials. Therefore it should be stored in a closed room with a roof and impermeable floor. It is transported in closed trucks and pumped into the storage tanks of CORE.

Sludge - slag former

Supplied by Waterboard Rijn & Issel, Amsterdam and De Dommel, the sludge is a product from water treatment plants. Once the water is treated, it is polluted with a high level of organic materials. CORE takes on these materials and uses in their recycling process. In most cases, the sludge needs to be dried due to containing high amounts of water before it can enter the process. Leftover heat from the oven is used for this system. Ideally, the process takes place by popping the sludge slowly out of the storage tank and placing it in a long line where it dries off. The sludge has a drying time of 1 week.

Polluted soil - slag former

Polluted soil is supplied by A. Jansen BV and POUV Group. This material needs to be dried before it can be used in the process, therefore is constrained to a drying time. The drying time is inversely proportional to the height of the soil. If it is stored flat then it will dry quicker, however then this also increases the required space. The drying rate can also change overtime depending on the season. During colder seasons drying rate is slower. Shed storage is preferred for soil.

Pyrolysis residual - slag former

This is the most toxic waste stream, and it is highly dusty. It does not require special treatment and can be fed to the system immediately. ATM material is residue from the pyrolysis operation, it needs to be stored in an inside storage because of weather conditions and the smell. The storage must have an impermeable concrete floor. The transportation of this material can be done through conveyor belts as it is not dusty.

Shredder waste - fuel

This stream consists of the following materials, HRK-G, HRK-V, pellets, and sludge. They can be delivered separately by the suppliers, A. Jansen, HKS Tiel and HVC Alkmaar. It is possible to combine different shredder material or store them separately to be used separately in the process, this depends on the recipes involved.

Dusty material - slag former

This stream consists of vezels, filtermix, Plastic M and Plastic D. It is supplied by HKS Tiel. These materials are very dusty and need extra precautions. They are flammable and can carry a static charge. In order to prevent the risk of dust explosions they need to be stored in vertical silos and with fire protection systems. The transportation of this material is through pumping in closed tubes, otherwise most of the material will be lost due to dustiness. When handling dusty material, ATEX (EU explosive atmosphere regulations) must be followed.

Polluted oil - support material

Polluted oil is a support material and is added to the mixer. This material is used to enable easier transportation of dusty material as it makes it more viscous.

2.2 Business process model

In this section the logistics flow in the CORE compound is visualised using business process modelling (BPM). The model is created through the information provided by the management team with in-depth interviews.

The waste material is transported with trucks from different suppliers located close to the compound. This waste is firstly dumped from the trucks in the unloading area and taken to the storage places. Different waste streams need to be stored separately as they have specific requirements (See Section 2.1). Depending on the waste stream, they are stored in silo, shed or tank storage. Sludge which can be stored in a tank or shed, is then taken to drying installations where drying takes place. After this point the waste streams are transported to the mixer where oil is added as well for dusty material. After the mixing operation, the combined waste material is transported to the day bunker. The day bunker creates a buffer of supply in case a bottleneck occurs in the previous process, and hence the process after can still run continuously at least for a day. The material is taken out from the day bunker and gets transported to the oven installation where the chemical process occurs. Operations after this, as highlighted with lighter grey are out of the scope of this research. In this part of the process the gas layer coming out is treated in a gas washing installation, the slag layer is dumped to the casting installation and in most cases the metal layer is very insignificant to be treated.

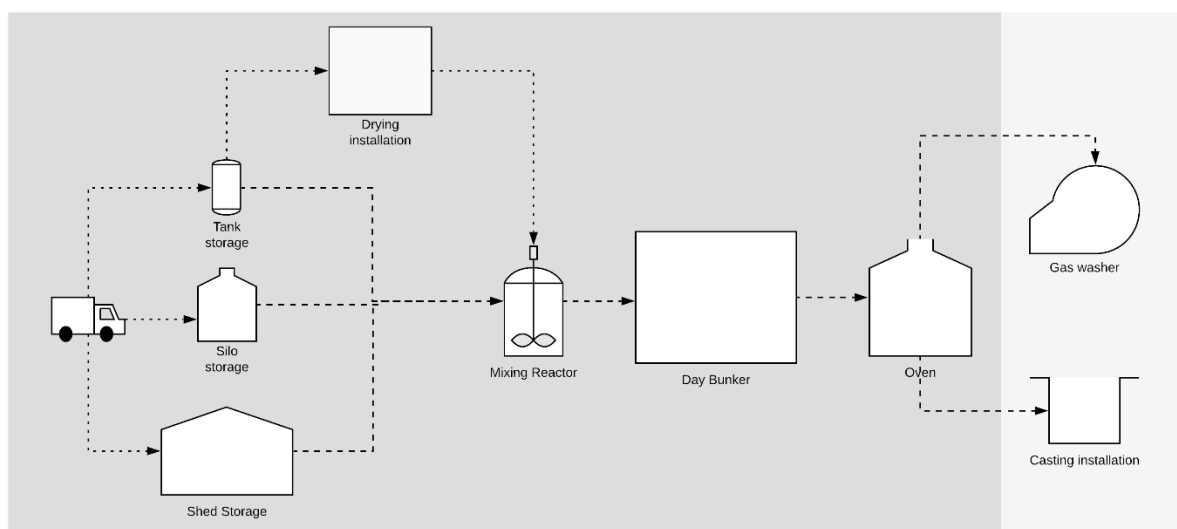


Figure 2: Visual representation of the factory process at CORE, scope of this project highlighted with dark.

Figure 2 is a visual representation of the above explained process in the factory. There can be multiple tanks, silo and shed storage and a variety of numbers of mixers. Different waste streams have different methods of transportation depending on the material type. Dusty material is removed from the trucks using a pneumatic system and pumped using screw conveyors in the factory. The other materials are transported using conveyor belts. This visual representation is used to create the business process model in Figure 3

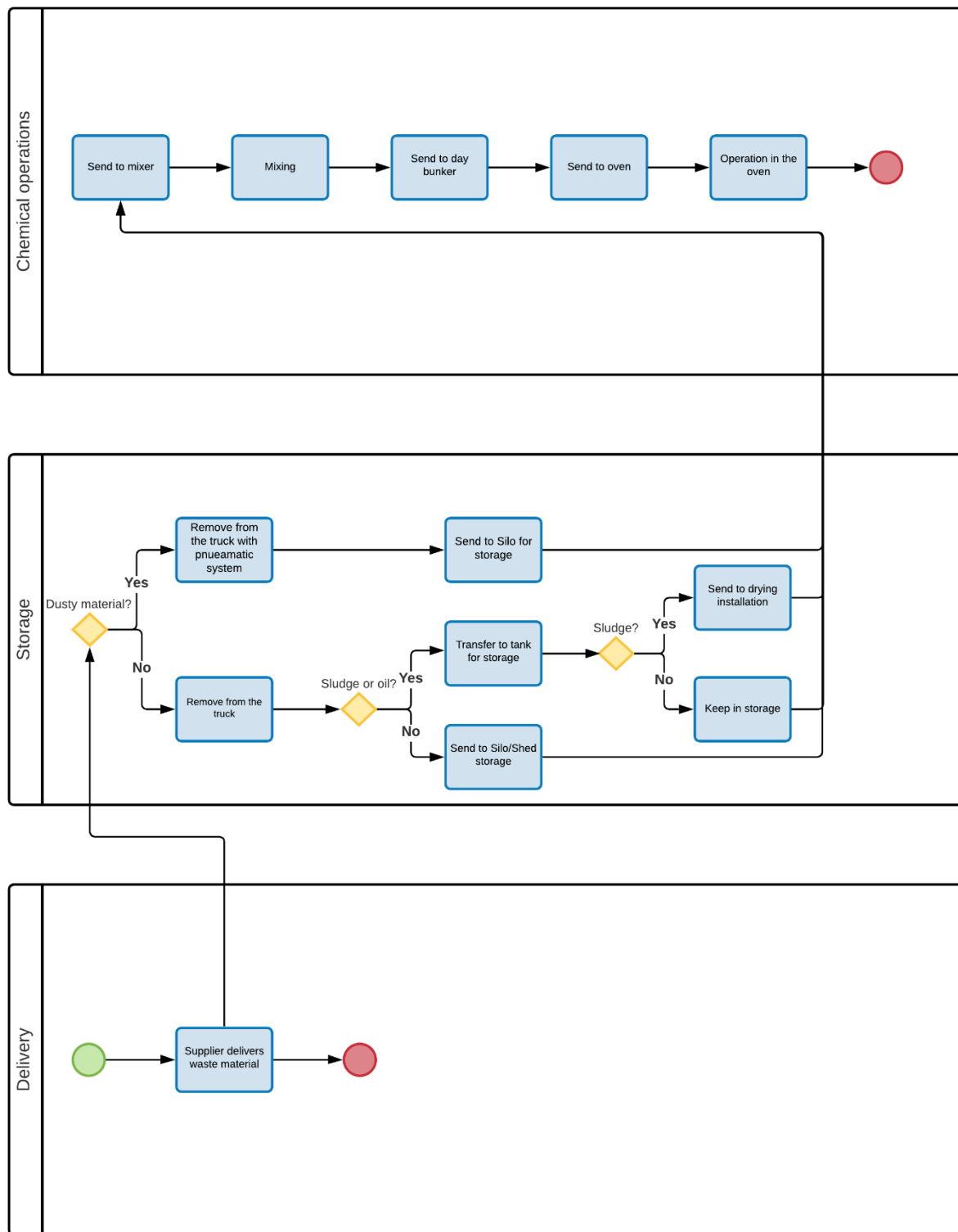
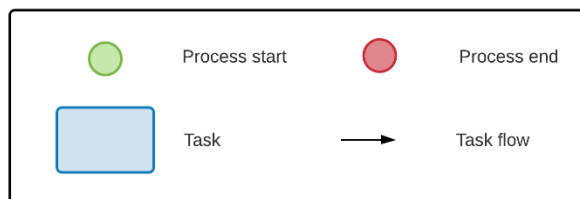


Figure 3: Business process model for CORE Chemistry



The activities in the compound are divided into three main groups, depending on the operation. Next, these are discussed briefly.

Delivery

The delivery occurs when a truck arrives from the supplier to the compound. There are two different types of deliveries, waste streams and other supply material. The delivery of other supply material depends on the compositions of the incoming waste streams and is not always necessary. If the slag material cannot meet the specific requirements, then the addition of these material to the process is necessary.

Storage

The process starts with checking if the material is dusty. As discussed in Section 2.1 these are fly ash and the dusty material waste stream containing vezels, filtermix, Plastic M and Plastic D. The dust is known upon delivery. It is included in the model to represent the different flow of incoming waste streams. These waste streams need to be removed from the trucks to the storage using a pneumatic system. Non-dusty materials are dumped from the truck to the storage area. Sludge and oil are supplied inside tanks and these tanks are emptied into the tanks of CORE.

The sludge needs to be dried with special drying installations before it can enter the process. The other material that requires drying, soil, can be dried in storage and does not require special treatment.

Chemical operations

The chemical operations consider the processes starting with mixing till reaching the oven. Materials that are mixed are sent to the day bunker and stored there for one day. After this point they are taken into the oven. As discussed with the management, the processes followed by the oven installation are out of the scope of this research and therefore not presented in the BPM.

2.3 Value stream mapping (VSM)

A more detailed overview of the material flow in the CORE compound is created by using value stream mapping (VSM). Firstly, a brief background on value stream mapping is provided in Section 2.3.1. This is followed by the Value Stream Map created for CORE Chemistry in Section 2.3.2.

2.3.1 Introduction to value stream mapping

As introduced by Rother & Shook (1999), a value stream considers all the operations that add value and non-value to the product, bringing the product through the main flows of the logistical activities. It is defined as the process of observing flows of information and materials, and visually representing these flows (Brunt, 2000). As a processing mapping tool, VSM can guide organizations in improvement as well as highlighting communication and flow of the different operations that form the whole process.

As identified by Rother & Shook (1999), value stream mapping is a qualitative tool that helps visualize multiple process level and makes decisions about the logistical flow apparent for discussion. Therefore, it is a good tool for representing the logistical process in a CORE factory in more detail. It enables the observation of material flow from the moment it is transported to the factory of CORE Chemistry till the end of the oven process.

VSM is a tool that enables the implementation of lean approach (Forno et al., 2014). lean approach, a concept driven by the Toyota Production System, has been widely studied and adapted by different organizations, as a methodology that eliminates waste and meets customer needs (Hines & Taylor, 2000). Implementation of Lean Approach allow organizations to adjust the various stages of an operation through continuous improvement (Álvarez et al., 2009). According to Slack et al. (2016), the focus of lean is achieving a flow of materials in perfect quality, exact quantity and when needed with the lowest possible cost.

2.3.2 Mapping the logistics flow

A VSM is created for the logistics flow of CORE Chemistry and can be seen in Figure 4. After the process is mapped on a general level through the BPM, more information added using the VSM methodology, in which cycle times of each main process are calculated, and inventory times in between are shown. The logistics flow is mapped until the oven process and the production processes that take place such as casting, energy recovery and gas cleaning are not included in the map as they are not considered in the scope of this research.

Several constraints are communicated from the management team about the compound:

- The maximum capacity of a compound is 120,000 tons of waste processed a year and the minimum capacity is 100,000 tons of waste processed a year.
- It is expected that the compound is in operation 320 days in a year.
- The process is continuous with 24 hours operating in a day in 6 hours long shifts.

Each process as represented in the VSM, namely unloading, drying, storage, mixing, day bunker and oven are discussed in this section with the cycle time calculations.

Unloading

The unloading process happens right after the waste is transported to the compound from the suppliers. At 120,000 ton/year and 320 days operational, 375 tons/day are processed in the compound. This translates into 10 trucks a day as a truck can transport at most 50 tons and least 25 tons. The average of this is taken to calculate the average amount transported by a truck, which is 37.5 tons.

The unloading process approximately takes 30 minutes (mins) per truck. This means 30 mins are spent to unload 37.5 tons of waste. Cycle time per ton of waste is calculated accordingly:

$$\text{Cycle time of unloading} = \frac{\text{Unloading time per truck}}{\text{Average number of tons per truck}} = \frac{30}{37.5} = 0.8 \text{ mins/ton}$$

Drying

This process is only relevant for certain waste streams and the cycle time varies accordingly. The drying time of sludge and soil are estimated to be 1 week.

$$\text{Drying time soil, sludge} = 1 \text{ week}$$

Storage

The minimum storage time of waste material takes 4 days in the shed, silo, or tanks. Usually, this time is 10 days. In the Value Stream Map this is shown with the inventory icon in between unloading and mixing.

Mixing

Mixing occurs after the drying or storage of materials and takes one day. The cycle time is dependent on the restriction of 120,000 tons a year of waste processed in the factory. Based on this, with 320 days operational, 375 tons a day are processed. As the operation takes 24 hours the cycle time is calculated accordingly:

$$\begin{aligned} \text{Cycle time of mixing} &= \frac{\text{number of mins in a day mixer is operational}}{\text{number of tons of waste processed in a day in the mixer}} = \frac{24 \times 60}{375} \\ &= 0.384 \text{ mins/ton} \end{aligned}$$

Day bunker

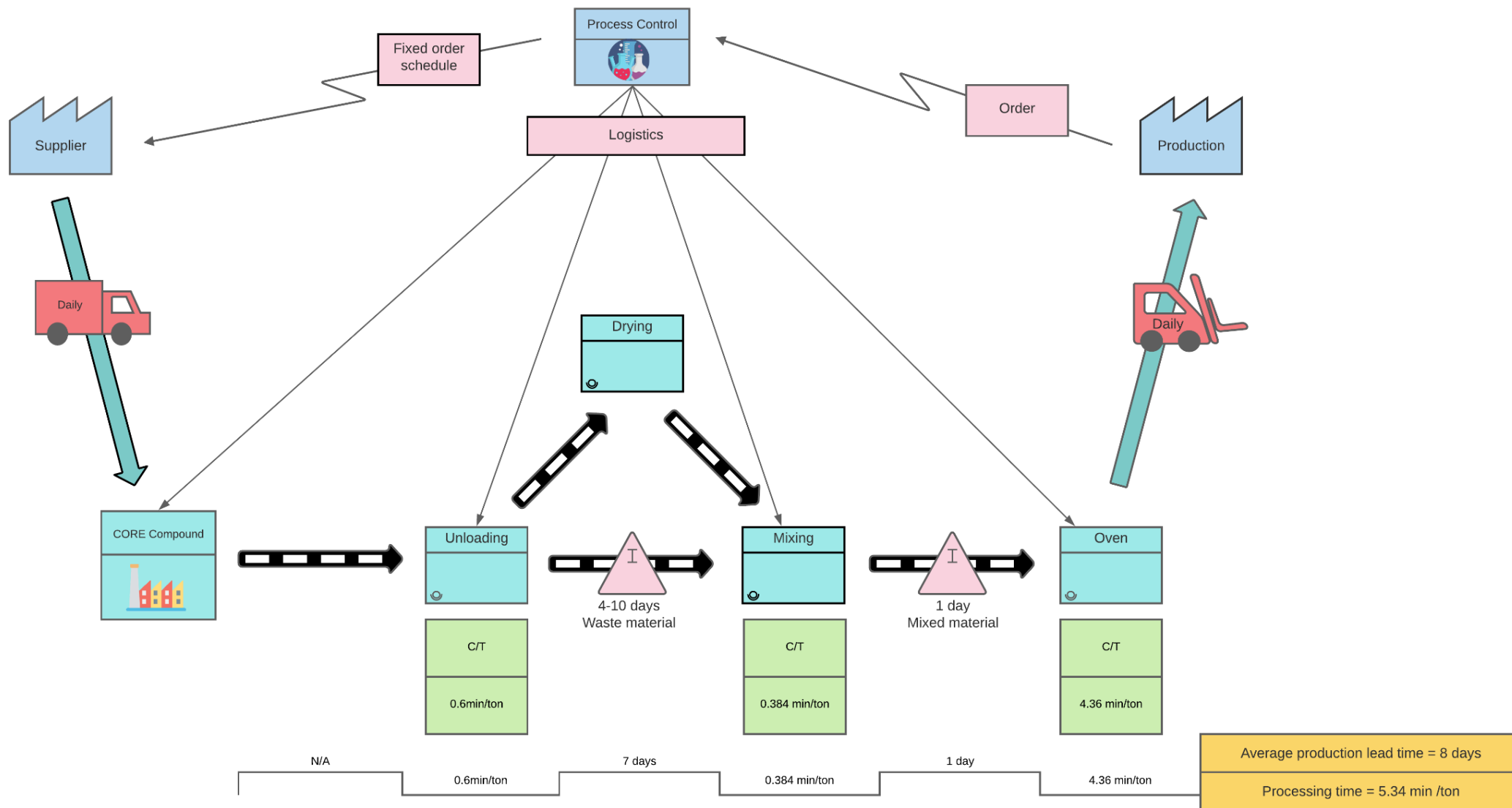
After the mixing, the mixture is kept in the day bunker for a day. This process is shown in the Value Stream Map with the inventory icon in between mixing and the oven process.

Oven

The Oven process is a continuous feed with a batch unload size of 330 tons of processed waste every day. This means 330 tons are processed in 24 hours. The cycle time is calculated accordingly:

$$\begin{aligned} \text{Cycle time of oven} &= \frac{\text{number of mins in a day oven is operational}}{\text{number of tons of waste processed in a day in the oven}} = \frac{24 \times 60}{330} \\ &= 4.36 \text{ mins/ton} \end{aligned}$$

Figure 5: Value Stream Map for CORE Chemistry



3 Theoretical framework

This chapter focuses on the related literature on mathematical modelling for resource planning. It aims to provide an answer to the main research question:

What methods/tools are there in the literature to support organizations in decision-making for resource planning in the process industry?

This main research question of this chapter is tackled by answering the sub-research question on mathematical modelling. As the main focus is on the process industry, the sub-research question is altered to be narrowed down to this industry. The following sub-research question is answered in this chapter with a literature review.

What mathematical modelling/optimization techniques are there in the literature to guide organizations in the process industry for resource planning and cost minimization?

Current system analysis enabled the placement of CORE Chemistry in the process industry. Further research in the literature is narrowed down to this industry as it is directly applicable to CORE Chemistry and more case specific information can be reached. Firstly, the process industry is introduced in Section 3.1. This is followed by a literature review on operations research in the process industry in Section 3.2. Lastly, batch process designs are discussed in Section 3.3 and other relevant literature in Section 3.4.

As a result of problem identification and proposed research questions, the research that will be conducted will focus on the estimation of resource requirements, namely land, machinery, and materials. As CORE would like to base their cost decisions on a systematic approach this can be done by adapting an OR approach. After introduction to the process industry, literature review on operations research and mathematical modelling in the process industry and additional related models are presented.

3.1 Process industries

Process industries can be categorized as types of organizations that add value by mixing, separating, forming or performing chemical reactions (Noroozi & Wikner, 2017). As defined by American Production and Inventory Control Society (APICS), these processes require maintained process control and high capital investment. Characteristic operations of process industries, mixing, separating, chemical reactions, are done to achieve non-discrete products or materials with large and costly installations (Fransoo & Rutten, 1993).

It is possible to make a distinction between organizations in the process industry depending on their nature of production systems. As identified by Kallrath (2002), this distinction can be made between continuous production systems and batch production systems. Fransoo & Rutten (1993) place this distinction on two extreme production systems, namely flow production and batch production. Depending on the demanded quantity, either batchwise or continuous production is adapted. Slack et al. (2016), defines batch processes as processes that produce more than one item at a time with parts of the processes having repeatable periods and continuous processes as processes that operate in an endless flow, enabling the smooth flow of material or products from one part of processes to another. These definitions can be supported by the definitions for process/flow and batch/mix from APICS, which highlight short production runs for batch processes and minimal interruptions in production runs for flow processes. In certain processing systems both extremes can be adapted, resulting in semi-continuous or semi-batch processes (Kallrath, 2002b). In general, the process industry includes a wide spectrum of businesses such as petrochemical industries with continuous production, steel and glass manufacturing organizations with large batch production and food and pharmaceutical industry with small batch productions (Van Donk & Fransoo, 2006).

In traditional literature, process industries are considered to be focusing on a single entity with straight characteristics (Noroozi & Wikner, 2017). However in most organizations in the process industry, this is not the case. Characteristics are not as straight forward, as discussed by Abdulmalek et al. (2006) process industries are referred to as being continuous however in most cases they are hybrid. The non-discrete products become discrete at a point in the process, and this is referred to as point of discretization by Abdulmalek et al. (2006), whereas in other literature it is classified as discretization decoupling point (DDP) (Noroozi & Wikner, 2017).

CORE can be placed in the process industry, as the operations in the chemical plant are established through mixing of materials followed by chemical reaction in the oven. The process flow is continuous and results in non-discrete products until the point after the oven installation. With casting and gas installations, the process turns into a discrete production process and can be referred to as the point of discretization (DDP). In Section 3.1.1, a detailed overview on the characteristics of process industries and further discussion on how CORE Chemistry holds these characteristics are given.

Characteristics of process industries

Flapper et al. (2002) identify main characteristics of process industries as follows: uncertain composition of input materials, alternative recipes, variable yield, production of co- and by-products, limited storage capacity and time limitations in storage. Further discussion on these characteristics as supported by different literature follows.

In a variety of process industries, deficits occur in the end product due to unknown compositions of input materials (Flapper et al., 2002). This so-called input problem is expressed further by Kılıç (2011), through the variable quality of the raw materials supplied for the process. Mainly the process industry obtains their input from mining and agricultural industries, and as a result the raw material inputs have natural variations in quality (Fransoo & Rutten, 1993). As the yield or variance is not known beforehand, it could happen that the supplied raw materials do not have the desired composition to result in specific end product qualities. It might be the case that reordering of raw materials is necessary, or additional material is required. Even though the supply does not originate from mining or agriculture, this also holds true for the case of CORE Chemistry as the waste material compositions are not known until a sample is tested from the supply. In case compositions do not meet specific requirements, additives for the reactor, namely CaO and CaCO₃ might be necessary for the reactor. Due to variations in the composition of waste material having a safety stock of the additives might be necessary. As suggested by Fransoo & Rutten (1993), if safety stocks are established in consideration with how frequent these variations occur, flaws can be minimized.

It is commonly seen in the process industry that products can be a result of different mixes of different ingredients, called recipes (Flapper et al., 2002). The recipes include different compositions of materials with specifying different production steps (Kılıç, 2011). As process industries are based on a low number of raw materials, in certain productions it is possible to alternate between different products. CORE Chemistry owns different recipes that hold different combination or composition of the waste streams. In case of shortages from one supply, production can still continue to a certain point by alternating between different recipes. Decisions on which recipes to focus on needs to be made by considering the cost outcomes, seasonal changes, and availability of materials.

Fluctuating yield rates could occur in certain steps in a process operation (Flapper et al., 2002). As mentioned by Fransoo & Rutten (1993) these steps could result in complicated production scheduling and occur due to the nature of the process. As for CORE Chemistry, it is expected that this variety occurs in the casting installation and gas treatment section with energy recovery and gas scrubbing. Although the inputs are known, the output and the amount are not certainly studied by CORE. Even though these steps are left out of this research, it supports the placement of CORE in the process industry and therefore are mentioned.

Often in process industries, when producing one specific product other products are also generated. If they are included in the business portfolio, they are referred to as co- and if not as by-products (Flapper et al., 2002). It is expected that there will be a small amount of metal produced during the process of CORE Chemistry, and it can be sold to third parties depending on the amount in the incoming feeds, therefore it can be classified as co-product. The gas layer from the process is combusted to generate steam and can be used to provide electricity for oxygen production or can be sold to adjacent companies. In both cases, the gas is also seen as a co-product.

3.2 Review on operations research in the process industry

In this section a brief introduction to operations research (OR) in the process industries are given. Very little work has been done so far with regards to OR in the process industry. Even though the process industry contributes greatly to the Gross Domestic Product (GDP) in most countries, operations research is not given significant attention to in this industry (Van Donk & Fransoo, 2006).

The first contribution to the operations research field in the process industry is done by Taylor et al. (1981), in which process industries are distinguished from fabrication and assembly industries. These differences are tackled by the need of production and inventory management systems specific to process industries. This is followed by more research on the specific characteristics of process industries, however the shift has focused on the differences within process industries rather than differences between process and manufacturing industry (Van Donk & Fransoo, 2006). As discussed in Section 3.1, Fransoo & Rutten (1993) distinguish between two extremes of process industries: flow and batch process industries. They argue that all process industries can be placed on a spectrum limited by these extremes. Also supported by Kallrath, (2002), these distinctions demonstrate that there is a great variety within what is traditionally referred to as a single entity, the process industry.

Before diving into the previous OR work done in the process industry, it is relevant to first give a definition of OR. As defined by Winston (2004) *operations research is a scientific approach that decision making seeks to best design and operate a system, usually under conditions requiring the allocation of scarce resources.* Many definitions of OR exist underlining the involvement of a scientific method alongside analytical methods and mathematical models to assist organizations in their decision making (Dyson et al., 2021). Winston (2004) describes the scientific approach to decision making as usually constituted by mathematical modelling. OR is applied to problems that concern how to operate activities within an organization by allocating available resources to various activities in a cost-effective manner. OR emerged from the military context and was initially applied already during World War II, when a team was devoted to resolve air defence problems. It was later on used for optimization and stock management, when it was introduced to the modern world with the Wilson formula (Réveillac, 2016). Today OR is regarded as a *decision support tool*.

The operations research field within the process industry context is mostly tackled in terms of planning and scheduling. According to Kallrath (2002), distinguishing between planning and scheduling is often not feasible, and there are strong overlaps in scheduling and planning in production, distribution or supply chain management and strategic planning. In planning problems, previous work mostly discusses production, distribution, sales and inventory plans based on demand. In the literature, mostly time-indexed models for multi-period analysis are tackled. Detailed schedules are formulated which aim to outline the timing and the sequence of activities in an operation, as well as assigning resources (Kallrath, 2002b). In the work of Neumann et al. (2002), where the focus is on the production section of the supply chain, long-term decision regarding network design with facility location problems, mid-term decisions for plant requirements formed from demand and short-term allocation of resources over time are treated.

Strategic level

There are three distinct levels of planning in operations: strategic, tactical and operational (Hax & Candea, 1984). Literature on Operations Management distinguishes tactical and strategic capacity

planning in terms of time horizon. Benedito et al., (2016) differentiates between strategic and tactical not in terms of this, but in terms of whether assets are given or need to be decided in the decision problem. Strategic decisions may be forced to be taken in a short amount of time, and thus differentiating between strategic and tactical in terms of time is not always feasible. (Martínez-Costa et al., 2014).

Quantitative methods, particularly mathematical modelling have been widely used to guide decisions on tactical or operational levels. Solving a strategic capacity problem brings along a variety of decisions that need to be quantified and that are subjected to complex conditions. A mathematical program can guide as a tool to support decision making and is an appropriate way to express the objective and constraints. operations research problems in process industries are mostly tackled with Linear Programming at the tactical level (Taylor et al., 1981). As suggested by Martínez-Costa et al. (2014) applications of mathematical modelling on strategic level should also be addressed in research, as these decisions can have a greater impact on the result on the research. Process industries have distinctive characteristics (Section 3.1.1) and as discussed by Dennis & Meredith (2000) process industries require production planning and control processes that match with these characteristics. Process industries fall behind in the implementation of OR techniques that match with their specific characteristics, mostly in the strategic and tactical level (Noroozi & Wikner, 2017). Most work in literature tackling the strategic decision level in the process industry occur in combination with operational or tactical decisions. This brings a need to tackle strategic decision issues in the process industries.

In the work of Kallrath (2002) strategic and operational decision levels are combined with a Mixed-Integer Linear Programming model based on a time-indexed formulation. Strategic level is studied from a supply chain design perspective with expansion, opening and shutting down decisions of plants. The model, like many in this field, defines a lot sizing and scheduling problem considering a time window.

In capacity planning literature, most mathematical modelling for strategic decision-making deals with capacity expansion in terms of sizes, types, location as well as scheduling capacity expansion, and replacement of equipment. In the work of Norton & Grossmann, (1994) strategic planning is studied with capacity expansions by describing a multi-period investment model for flexible processes. The decisions are made for expansion of processes, capacity of processes and production rate. Most work with regards to strategic planning deals with this kind of decisions as well as finding optimum production batch size and scheduling. Since no relevant work to the problem of this thesis is found in the process industry, strategic planning on manufacturing is also studied by looking at papers on this field. The review by Martínez-Costa et al. (2014) present strategic mathematical models for capacity expansion and reduction in the manufacturing industry. The work shows that strategic planning is not very different for the process industry, as on this decision level same type of decisions are needed to be made. The reviewed models also tackle decisions on location of facilities.

In most literature, production capacity is defined as the volume of products generated by a system in a certain time period. However, what is generally defined by capacity in strategic planning problems is not the volume of outputs from a system, but the availability of different production resources (Benedito et al., 2016). As this definition beholds, literature on this type of planning is missing when looking into the process as well as the manufacturing industry.

3.3 Review on batch plant design

On the design aspect of plants, relevant literature is found related to batch plant design. Barbosa-Póvoa (2007) presents a review on the design of batch plants, by considering two types of plants multi-product and multi-purpose. She argues that there is still a need for further development in the present models, with special attention given to multi-objective design. According to Barbosa-Póvoa (2007) batch production involves flexible facilities where a variety of products can be produced with the available resources such as equipment, manpower, and utilities. Different sequences, hence recipes, can lead to the same product. According to Barbosa-Póvoa, (2007) the main aspects of a design problem are the

resources, tasks and time. The author differentiates between resources as processing or storage units, connections amongst (auxiliary) equipment's, and utilities. The processing unit capacity can be defined nominally or by a range (Barbosa-Póvoa, 2007).

Reklaitis, (1989) reviews the design of such systems. The conceptual batch process design is studied from four decision levels:

1. Determination of the processing network involving the definition of the product recipe and tasks for each product.
2. Selection of best operating strategy with decisions on the operating mode.
3. Allocation of equipment items to tasks and storage of material.
4. Sizing of equipment.

The work by Modi & Karimi (1989), where the design of multiproduct batch processes with finite intermediate storage are studied, determines the equipment size of each batch unit, number of units at each batch stage, the processing rate of each unit and size of all intermediate storage tanks. It classifies the design problem of the paper as a sizing problem with the exception of determining the number of units at each stage. The objective of this paper is to present a heuristic process to minimize equipment costs.

In most cases, the product recipes, possible equipment units and their associated tasks, time horizon of planning, inventory availability, demand, storage policies, and operating and capital cost data are given. Optimal plant configuration and process schedules are to be determined by optimizing a plant objective such as the economic performance in terms of capital expenditure, operating costs and revenues. It is also possible that the plant objective defines several goals, leading to a multi-objective optimization problem.

Storage availability has a special importance in process industries. Unlike warehouses in traditional manufacturing processes where the storage is more flexible, the capacity of tanks for liquids can place a hard constraint (Crama et al., 2001). As identified by Voudouris & Grossmann (1996) five main storage policies influence the final design. These are as follows:

- Zero-wait: Material cannot be stored as it is unstable and must be processed.
- Unlimited Intermediate Storage: Material can be stored in a dedicated vessel with finite capacity.
- Shared Intermediate Storage: Material can be stored in one or more vessel that can be shared with other materials, but not at the same time.
- No Intermediate Storage: Material can be temporarily stored in the process equipment when there are no vessels available.

It is also possible to adapt a combination of these policies, defined as Mixed Intermediate Storage policy Barbosa-Póvoa (2007).

Many models consider physical characteristics as well as operational characteristics such as task allocation, inventory, and utility consumption. Barbosa-Póvoa (2007) distinguishes between design problems as grassroots and retrofit. Grassroot problems focus on the design of a plant structure and operation from scratch whereas retrofit problems focus on the redesign of an existing plant. The focus of this research lies in the grassroot problems, where a plant is designed from scratch.

Grassroots design

Design of plants can consider choosing the processing units and their capacity to minimize the design objective in consideration such as costs (Barbosa-Póvoa, 2007). There has been previous literature on design problems with an objective to minimize capital cost without considering scheduling. In the work of Loonkar & Robinson (1970), a procedure for calculating the sizes of equipment to minimize the

capital investment in a batch processing plant is established. The design problem is tackled without scheduling, the equations of the model are solved by iteration. The paper considers linear processes with non-continuous batches (one batch in the process at any time).

There has been a variety of work in literature with regards to the design problem in which storage considerations are not taken into account. For example the work by Grossmann & Sargent (1979) where a nonlinear model is formulated for flexible chemical plants that are economically optimal, does not take into account storage of materials. It is also assumed that the plant in consideration is subjected to different operating conditions.

Works of Takamatsu et al. (1982) and Modi & Karimi (1989) introduce storage consideration in terms of intermediate storage. Both papers adapt a heuristic solution approach with storage costs. Takamatsu et al. (1982) consider the operation schedule to determine the sizes of batch items. The objective is to minimize capital costs by determining the number of equipment, volumes of storage tanks and number of parallel batch items. Modi & Karimi (1989) on the other hand, optimizes the equipment costs in a sequential process by determining the optimal storage locations and sizes.

Scheduling considerations in works of grassroots design are limited to storage. In the work of Voudouris & Grossmann (1996) scheduling is incorporated to the design problem of batch plants. The paper aims to minimize the cycle time for unlimited intermediate storage and zero wait policies by solving a non-linear programming model. In most literature where scheduling is included, the model on hand is a non-linear model. The paper from Vasillos & Grossmann (1992) formulates these problems with Mixed-Integer Linear Programming by transforming the continuous sizes of equipment and storage into discrete values. As opposed to rounding schemes for continuous models, global optimum solutions are obtained.

3.4 Other relevant literature

This section presents other papers in different directions that have models relevant to the scope of this research.

The paper by Hugo et al. (2005) introduces the strategic planning of hydrogen infrastructure using multi-objective optimization. Due to its simple supply chain, the process of CORE can be optimized using some aspects of the model. The model considers both investment and environmental criteria and is solved by forming a Mixed Integer Linear Program. There are potential supply chain configurations that can be invested in, the paper aims to form a general optimization-based model to facilitate design and planning. Figure 6 represents the model structure of a hydrogen supply chain. As it can be seen there are several possible alternatives and interactions between various supply chain components.

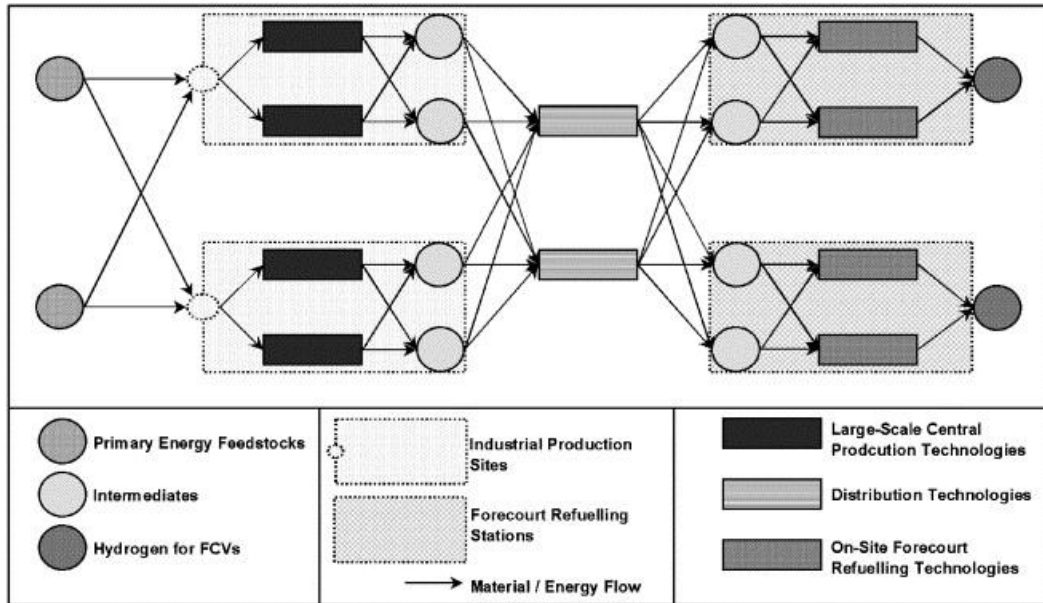


Figure 6: Superstructure of hydrogen supply model (Hugo et al., 2005)

The model defines different classes for each component of the supply chain. For instance primary energy resources are defined by the set consisting of natural gas, coal, biomass, and renewable energy:

$$r \in R := \{Natural\ Gas, Coal, Biomass, Renewable\ Energy \dots\}$$

Other supply chain components, intermediates, industrial production sites, production technologies etc., are all defined with sets of possible alternatives. The main objective of the model is to give insight into the optimal strategic investment planning and asset management over a long term (Hugo et al., 2005). The model considers four levels of decision making: strategic supply chain design with allocation of technologies, capacity and shut-down planning, production planning and performance index analysis.

The possible different combinations of components from different sets reflect the possible supply chain directions. The scope of this thesis does not have a supply chain perspective, however there are different routes a waste entering the CORE factory can take, dependent on which storage they are stored in and if drying is necessary. Therefore the set construction in terms of supply chain components from the model of Hugo et al. (2005) are used to construct sets in the model of this thesis. The sets constitute the waste material types, storage types and machinery type. In Section 4 the model is discussed further.

3.5 Conclusion

The literature review on mathematical modelling and resource planning in the process industry is presented in this chapter. The investigation in Chapter 2 on the current system of CORE Chemistry, followed by the initial analysis of literature revealed that CORE Chemistry can be placed in the category of process industry. Further analysis is done on CORE Chemistry in terms of process industry characteristics from the literature. Recipes, fluctuating yield rates, generation of co- and by-products and limited storage capacity are all applicable process industry characteristics to the CORE process. Characteristics initially identified are important and the decision-making approach must be customized to these characteristics. Due to this the research scope is narrowed down to the process industry initially.

An operations research approach is applicable to this thesis. Work in the operations research literature focusing on the process industry is studied further in Section 3.2. The literature in operations research in this field is mainly focused on planning and scheduling. Literature mostly focuses on time-indexed and multi-period analysis. These are mostly done in the tactical and operational level planning. However, in this research the interest is on the strategic side of the planning. In strategic planning a decision about the assets is taken. Mathematical modelling techniques have been widely used to guide

process industries, but when the decision level of these models are studied, strategic decisions are not common. The models are mostly used to guide organizations in terms of tactical or operational decisions, and if strategic decisions are present, they are always combined with another level of decision making. Studies in the process industries fall behind in implementing production planning and control processes that match with their specific characteristics in the strategic level. This brings up a need to tackle strategic decisions in process industries and creates the basis of this research.

When capacity planning literature in strategic level is studied, it can be seen that most models deals with capacity expansion in terms of sizes, location and types. Scheduling capacity expansions and replacement of equipment are also studied. Most work deals with this type of capacity planning and this is also the case for the manufacturing industry. This brings up the fact that strategic planning in the process industry does not differ much from the manufacturing industry. Production capacity planning in terms of availability of different production resources are missing when looking into the process as well as the manufacturing industry.

On the design aspect of plants, batch designs are also studied in this literature review as they are found to be relevant to the CORE process due to the similarities. It is argued in most literature that there is also a need for development in this type of problems in terms of considering multi-objective design. Design of batch systems are studied from four decision levels: determination of the network, selection of operating strategy, allocation of equipment items and sizing of equipment. These are all relevant decision levels to the research of this thesis and are considered in the model presented in Chapter 4.

Storage considerations are important in these kinds of problems. Unlike traditional warehouses where storage is more flexible, the capacity of tanks for liquids can place a hard constraint. Storage considerations in the process of CORE are also important, as some material can only be stored in certain conditions and certain type of storage, whereas some material can alternate between different storages.

Grassroot designs which deal with problems where a plant is designed from scratch, consider choosing the processing units and their capacity to minimize a design objective. There are many work in literature where storage considerations are not made with regards to grassroot design. The consideration of storage takes place in terms of introducing a cost that is added to the objective function. Many of these papers solve the optimization problem in terms of Mixed-Integer Linear Programming.

4 Model development

This chapter formulates a mathematical model that optimizes the resource requirements, namely, land, machinery, and materials by minimizing the costs. The following research question is answered in this chapter:

Based on the literature and available data, how can a model be designed to be implemented in the process of CORE?

As CORE Chemistry currently does not have a systematic approach to estimate the costs of building a new factory and optimize the resource requirements, a mathematical model is developed to assist them with this. The current system analysis in Chapter 2 enabled to visualize the process in the factory by means of a Business Process Map and a Value Stream Map. Materials and their specific requirements are also introduced. This process in line with the literature review in Chapter 0, enabled the placement of CORE Chemistry in the process industry. It is found out that literature on solely strategic planning is lacking behind, and hence studied in this research. The resource problem of CORE Chemistry is translated into a Mixed-Integer Linear Programming (MILP) model and the following sections explain the model development process. Section 4.1 explains the model selection. Section 4.2 introduces the model notation with indices and parameters used in the MILP model. Section 4.3 and Section 4.4 describe the decision variables and the objective function, respectively. Section 4.5 explains the constraints of the MILP model. The entire MILP model can be found in Section 4.6.

4.1 Model selection

Many operations research (OR) problems for resource planning in the process industry are tackled with mathematical modelling. Mainly, the mathematical models are formulated by Linear Programming (LP), Non-Linear Programming (NLP) or Mixed-Integer (non) Linear Programming (MILP/MINLP) (Chapter 3). In this research, firstly a MINLP is created. Then by means of linearization the model is converted to a MILP model. A MI(N)LP model is well suited to this research since the decision variables are both continuous and integer. The cost relationships can be modelled linearly, however as the model aims to assign the most suitable storage location to each waste type in terms of cost effectiveness, the model has a nonlinear element in the cost function. This element is a product of a continuous variable and a binary variable. This is linearized by means of introducing a dummy variable, further explained in Section 4.5.

One advantage of MILP models is that the mathematical investigation can be assisted with widely available quality software and is commonly used in research. The proposed MILP model of this research aims to optimize the land requirements in terms of storage types and locations, number of machines and amount of waste to be produced.

4.2 Model notation

Firstly, the model notation is introduced to give an overview of the indices and parameters used. Table 1 gives an overview of each waste stream, how they are classified and what kind of storage is required. A recipe from CORE Chemistry to form obsidian combines slag former, fuel, and support material if dusty material is used.

Table 1: Waste streams

Waste type	Storage type	Material	Classification	Storage Location
1	1 / 2	Pyrolysis residue	Fuel	Silo/Shed
2	1	Dusty material	Fuel	Silo
3	3	Sludge	Fuel	Tank
4	1 / 2	Shredder waste	Fuel	Silo/Shed
5	1	Fly ash	Slag former	Silo
6	1 / 2	Polluted soil	Slag former	Silo/Shed
7	3	Oil	Support	Tank

Table 2 illustrates the notations of indices and parameters that are used in the model.

Table 2: Indices and parameter of the MILP model

Notation	Description	Value
<i>Sets</i>		
I	Waste type, $i \in I$	$i = \{1,2,3,4,5,6,7\}$
J	Fuel type, $J \subset I, j \in J$	$j = \{1,2,3,4\}$
K	Slag type, $K \subset I, k \in K$	$k = \{5,6\}$
L	Storage type, $l \in L$	$l = \{1,2,3\}$
M	Machine type, $m \in M$	$m = \{1,2\}$
Q	Waste type that requires drying, $Q \subset I, q \in Q$	$q = \{2,5\}$
<i>Parameter</i>		
r_o	Ratio for amount of oil to amount of dusty material	
r_s	Ratio for amount of fly ash to amount of polluted soil	
K_m	Capacity of machine m in tons per year	
e_i	Energy density of waste i in J per ton, $\forall i \in J$	
E	Energy required by the one ton of slag stream to be processed in J per ton	
C_{min}	Minimum amount of waste that can be processed in the plant in ton per year	
C_{max}	Maximum amount of waste that can be processed in the plant in ton per year	
$W_{i,min}$	Minimum amount of waste i required to be processed in ton per year	
$W_{i,max}$	Maximum amount of waste i to be processed in ton per year	
t_i	Required storage at all times of waste i in years	$\frac{7}{320} \text{ years } \forall i,$ $t_i = t + t_{i,dry} \quad \forall i \in q$

$t_{i, dry}$	Time required for drying waste i , $\forall i \in q$	
t_d	Required storage in the day bunker at all times in years	$\frac{1}{320} years$
ρ_i	Density of waste i	
h_l	Height of storage l in meters	
$c_{A,l}$	Cost per square meter per year of storage l	
c_v	Cost per cubic meter of tank storage	
D_m	Depreciation for m	
p_i	Price of processing per ton of waste i	

Index i constitutes the waste type such that every waste represented in Table 1 corresponds to a number from set I , in order. For instance, $i = 3$ corresponds to the third row of Table 1 and defines sludge. Subsets J and K of I , classify the waste material into fuel and slag. Index l corresponds to the storage type such that silo, shed and tank are defined, respectively. Index m corresponds to the machine type such that dryer and mixer are defined, respectively. Another subset Q of I is formed to represent the material that needs drying, sludge, and polluted soil.

The relevance of each parameter is discussed with their prospective constraints in Section 4.4.

4.3 Decision variables

In this section the decision variables of the MILP model are introduced.

Table 3: Decision variables of the LP model

Notation	Description
<i>Decision Variable</i>	
W_i	Amount of waste i in tons per year
$y_{il} \in \{0,1\}$	Equals 1 if storage l is used for waste i , 0 otherwise
A_{il}	Total area required for storing waste i in storage l in square meters
A_d	Total area required for daybunker
V_{il}	Total volume required for storing waste i in storage l in cubic meters
n_m	Number of machine m
$z_{1,il}$	Dummy variable introduced for linearization of $A_{il} \times y_{il}$ for waste i in storage l
$z_{2,il}$	Dummy variable introduced for linearization of $V_{il} \times y_{il}$ for waste i in storage l

Decision variable W_i constitutes the optimal number of waste i to be processed in one year. In order for the model to decide between what storage to assign to the waste streams that can alternate between silo and shed, binary variable y_{il} is introduced. A_{il} and V_{il} represent the land required for storages in a year. Final decision variable n_m defines the optimal number of machines needed.

4.4 Objective function

The MILP model aims to maximize the following objective function:

$$\sum_i W_i p_i - \sum_i \sum_l z_{1,il} c_{A,l} - A_d c_d - \sum_i \sum_l z_{2,il} c_v - \sum_m n_m D_m \quad (1)$$

The objective is to minimize the first-year resource costs of the factory and maximize the profit coming from processing waste. For each resource, the main cost parameter is considered. For instance, for silo and shed storage the most significant cost is related to the cost per area, and for tank this is per volume. Here, the dummy variable $z_{1,il}$ and $z_{2,il}$ are introduced in the cost function and it corresponds to the multiplications of A_{il} and y_{il} , and V_{il} and y_{il} respectively. Further explanation on this linearization can be found in Section 4.5.

For machinery, the most significant cost is the investment costs, which are represented in terms of depreciation cost. The depreciation cost is calculated as follows:

The salvage value of the machine m , represented by F_m in the future needs to be converted to its equivalent today, the present worth P_m . This is calculated by using the interest rate i and useful life of machinery N . In the process industry the interest rate value i is taken to be 0.02.

$$P_m = F_m(1 + i)^{-N} \quad \forall m \quad (2)$$

The value of equipment decreases over time, and the recovery of money from the earnings of equipment is referred to as depreciation fund (Panneerselvam, 2001).

Using the present value of the salvage value, the depreciation cost is calculated using the straight line method of depreciation (Panneerselvam, 2001). With this method the value the equipment will add throughout its lifetime in terms of cost can be calculated, as the investment cost is distributed throughout the lifetime of the equipment and is not considered at once. The depreciation cost for machine m represented by D_m , is calculated by deducting the present worth of salvage value P_m from the initial investment I_m divided by the lifetime l_m .

$$D_m = \frac{I_m - P_m}{l_m} \quad \forall m \quad (3)$$

This value is calculated beforehand and is included in the cost function.

4.5 Constraints

This section explains the constraints of the MILP model.

Linearization

The quadratic expressions in the cost function, $A_{il} \times y_{il}$, and $V_{il} \times y_{il}$, are linearized by introducing the dummy variables $z_{1,il}$ and $z_{2,il}$. Suppose an upper bound for A_{il} and V_{il} are given as M_1 and M_2 respectively. Then the quadratic expression can be linearized by using the big M method and introduces the following constraints:

$$z_{1,il} \geq A_{il} - (1 - y_{il})M_1 \quad (4)$$

$$z_{2,il} \geq V_{il} - (1 - y_{il})M_1 \quad (5)$$

The product that is now modelled by $z_{1,il}$ can equal 0 if $y_{il} = 0$ for some i and j , and can take any value between 0 and M_1 if $y_{il} = 1$ for some i and j . This can be shown with:

$$z_{1,il} \leq y_{il}M_1 \quad (6)$$

The product is always non-negative and smaller than A_{il} ($z_{1,il} = 0$ if $y_{il} = 0$) Hence we have:

$$0 \leq z_{1,il} \leq A_{il} \quad (7)$$

In case $z_{1,il} = A_{il}$, then this is only possible by $y_{il} = 1$. This is obtained from (4).

Equation (4) is included in the model as the first linearization constraint in terms of $z_{1,il}$. The same principle applies to $z_{2,il}$ and is expressed by (5).

Storage classification

There are three types of storage; silo, shed and tank. Each waste type has their own storage requirement such that some can only be stored in tanks, some in silos and some either in silos or sheds (Table 1). For the model to assign this, the binary variable y_{il} is introduced. The following constraints enable the model to know that specific waste material cannot be stored in a specific storage type.

Waste material that cannot be stored in a tank (fly ash, polluted soil, pyrolysis residue, dusty material, and shredder waste) are defined with the following constraint:

$$y_{il} = 0 \text{ for } i = 1,2,4,5,6 \text{ and } l = 3 \quad (8)$$

Waste material that cannot be stored in a shed (fly ash, dusty material, sludge, and oil) are defined with the following constraint:

$$y_{il} = 0 \text{ for } i = 2,3,5,7 \text{ and } l = 2 \quad (9)$$

Waste material that cannot be stored in silo (sludge and oil) are defined with the following constraint:

$$y_{il} = 0 \text{ for } i = 3,7 \text{ and } l = 1 \quad (10)$$

Following constraints ensure that one type of storage is assigned to the waste.

$$y_{i1} + y_{i2} + y_{i3} = 1 \quad \forall i \quad (11)$$

For some waste material (pyrolysis residue, shredder waste, polluted soil) both shed or silo storage is possible. However, one needs to be chosen. Constraints (8), (9), (10), (11) ensure that waste can only be stored in suitable storage, and furthermore constraint (11) selects the best one from the suitable storages.

Chemical Process

The following constraints deal with specific chemical requirements. Oil is added in the mixer stage to the process and is used in presence of dusty material. The amount of oil per year depends on the amount of dusty material per year, and there is an experimentally determined ratio r_o that needs to hold. The following constraint (12) defines this. W_7 represents the amount of oil and W_2 represents the amount of dusty material to be determined.

$$W_7 = W_2 \cdot r_o \quad (12)$$

The recipes have a certain amount of fly ash to polluted soil ratio, represented by r_s which the system needs to meet. The following constraint defines this:

$$W_5 = W_6 \cdot r_s \quad (13)$$

Each fuel waste $W_{i \in j}$ has a specific energy density, e_i . The total slag one ton of slag requires energy E to be processed. Therefore to process the total slag, $\sum_i W_{i \in k}$, the total energy entering the system is required to be equal to or larger than $\sum_i W_{i \in k} E$.

$$\sum_{i \in J} W_i e_i \geq \sum_{i \in K} W_i E \quad (14)$$

Capacity

There is a lower and upper limit to the total amount of waste that can be processed in the plant in a year. Following constraint defines this and bounds the total of values of W_i to the minimum and maximum plant capacity:

$$C_{min} \leq \sum_i W_i \leq C_{max} \quad (15)$$

There are also minimum values of W_i that needs to be processed and for certain waste material a maximum amount. This is due to specific supplier arrangements and puts a constraint on some waste amounts. Certain waste material supply is already established, and for the ones without a minimum or a maximum, $W_{i,min}$ and $W_{i,max}$ will equal to zero.

$$W_{i,max} \geq W_i \geq W_{i,min} \quad \forall i \quad (16)$$

There are also capacity constraints on the machines, as both the dryer and mixer can handle a certain amount of waste material daily. Therefore, the amount of sludge a dryer can take is limited. The capacity of one dryer is multiplied by the number of dryers. This total capacity of dryers in the process needs to be able to satisfy the amount of sludge that the model determines. Following constraint denotes this:

$$W_3 - n_1 K_1 \leq 0 \quad (17)$$

The total capacity of the mixers needs to satisfy the total amount of waste.

$$\sum_i W_i - n_2 K_2 \leq 0 \quad (18)$$

Storage

Before discussing the storage constraints, it should be mentioned that t_i denotes the required storage at of waste i all times in years and is equal to 7/320 years. There needs to be a supply of 1 week of storage at all times in terms of every waste stream. This is represented in terms of years by dividing it by 320, as the factory is operational 320 days in a year. For polluted soil and sludge, this storage time is increased by a particular value $t_{i,dry}$, which depends on how long it takes to dry these products:

$$t_i = t + t_{i,dry} \quad \forall i \in q \quad (19)$$

In terms of storage requirements, for the silo and shed based storage, there is a specific storage height h_l where $l = 1,2$ and a density ρ_i for individual waste stream. Given a required storage time, t_i total area required for silo and shed can be found by Equation (18):

$$A_{il} = \frac{W_i \cdot t_i}{\rho_i} \cdot \frac{1}{h_l} \quad \forall i, l \quad (20)$$

For the tanks, the costs are incurred per cubic meter of storage. Total volume required for storing enough material for time t_i is given by:

$$V_{il} = \frac{W_i \cdot t_i}{\rho_i} \quad \forall i, l \quad (21)$$

It is also required that there is one day of storage at all times kept in the day bunker. This ensures that if any step in the process fails before the oven, the process can still continue and produce obsidian for a day. The day bunker stores all the waste that gets mixed in the mixer before they are in the oven. To calculate the total area required for the day bunker all waste processed in a year is used with the average density:

$$A_d = \frac{\sum_i W_i \cdot t_d}{\frac{\sum_i \rho_i}{7}} \cdot \frac{1}{h_d} \quad \forall i \quad (22)$$

Additional Constraints

Following sign restrictions on the decision variables are also in place for the MILP model:

$$W_i \geq 0 \quad \forall i \quad (23)$$

$$A_{il} \geq 0 \quad \forall i, l \quad (24)$$

$$V_{il} \geq 0 \quad \forall i, l \quad (25)$$

Equations (23)-(25) make sure that the amount of waste, the area and the volume required for storage cannot be negative.

The process can only occur if there is at least one dryer and one mixer. Therefore n_m has a lower bound of 1. Also, it is only possible to have integer numbers for the number of machines and the Constraint (26) enables this.

$$n_m \geq 1 \quad \forall m \quad (26)$$

$$n_m \in \mathbb{Z} \quad \forall m \quad (27)$$

4.6 The MILP Model

This section highlights the complete MILP Model. Sets, parameters, and decision variables can be found in Section 4.2 and Section 4.3 respectively.

The MILP model is as follows:

$$\begin{aligned} & \sum_i W_i p_i - \sum_i \sum_l z_{1,il} c_{A,l} - A_d c_d - \sum_i \sum_l z_{2,il} c_v - \sum_m n_m D_m \\ & \quad z_{1,il} \geq A_{il} - (1 - y_{il}) M_1 \\ & \quad z_{2,il} \geq V_{il} - (1 - y_{il}) M_1 \\ & \quad s.t \quad y_{il} = 0 \text{ for } i = 1, 2, 4, 5, 6 \text{ and } l = 3 \\ & \quad \quad y_{il} = 0 \text{ for } i = 2, 3, 5, 7 \text{ and } l = 2 \\ & \quad \quad y_{il} = 0 \text{ for } i = 3, 7 \text{ and } l = 1 \\ & \quad \quad y_{i1} + y_{i2} + y_{i3} = 1 \text{ for } \forall i \\ & \quad \quad W_7 = W_2 \cdot r_o \\ & \quad \quad W_5 = W_6 \cdot r_s \\ & \quad \quad \sum_{i \in J} W_i e_i \geq \sum_{i \in K} W_i E \end{aligned}$$

$$\begin{aligned}
C_{min} &\leq \sum_i W_i \leq C_{max} \\
W_{i,max} &\geq W_i \geq W_{i,min} \quad \forall i \\
W_3 - n_1 K_1 &\leq 0 \\
\sum_i W_i - n_2 K_2 &\leq 0 \\
A_{il} &= \frac{W_i \cdot t_i}{\rho_i} \cdot \frac{1}{h} \quad \forall i, l \\
V_{il} &= \frac{W_i \cdot t_i}{\rho_i} \quad \forall i, l \\
A_d &= \frac{\sum_i W_i \cdot t_d}{\frac{\sum_i \rho_i}{7}} \cdot \frac{1}{h_d} \\
W_i &\geq 0 \quad \forall i \\
A_{il} &\geq 0 \quad \forall i, l \\
V_{il} &\geq 0 \quad \forall i, l \\
n_m &\geq 1 \quad \forall m \\
n_m &\in \mathbb{Z} \quad \forall m
\end{aligned}$$

4.7 Conclusion

In this section, an overview of the MILP model that is developed for CORE Chemistry is given. The model considers the highest costs for each resource. For shed and silo storage this is the area, for tank storage it is the volume. For machinery, the highest known costs are in terms of the initial investment. A depreciation cost is used for these to account for the initial investment in terms of the useful life of the machinery and the salvage value. The objective of the model is to maximize profit by minimizing these costs. Several constraints with regards to the storage, capacity and chemical process are explained in this section. Finally, the entire MILP model is presented.

5 Model analysis and case study on CORE Chemistry

This chapter answers the following research questions:

What data is required and available for implementing the methods?

Based on the developed model, what are the most profitable decisions for CORE in terms of resource allocation?

An analysis on the results of the MILP model is presented in this chapter. The model is coded in Python and solved with GUROBI Optimization Solver. The code can be found in Appendix B, the python code for the MILP model. As CORE Chemistry would like to input their own data, a user-friendly tool is made in Excel to enable this. The code reads the data from the Excel file and executes the results accordingly.

Firstly, the initial inputs to the MILP model are presented in Section 5.1. This is followed by the results of the MILP model with the given inputs in Section 5.2. This is followed by a sensitivity analysis and discussion of results in Section 5.3.

5.1 Input data

In this section parameter data as the input for the MILP model is collected. The data is collected by consulting the management team of CORE Chemistry as well as accessing waste data spreadsheets collected by experiments done by CORE.

Table 4: Input data for waste streams

Waste	Type	Energy (J)	Density (tons/m ³)	Processing price (€)	Minimum processing amount (tons)	Maximum processing amount (tons)
		e_i	ρ_i	p_i	$W_{i,min}$	$W_{i,max}$
Pyrolysis residue	Fuel	11.84	500	150	8000	24000
Dusty material	Fuel	21	244	85	8000	-
Sludge	Fuel	13.3	451	100	-	-
Shredder waste	Fuel	29	1100	120	-	-
Fly ash	Slag		800	150	2000	-
Soil	Slag		1500	60	8000	-
Oil	Support		900	200	-	-

Table 4 contains the initial collected parameter data for the waste set. The energy data for the waste are taken from the sample values that CORE Chemistry received from their suppliers. For pyrolysis residue and shredder the energy is calculated from the average of the measured energy values of the samples. For dusty material and sludge, the average energy of different incoming materials of those streams (HRK-G, Pellets, HRK-W for sludge and Plastic M, Vezels, Filtermix, Plastic D) are considered when calculating the energy values used in the optimization model. The density values are provided by the management team, measured from the samples. The processing price are provided by the management team.

The minimum and the maximum processing amount are also provided by the management team and is purely due to arranged supplier relationships. Pyrolysis residue is the only waste stream with an upper limit, and this is due the fact that no more than 24,000 tons can be supplied by the current supplier.

Table 5: Input data for machinery

Machinery	Depreciation Cost	Capacity
	D_m	K_m
Dryer	60099	57600
Mixer	9390	48000

Table 5 contains the initial collected parameter data for the machinery. The capital cost is calculated by Equation (3). Capacity data are provided by CORE Chemistry.

Table 6: Input data for storage

Storage	Cost	Height
	$c_{A/V,l}$	h_l
Silo	160	3
Shed	260	3
Tank	400	-
Day bunker	35	1.25

Table 6 contains the input data for storage. Cost information on shed, silo and day bunker are provided by CORE Chemistry. As there are no other factors and it is less expensive, silo storage will be assigned to every waste that can be stored in either silo or shed with these parameter values. This eliminates the usefulness of the decision variable y_{il} , however it is chosen to be still included in the model as sometimes due to municipality regulations of the factory location, shed storage is required for some waste. Then this can be assigned by making use of the variable and the constraints. Also, as these parameter values can be changed, there might be scenarios where shed is preferred over silo.

Due to lack of data, there was no information on the cost of tanks. Therefore the tank costs are approximated by the formula provided by Smith (2005):

$$C_E = C_B \left(\frac{Q}{Q_B} \right)^M \quad (28)$$

Where C_E = equipment cost with capacity Q

C_B = known base cost for equipment with capacity Q_B

M = constant depending on equipment type

The values for Equation (28) are taken from Smith (2005) for tank storage. As C_E is the equipment cost with capacity Q , to find the cost per m^3 this value is divided by Q . Results of the MILP problem.

5.2 Results of the MILP problem

After collecting parameter input data, the MILP problem is solved using Gurobi Optimization Solver. Figure 7 depicts the output received from the solver.

Figure 7: Optimization output from Gurobi

```
Gurobi Optimizer version 9.1.2 build v9.1.2rc0 (win64)
Thread count: 6 physical cores, 12 logical processors, using up to 12 threads
Optimize a model with 116 rows, 115 columns and 257 nonzeros
Model fingerprint: 0xbc6399d6
Variable types: 92 continuous, 23 integer (21 binary)
Coefficient statistics:
  Matrix range      [7e-03, 1e+05]
  Objective range   [6e+01, 6e+04]
  Bounds range      [1e+00, 2e+04]
  RHS range         [1e+00, 1e+05]
Found heuristic solution: objective 1.257188e+07
Presolve removed 107 rows and 100 columns
Presolve time: 0.00s
Presolved: 9 rows, 15 columns, 29 nonzeros
Variable types: 11 continuous, 4 integer (3 binary)

Root relaxation: objective 1.682784e+07, 7 iterations, 0.00 seconds
```

Nodes		Current Node			Objective Bounds			Work	
Expl	Unexpl	Obj	Depth	IntInf	Incumbent	BestBd	Gap	It/Node	Time
	0	0	1.6828e+07	0	2	1.2572e+07	1.6828e+07	33.9%	- 0s
H	0	0			1.682440e+07	1.6828e+07	0.02%	- 0s	
	0	0	cutoff	0	1.6824e+07	1.6824e+07	0.00%	- 0s	

```
Cutting planes:
  Gomory: 1
  RLT: 3

Explored 1 nodes (8 simplex iterations) in 0.07 seconds
Thread count was 12 (of 12 available processors)

Solution count 2: 1.68244e+07 1.25719e+07

Optimal solution found (tolerance 1.00e-04)
Best objective 1.682439678529e+07, best bound 1.682439678529e+07, gap 0.0000%
```

The objective function value is 16.8 million. This means in the first year of production, CORE Chemistry will have a profit of 16.8 million € considering processing prices of waste, storage area required for each stream and machine investment. This is a very high value for the first year of production, in which many initial big investments are made, and the process is being initialized. It is unlikely that an organization can achieve such a high profit in the first year of factory operation. Many factors are not considered in the overall model due to simplicity and lack of data, and these play a role in the high objective function value. The costs that are the most influential for each element are taken into account, this being area and volume for storage and investment for machinery. Even though the

objective function value is high, when other elements of the factory are accounted for in detail it is very likely that the total profit will stay positive.

Table 7 shows more detail about the results in terms of waste type. As it can be seen, sludge is the only waste stream that is not included in the production. This could be due to the fact that once sludge is included, a drying installation is required to dry sludge and for other waste this additional cost element is not necessary. Since there is also not yet a minimum processing bound for sludge, the optimal value is found to be zero. The drying increases the storage time of sludge as well as the overall cost. This does not compensate with the relatively low processing price of sludge, which is less than the average of 123.57 euros. Moreover, sludge needs to be stored in a tank which has much higher storage costs compared to shed and silo storage. Therefore the presence of sludge will greatly decrease the profit and hence is not present in the optimal solution.

Table 7: Production and storage results from the MILP model

Waste type	Processing amount (tons/year) W_i	Storage type	Required Storage Area/Volume A_i or V_i
Pyrolysis residual	24,000.0	Silo	350 m ²
Dusty material	8,000.0	Silo	239.07 m ²
Sludge	0	Tank	0
Shredder	910.145	Silo	6.03 m ²
Fly ash	69,607.884	Silo	634.45 m ²
Soil	17,402.0	Silo	169.17 m ²
Oil	80.0	Tank	1.94 m ³

Pyrolysis residual with one of the highest processing prices attains its maximum value of 24,000 tons and dusty material with one of the lowest processing prices attains its maximum value of 8,000 tons. As there is an energy balance constraint on the amount of slag formers and fuel present in the process, the necessary left-over fuel amount is assigned to shredder and not sludge as shredder is more profitable in terms of higher processing price and lower storage costs.

The high processing amounts of fly ash and soil are due to the energy balance constraints as the energy of fuel in the system needs to overcome the energy required by the slag formers. Therefore, these values are much higher than the minimum processing amounts of fly ash and soil.

The comparison of the minimum processing amount to the optimized processing amount of each waste stream can be seen in Figure 8. For half of the waste streams, a lot more than the minimum amount of production is found to be optimal. For waste streams that are costly and do not contribute to the profit positively, either nothing is produced as there is no minimum (i.e. sludge) or the minimum processing amount is produced (i.e. dusty material).

Figure 8: Comparison of minimum to optimized production amounts of each waste type in tons per year



Optimal decisions about the storage can be found in Table 8.

As expected, shed storage is not assigned to any waste type due to its high cost. Tank storage is only assigned once, namely to oil which is the only waste in the optimum production size that requires tank storage. As with the presence of dusty materials it is essential that a minimum value of oil is present as well and this is bounded with the chemical ratio between oil and dusty material. Oil is taking the minimum value possible as tank storage is highly expensive and the processing price of oil does not compensate for this.

Table 8: Storage insights from the MILP model

Storage type	Required Land
	$\sum A_{il}$ or $\sum V_{il}$
Silo	1398.72 m ²
Shed	-
Tank	1.94 m ³

Table 9: Machinery insights from the MILP model

Machinery	Amount
	m_n
Dryer	0
Mixer	3

Table 8 shows the optimal amount of machinery. As the MILP model does not suggest producing any slag, dryer is also not necessary and hence the amount zero. On the other hand, the mixer is assigned a value to maintain the capacity constraints of the model.

5.3 Sensitivity analysis on the MILP model

In this section a discussion on sensitivity analysis on the proposed MILP model for CORE Chemistry is given. In many cases, the values of model parameters can change and sensitivity analysis may enable to not solve the problem completely again (Winston, 2004). Since CORE Chemistry would like to try out different scenarios on the model when they have more data, and the initial inputs are just estimations the outcomes of the sensitivity analysis will be valuable. If a parameter is changed, it might not have an effect and the current solution may remain optimal.

With sensitivity analysis it is possible to analyse objective function coefficient ranges, reduced cost, shadow prices and dual prices. However, these attributes are only available to LP models. This information can be retrieved by fixing the MILP model and creating a fixed LP model. The python code can be found in Appendix B, python code for the LP model. Even though this method is prone to errors, it can be applied in the case of the MILP problem for CORE Chemistry. As discussed before, the values of the binary variable y_{il} is known beforehand since assignment of storage only relies on the costs and the model always assigns the waste to the cheapest storage. Therefore, with the initial parameters, the binary variable can be assigned fixed values. It cannot be taken out from the model since the area costs need to be taken into account if silo storage is used or volume costs need to be taken into account if tank storage is used.

The integer variable n_m is taken to be continuous to allow sensitivity analysis. When this change is made, it is seen that the optimal solution in terms of waste amounts do not change, however the optimization function value slightly increases. Figure 9 shows the output from GUROBI when the MILP model is converted to the LP model. The optimal objective function value of the LP amounts to approximately 16.8 million € and hence there is no significant shift from the MILP model. The exact change in the optimal function value amounts to 4695.00471 euros. When examined further it is seen that the mixer (m_2) is assigned a value of 2.5 in the LP model whereas in the MILP model this amounts to 3. Hence the difference of 0.5 is reflected in the profit as 4695 is half of the depreciation cost of mixers as seen in Table 5. Therefore, the slight increase in the profit can be explained through this and does not affect the optimal waste amount results.

Figure 9: Output from the LP converted MILP model

```
Gurobi Optimizer version 9.1.2 build v9.1.2rc0 (win64)
Thread count: 6 physical cores, 12 logical processors, using up to 12 threads
Optimize a model with 28 rows, 62 columns and 72 nonzeros
Coefficient statistics:
  Matrix range      [1e-02, 6e+04]
  Objective range   [6e+01, 6e+04]
  Bounds range      [2e+04, 2e+04]
  RHS range         [2e+03, 1e+05]
Iteration    Objective          Primal Inf.    Dual Inf.      Time
     0      5.7598379e+32    3.329531e+30    5.759838e+02     0s
     8      1.6829092e+07    0.000000e+00    0.000000e+00     0s

Solved in 8 iterations and 0.02 seconds
Optimal objective  1.682909179e+07
```

This way by fixing the binary variables and allowing integer variables to be continuous, sensitivity analysis data is achieved from GUROBI. The following sections discuss the numerical values of the

sensitivity analysis. In the simplified LP model, everything is expressed in terms of waste amount as area and volume can be expressed in terms of this.

5.3.1 Objective function coefficient ranges

It is possible to determine a range for the objective function coefficients that ensure that within this range the current solution remains optimal (Winston, 2004). The output attained from the Python code for this range is shown in Table 10 for the waste types. The coefficient minimum to coefficient maximum shows the allowable amount of decrease and increase.

Table 10: Output from GUROBI for sensitivity analysis of variables

Variable	Notation in the model	Value	Objective coefficient	Coefficient minimum	Coefficient maximum	Reduced cost
Pyrolysis residual	W_1	24000	197.555	124.589	inf	0
Dusty material	W_2	8000	80.1071	-inf	120.898	0
Sludge	W_3	0	61.0859	-inf	125.142	-64.0565
Shredder	W_4	910.145	118.828	65.8331	130.411	0
Flyash	W_5	69607.9	148.43	133.952	331.802	0
Soil	W_6	17402	58.333	0.418838	791.821	0
Oil	W_7	80	190.166	-inf	4269.23	0
Dryer	n_1	0	-6099	-inf	7.27596e-12	0
Mixer	n_2	2.5	-9390	-6.17108e+06	0	0

It is possible to increase the coefficient of pyrolysis residual and there is no upper bound on this. Since the variable is already attaining its maximum value bounded by 24,000 tons, no matter the increase in the coefficient maximum the model will always assign this to pyrolysis residue. This is also reflected in dusty material and there is a negative infinity coming from the lower side. As it is already attaining its minimum value, a decrease in the dusty material coefficient for instance in terms of processing price will not affect the optimal amount.

It can be seen that the only waste material taken to be zero, sludge, can escape this if the coefficient of this variable can exceed 125.142. Keeping the costs of storage, storage time and height of storage the same, if the sludge can be processed for a bit more than an additional $125.142 - 61.0859 = 64.0561$ euros, the zero amount will not be optimal anymore. Since due to sign constraints waste amounts cannot take values smaller than zero, the only option will be having a value greater than zero and hence including sludge in the business case of CORE. This is also visible in terms of the reduced cost, which shows how changing the coefficient of sludge by approximately 64.0561 will result in a new optimal solution. This can be achieved by changing the parameters: costs of storage, storage time, height of storage or the processing price.

Due to simplification of the model from MILP to LP, the machine number variable is converted from integer to continuous. As a result, it is attaining decimal numbers. Since this change is very insignificant in the objective function, it can be disregarded. From the allowable range output, it can be observed that there is room for including more machinery costs and hence the solution will stay optimal. The mixer

costs can go until 7.27596×10^{12} euros. The model only included the initial investment for machinery, and if other costs are accounted for it will still give the same outcome. Hence this shows that neglecting other costs did not play a significant role.

5.3.2 Shadow and dual Prices

The shadow price of an LP's constraint can be defined as the amount that the optimal value is improved if the right hand side is increased by one unit (Winston, 2004). As it can be seen from Table 11, the dual price of capacity 1, the constraint that defines the maximum and minimum waste to be processed in a year, is 128.369. This shows that a one unit of increase in the maximum capacity will increase the profit by 128.369 euros.

5.3.3 Right hand side ranges

The RHS minimum and RHS maximum in Table 11 shows the range of values for the right hand side of the constraints within which the current solution remains optimal. The maximum RHS value for the chemical constraint 3, which is the energy balance constraint between fuel and slag is relatively high. This shows that the current optimal fuel supply can meet very high amounts of slag. It is possible to add more slag into the process as this would increase the amount of products produced as well and this can be attained with the current fuel amounts.

5.3.4 Slack values

The slack value is reported for each constraint in Table 11. If a constraint is binding, then it has a slack value of zero. The slack value refers to the amount of resource that is not being used, and represented by the constraint. For capacity 2 constraints on sludge and flyash, this value amounts to the minimum bound minus the optimal amount. The negativity shows that the minimum constraint on these waste are not binding, and hence higher values are assigned. In the case of shredder this might be due to its relatively high processing price which brings more profit and relatively high density which lowers the area required for storage hence the costs. For flyash, there is a certain amount it needs to attain to meet the energy balance equations and to enable the process to occur successfully. As it is not the only fuel, it is more profitable than shredder which requires extra costs and storage time due to drying.

Table 11: Output from Gurobi for sensitivity analysis of constraints

Constraint	Sign	Slack	Dual Price	Right hand side (RHS)	RHS minimum	RHS maximum
Chemical Process 1	=	0	61.6021	0	-80	5709.09
Chemical Process 2	=	0	18.0194	0	-338039	47009.9
Chemical Process 3	>	0	-0.335734	0	-31400	1.62e+06
Capacity 1	=	0	128.369	120000	114291	Inf
Capacity 2 Pyrolysis Residual	>	-16000	0	8000	-Inf	24000
Capacity 2 Dusty material	>	0	-40.7907	8000	-Inf	9182.45
Capacity 2 Sludge	>	0	0	0	-Inf	0
Capacity 2 Shredder	>	-910.145	0	0	-Inf	910.145
Capacity 2 Flyash	>	-67607.9	0	2000	-Inf	69607.9
Capacity 2 Soil	>	-9401.97	0	8000	-Inf	17402
Capacity 2 Oil	>	-80	0	0	-Inf	80
Capacity 3	<	0	1.04339	0	-Inf	0
Capacity 4	<	0	0.195625	0	-Inf	120000
Capacity 5	<	0	72.9661	24000	8000	25810.8

5.4 Conclusion

This chapter analyses the results of the MILP model which is coded using Python and solved with Gurobi optimization solver. Firstly the input data are introduced. This is followed by a discussion on the results of the optimization model. The objective function value of 15 million euros suggests that some significant factors are neglected in the model, as according to the management team it is not possible to achieve this much of a profit in the first year of factory operation. The results are further analysed by means of a sensitivity analysis, and it is found out that due to high range of allowable increase in the cost coefficients with the current optimal solution, the model is successful with analysing the most effective cost parameters.

6 Design of the decision support tool

In this chapter the decision support tool (DST) designed for CORE Chemistry is introduced. From the MILP model, a DST is created to enable CORE Chemistry to input different parameters via a user interface and test the optimization model. The DST is created in Excel and the python code of the MILP code is expressed as a batch file. As the Python code requires Anaconda activation, this batch code also provides this command before executing the code. The batch code is then called from the Excel file CORE_DST.xlsm with a macro button coded in Visual Basics for Applications (VBA).

The DST aims to assist CORE Chemistry with the optimal amount of waste to produce, required area for storage and gives an estimation of the profit calculated by considering the highest cost parameters. The user manual provided to CORE Chemistry is included in Appendix C.

Section 6.1 introduced the DST through the user interface, followed by an explanation on the creation of the DST in Section 6.2. The chapter is concluded with the technical requirements in Section 6.3.

6.1 User interface

The DST is designed to create a user-friendly interface to the Python code and to have a separate input environment. An overview of the initial input screen of the DST is given in Figure 10. The design is created such that it is easily understandable by the management team of CORE Chemistry.

CORE Chemistry - Decision Support Tool

Waste Inputs								
Waste	Type	Storage	Energy	Density	Processing price	Minimum Process Amount	Maximum Process Amount	Drying
Pyroresidue	Fuel	Silo	11.84	0.5	200	8000	24000	no
Dusty	Fuel	Silo	21	0.244	85	8000	1000000	no
Sludge	Fuel	Tank	13.3	0.451	100	0	1000000	yes
Shredder	Fuel	Silo	29	1.1	120	0	1000000	no
Flyash	Slag	Silo		0.8	150	2000	1000000	no
Soil	Slag	Silo		1.5	60	8000	1000000	yes
Oil	Support	Tank		0.9	200	0	1000000	no

Start Optimization

Storage Constraints		Time (in days)
Daybunker storage		1
General Storage		7
Drying time		7

Machine Data					
Machinery	Investment cost	Salvage value	Salvage value present	Depreciation Cost	Capacity
Dryer	1600000	160000	97524.93928	60099	57600
Mixer	250000	25000	15238.27176	9390	48000

Storage Data		
Storage	Cost	Height
Silo	160	3
Shed	260	3
Tank	400	3
Daybunker	35	1.25

Chemical constants		Value
Dusty/Oil ratio		0.01
Flyash/Soil ratio		4
Energy for Slag		5.5

Figure 10: User interface for the decision support tool

Instructions to use the DST
Make sure following files are downloaded and saved in the same directory: CORE_operation_data.xlsx, MILP_CORE.bat, MILP_CORE.py Parameters for the MILP model can be inputted through Waste Data, Machine Data, Storage Data, Storage Constraints, Operation Constraints, Chemical Constraints. If values are not changed, the model runs with the initially inputted parameter values. After values are entered to the DST, the MILP model can be run by clicking the button Start Optimization. This will pop up a command window where the model is executed and the results are listed. For a summary of results refer to the file OptimizedAmounts.xlsx

Initial instructions are included with a box in the DST and a screenshot is provided in Figure 11.

The Excel file initially includes the parameters used in this research. Different values can be entered through designated tables and boxes. The DST only provides an environment to input these parameters and the outputs of the optimization model are not represented in this file. The following section discusses how the DST functions and which steps are necessary to be taken.

Figure 11: Instructions of use for the DST

6.2 Creation of the DST

This section highlights how the decision support tool is created. Firstly, the Python code MILP_CORE.py is called from a batch file MILP_CORE.bat. This batch file firstly enables the Anaconda environment and then executes the python code. The batch file is called by the macro-enabled Excel file CORE_DST.xlsm which is the input environment for the MILP model. The python code extracts data from the Excel file CORE_operation_data.xlsx with the Pandas module in python. This file is linked to the user interface file, CORE_DST.xlsm. When a value in CORE_DST.xlsm is changed by the user, this is updated in the data file CORE_operation_data.xlsx of the python code.

The CORE_DST.xlsm Excel file executes the batch file when the “Start Optimization” button is created. This button is a link to the macro in VBA that executes the batch file. After execution, the command window pops up and the decision variable values can be examined from there. For a better representation, OptimizedValues.xlsx file can be visited which is saved in the same file directory and is created by the python code. It includes a table with the significant decision variables and their optimized values.

6.3 Technical requirements of the DST

The following steps are required from the user:

- All the following files need to be downloaded and saved in the same file directory locally:
- The path of these files must be updated in the python code, the batch file and the VBA code.
 - CORE_operation_data.xlsx
 - MILP_CORE.bat
 - MILP_CORE.py
 - CORE_DST.xlsm
- CORE_operation_data.xlsx is linked to CORE_DST.xlsm and gets its values from there. Therefore to have right initial configuration, firstly CORE_DST.xlsm needs to be opened and then CORE_operation_data.xlsx.
- The python pandas module cannot work with an open excel file. When the DST wants to be run, the data provider of the python code, CORE_Operation_data.xlsx cannot be open.
- System requirements are the following: GUROBI, Python (Anaconda), Visual Basics for Applications (VBA).

If the above mentioned are required, the DST is expected to run smoothly.

6.4 Conclusion

In this chapter the Decision Support Tool created for CORE Chemistry is introduced. It aims to support CORE Chemistry with decisions for material, land, and machinery requirements by creating a user-friendly execution environment of the MILP model.

7 Conclusions, recommendations, and future research

Within this research, a Mixed-Integer Linear Programming Model is developed to provide CORE Chemistry with material, land and machinery requirements of building a waste processing factory. The following research question is answered in this thesis:

How can the land, machinery, and material requirements of building an installation for complex waste streams at CORE Chemistry be estimated?

All the chapters of the thesis aimed at answering sub-research questions related to the main research question. The conclusions drawn from these chapters contributed to answering the main research question and hence provides a solution to the core problem of CORE Chemistry.

In this chapter the main conclusions of the research, recommendations and possible future research are discussed by answering the final sub-research question:

What conclusions and recommendations can be drawn from this research conducted for CORE Chemistry?

The result of the thesis is presented to CORE Chemistry. Section 7.1 highlights the conclusions of the research, followed by recommendations in Section 7.2. Contributions and directions of future research are discussed in Section 7.3 and 7.4 respectively.

7.1 Conclusions of the research

The logistics flow defined by the flow of materials from arrival to the factory till the oven process of CORE Chemistry are mapped by business process models. Specific requirements of the process related to the waste materials are initially identified given by CORE Chemistry. In order to have a better visual representation of the factory, value stream mapping is used to identify the main tasks and the cycle times. The identification of specific requirements of CORE Chemistry such as unknown compositions of input materials, products resulting from different mixes of different ingredients (known as recipes), fluctuating yield rates and the existence of co- and by-products are specific characteristics of the process industry. This was revealed by the literature review and hence formed the scope of the later stages of the thesis. Further in the literature review, it is revealed that there is a lack of research on strategic decision making in the process industry in terms of resource requirements. A MILP model is created to assist CORE Chemistry in strategic decision making for land, machinery and material requirements when opening a factory. A decision support tool is created to enable CORE Chemistry to test different scenarios as the input data for the initial model are not known with full certainty and are subjected to changes. In conclusion, following are the main outcomes of this research conducted for CORE Chemistry:

1. CORE Chemistry has specific requirements present in many organizations in the process industry, and these need to be taken into account when CORE Chemistry is assisted with decision making.
2. There is a lack of literature in the operations research field with regards to capacity in the process industry. Mathematical modelling techniques have been widely used to guide process industries, but when the decision level of these models are studied, strategic decisions are not common.
3. Storage considerations are important in process industry problems. Unlike traditional warehouses where storage is more flexible, the capacity of tanks for liquids can place a hard constraint. Storage considerations in the process of CORE is important, as some material can only be stored in certain conditions and certain type of storage, whereas some material can alternate between silo and shed storage.
4. The first-year profit of CORE Chemistry can be optimized by using a MINLP model that considers the most significant cost parameters of each variable. For storage this is the cost of land and for machinery this is the initial investment cost represented in terms of depreciation.
5. The MINLP model can be linearized by the introduction of dummy variables.
6. Constraints on storage and its classification, capacity, chemical requirements can be introduced in the MILP model and with the initial parameters a feasible solution is found.
7. The first-year profit is 16 million € for CORE Chemistry, and this is significantly high due to the fact that only a small scope of cost are included in the research. However according to the management team this high amount promises a real profit when other cost parameters are also introduced.
8. It is possible to conduct a sensitivity analysis on the MILP in terms of objective function coefficient ranges, shadow and dual prices, right hand side ranges and slack values by converting it to an LP model. This is achieved by fixing the binary variable values and assigning

continuous values to the machine number variable. This does not shift the objective function value significantly, as the binary variable values of storage are known beforehand and still kept in the model as a request from CORE Chemistry for future research. The shift for the integer variable is also not significant and gives the same optimal results for every other decision variable as the MILP model.

9. The sensitivity analysis showed that pyrolysis residual is very valuable for the business case of CORE Chemistry whereas with the current parameters' slag is not profitable to include in the business portfolio. However with an increase on its objective coefficient by approximately 64 € it will be profitable to include it in the portfolio. This can be achieved by changing the supplier arrangement and hence increasing the processing price, increasing the storage height or decreasing the storage time of sludge.
10. Only including the most significant cost can decrease the validity of the model in terms of the profit, however the waste amounts, machine numbers and storage decisions will remain optimal even if these are included. This is shown by the very high allowable optimization coefficient increase for the mixer. Even though only investment cost is included, the optimal solution will remain valid if more costs are introduced. Hence the model is close to being valid.
11. The highest dual price is on the capacity constraint of the whole factory. CORE Chemistry can make 128 € more profit with each unit increase on the waste capacity of the whole factory.
12. As the allowable right-hand side on the energy balance constraint is relatively high, this shows that more slag can be added to the process and the fuel amounts present can handle this. As more slag will result in more products this can have a positive effect on the profit of CORE Chemistry.
13. Using the DST, CORE Chemistry can test different parameter values and obtain related optimized results. This provides CORE Chemistry with a good user-interface.

7.2 Recommendations

This section introduces the recommendations drawn for CORE Chemistry using the developed MILP model. The recommendations are based on the research and the results from the optimization model.

1. In order to calculate the optimal land, machinery and material requirements of building a CORE Chemistry factory, it is recommended to make use of the user-friendly DST built upon the MILP model. It is essential that the data are kept updated to keep the model valid and useful.
2. If CORE Chemistry desires to include sludge in their business portfolio, then work must be done in terms of increasing the value of sludge. This can be achieved in several ways: by having different supplier arrangement and higher processing prices, increasing the height of the storage for sludge, acquiring cheaper drying installation, or lowering the storage time for sludge.
3. As more is known, CORE Chemistry is encouraged to test the model with better data estimations to get results closer to reality. Including more cost parameters can also increase the validity of the model.
4. When possible, CORE Chemistry should aim to process more waste than the defined capacity at the moment, as this will be the most profitable action with the highest dual price in terms of the constraints in the MILP model.
5. As the energy balance constraint allows, CORE Chemistry can introduce more slag than the optimized values and they can achieve this with the set fuel amounts. This can introduce a good profit as more slag will result in more output.
6. It will be beneficial to know the production output rates and implement this in the model, as profit is also achieved by the final product of CORE Chemistry and this can be added to the model.

7.3 Contributions of research

In this research it is enlightened that there is a lack of research on strategic capacity planning in the research industry. Mathematical models have been widely used to guide organizations in planning, however strategic decisions are not commonly treated. Hence this research aims to provide a way to address purely strategic decision making for organizations. The research is performed with CORE Chemistry, and the organization is provided with a decision support tool based upon a MILP optimization model. The theoretical aspects of the CORE Chemistry process are transferred to a practical tool which can be used to assist CORE Chemistry with resource decisions and cost requirements.

7.4 Directions for future research

This research is conducted in a time frame of ten weeks, only focusing on a part of the process of CORE Chemistry. Therefore it brings up the opportunity for more extensive research as described:

- The research only focused on the logistics flow till the oven. The process after the oven can also be introduced into the model in later stages of the organizations when more is known.
- Presenting the optimization data in a visual friendly format was a bottleneck in the process. Work on this can be done to integrate the results into the same DST file and will allow more ease of use.
- More cost components can be added to the model once CORE Chemistry has more data on it. This is most likely not possible before starting to operate a real factory. This will increase the validity of the model.

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Appendix A: Schematic overview of research design per research question

Table 12: Research design for each sub-research question

Research question	Type of research	Research population	Subjects	Research strategy	Method of data gathering	Method of data processing	Activity plan
<i>How can the logistics of building an installation be mapped for CORE Chemistry?</i>	Cross-sectional, exploratory research	Company	Management team	Deep qualitative	Observation, structured-interviews, analysis of primary sources	Deep qualitative	- Interview stakeholders - Gather information on the process - Construct process map
<i>What methods/tools are there in literature to support organizations in decision making for resource allocation?</i>	Cross-sectional, descriptive research	Organizations	Organizations using decision support tools	Broad qualitative	Literature study	Broad qualitative	Conduct literature review for sub-questions.
<i>What data is required for implementing the methods and is available within the organization?</i>	Cross-sectional, descriptive research	Company	Management team	Deep qualitative	Interviews, analysis of primary sources	Deep qualitative and quantitative	- Identify required data - Interview stakeholders - Analyse company documents
<i>Based on the literature how can a model be designed to be implemented in the process of CORE?</i>	Cross-sectional, explanatory research	Company	Compound	Deep qualitative and quantitative	Observation and use of primary data	Deep qualitative and quantitative	- Choose a suitable modelling method - Motivate choice - Formulate the model
<i>Based on the developed model, what are the most profitable decisions for CORE in terms of resource allocation?</i>	Cross-sectional, explanatory research	Company	Compound	Deep qualitative and quantitative	Observation and use of primary data	Deep qualitative and quantitative	Sensitivity analysis on sensitive parameters
<i>What conclusions and recommendations can be drawn from this research conducted for CORE Chemistry?</i>	Cross-sectional, descriptive research	Company	Compound	Deep qualitative and quantitative	Observation and use of primary data	Deep qualitative and quantitative	- Assess different scenarios - Provide conclusions and recommendations for CORE

Appendix B: The Python codes for the model

The python code for the MILP model

```
#import gurobi library

import pandas as pd
import gurobipy as gp
from gurobipy import GRB
import openpyxl
from openpyxl import Workbook
from openpyxl import load_workbook

#Read excel file and data sheets
fuel_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                          sheet_name = "FuelData", index_col=0)
slag_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                          sheet_name = "SlagData", index_col=0)
waste_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                           sheet_name = "WasteData", index_col=0)
storage_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                              sheet_name = "StorageData", index_col=0)
daybunker_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                                sheet_name = "DayBunkerData", index_col=0)
machine_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                              sheet_name = "MachineData", index_col=0)
notank_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "NoTank", index_col=0)
noshed_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                              sheet_name = "NoShed", index_col=0)
nosilo_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                              sheet_name = "NoSilo", index_col=0)
operation_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                                sheet_name = "AdditionalData", index_col=0)
drying_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                              sheet_name = "Drying", index_col=0)

#Sets
waste = waste_data.index.to_numpy()
fuel = waste_data.index.to_numpy()[waste_data["Type"] == "Fuel"]
slag = waste_data.index.to_numpy()[waste_data["Type"] == "Slag"]
storage = storage_data.index.to_numpy()
machine = machine_data.index.to_numpy()
notank = waste_data.index.to_numpy()[waste_data["Not suitable"] == "Tank"] | (waste_data["Not suitable"] == "Shed & Tank")]
noshed = waste_data.index.to_numpy()[waste_data["Not suitable"] == "Shed & Tank"] | (waste_data["Not suitable"] == "Silo & Shed")]
nosilo = waste_data.index.to_numpy()[waste_data["Not suitable"] == "Silo & Shed"]
drying = drying_data.index.to_numpy()

silo = waste_data.index.to_numpy()[waste_data["Storage"] == "Silo"]
tank = waste_data.index.to_numpy()[waste_data["Storage"] == "Tank"]

#parameters linked to indices
capacity_machine = machine_data["Capacity"].to_dict()
energy_waste = fuel_data["Energy"].to_dict()
waste_min = waste_data["Minimum processing"].to_dict()
storage_t = waste_data["Storage time"].to_dict()
density_waste = waste_data["Density"].to_dict()
height_storage = storage_data["Height"].to_dict()
costA_storage = storage_data["Cost"].to_dict()
capital_machine = machine_data["Capital cost"].to_dict()
price_waste = waste_data["Processing price"].to_dict()
waste_max = waste_data["Maximum processing"].to_dict()

#single value parameters
ratio_dusty_oil = operation_data["Ratio dusty to oil"].values.tolist()
ratio_flyash_soil = operation_data["Ratio flyash to soil"].values.tolist()
energy_slag = operation_data["Energy slag"].values.tolist()
height_daybunker = daybunker_data["Height"].values.tolist()
capacity_min = operation_data["Min capacity"].values.tolist()
capacity_max = operation_data["Max capacity"].values.tolist()
daystorage_t = operation_data.index.to_numpy()
costV_storage = operation_data["Tank cost"].values.tolist()
costd_storage = operation_data["Daybunker cost"].values.tolist()

#arbitrary variable to prevent division error
sumdensity_waste = waste_data["Density"].values.tolist()
variable_density_height = [i*sum(sumdensity_waste)/7 for i in height_daybunker]

M = 100000 #very large value

opt_mod = gp.Model(name = "LP Core Chemistry")
```

```
#Decision variables
w_amount = opt_mod.addVars(waste, vtype=GRB.CONTINUOUS, name = "waste_amount")
s_area = opt_mod.addVars(waste, storage, vtype = GRB.CONTINUOUS, name = "storage_area")
s_volume = opt_mod.addVars(waste, storage, vtype = GRB.CONTINUOUS, name = "storage_volume")
m_number = opt_mod.addVars(machine, vtype = GRB.INTEGER, name = "machine_number")
y_storage = opt_mod.addVars(waste, storage, vtype = GRB.BINARY, name = "type_storage")
z_variable1 = opt_mod.addVars(waste, storage, vtype = GRB.CONTINUOUS, name = "z_arbitrary_variable1")
z_variable2 = opt_mod.addVars(waste, storage, vtype = GRB.CONTINUOUS, name = "z_arbitrary_variable2")

obj = (gp.quicksum(w_amount[w]*price_waste[w] for w in (waste))-(gp.quicksum(w_amount[w] *daystorage_t for w in waste )
/ (variable_density_height[0]) * costd_storage[0])-(gp.quicksum(z_variable1[w,s]*costA_storage[s] for w in waste for
s in storage))-(gp.quicksum(z_variable2[w,s] for w in waste for s in storage)*costV_storage[0])-(gp.quicksum(m_number[m]
*capital_machine[m] for m in machine))

opt_mod.setObjective (obj, GRB.MAXIMIZE)
```

Linearity constraint

```
Linearity3 = opt_mod.addConstrs ((z_variable1[w,s]>= s_area[w,s]-(1-y_storage[w,s])*M for w in waste for s in storage),
name = "Linearity3")
Linearity4 = opt_mod.addConstrs ((z_variable2[w,s]>= s_volume[w,s]-(1-y_storage[w,s])*M for w in waste for s in storage),
name = "Linearity4")
```

1. Storage classification

```
StorageClass1 = opt_mod.addConstrs((y_storage[w,storage[2]]== 0 for w in notank) , name ="StorageClass1")
StorageClass2 = opt_mod.addConstrs((y_storage[w,storage[1]]== 0 for w in noshed) , name ="StorageClass2")
StorageClass3 = opt_mod.addConstrs((y_storage[w,storage[0]]== 0 for w in nosilo) , name ="StorageClass3")
StorageClass4 = opt_mod.addConstrs((y_storage.sum(w,"*") == 1 for w in waste), name="StorageClass4")
```

2. Chemical process

```
Chemicalprocess1 = opt_mod.addConstr((w_amount[waste[6]]== w_amount[waste[1]]* ratio_dusty_oil[0]), name ="Chemicalprocess1")
Chemicalprocess2 = opt_mod.addConstr((w_amount[waste[4]]== w_amount[waste[5]]* ratio_flyash_soil[0]), name ="Chemicalprocess2")
Chemicalprocess3 = opt_mod.addConstr((gp.quicksum(w_amount[f]*energy_waste[f] for f in fuel)
=> gp.quicksum(w_amount[s]*energy_slag[0] for s in slag)), name="Chemicalprocess3")
```

3. Capacity

```
Capacity1 = opt_mod.addRange(gp.quicksum(w_amount[w] for w in waste), capacity_min[0], capacity_max[0], name="capacity1")
Capacity2 = opt_mod.addConstrs ((w_amount[w] >= waste_min[w] for w in waste), name="capacity2" )
Capacity3 = opt_mod.addConstr ((w_amount[waste[2]]- m_number[machine[0]]* capacity_machine[machine[0]] <= 0), name="capacity3")
Capacity4 = opt_mod.addConstr((gp.quicksum(w_amount[w] for w in waste) - m_number[machine[1]]*
capacity_machine[machine[1]] <= 0), name ="capacity4")
Capacity5 = opt_mod.addConstr((w_amount[waste[0]]<= waste_max[waste[0]]), name ="capacity5")
```

4. Storage

```
Storage1 = opt_mod.addConstrs((s_area[w, s]== w_amount[w]* storage_t[w]/
(density_waste[w]*height_storage[s]) for w in silo for s in storage), name = "storage1")
Storage1 = opt_mod.addConstrs((s_area[w, s]== 0 for w in tank for s in storage), name = "storage1")

Storage3 = opt_mod.addConstrs((s_volume[w, s]== (w_amount[w]* storage_t[w])/
(density_waste[w]) for w in tank for s in storage), name = "storage2")
Storage4 = opt_mod.addConstrs((s_volume[w, s]== 0 for w in silo for s in storage), name = "storage3")
```

```
opt_mod.update
opt_mod.optimize()
opt_mod.write("model.lp")
```

The python code for the LP model for Sensitivity Analysis

This MILP code is converted to a LP code. The first part of the code where parameters are defined are the same. Only the different parts are included here.

```
#Decision variables
w_amount = opt_mod.addVars(waste, vtype=GRB.CONTINUOUS, name = "waste_amount")

m_number = opt_mod.addVars(machine, vtype = GRB.CONTINUOUS, name = "machine_number")

obj = (gp.quicksum(w_amount[w]*price_waste[w] for w in (waste))-(gp.quicksum(w_amount[w] *daystorage_t for w in waste )
/ (variable_density_height[0]) * costd_storage[0]) - (gp.quicksum(w_amount[w]* storage_t[w]/(density_waste[w]
*height_storage[storage[0]])*costA_storage[storage[0]] for w in silo))- (gp.quicksum((w_amount[w]* storage_t[w])/
(density_waste[w])*costV_storage[0]for w in tank))- (gp.quicksum(m_number[m] *capital_machine[m] for m in machine))

opt_mod.setObjective (obj, GRB.MAXIMIZE)
```

```

# 2. Chemical process
Chemicalprocess1 = opt_mod.addConstr((w_amount[waste[6]]== w_amount[waste[1]]* ratio_dusty_oil[0]), name ="Chemicalprocess1")
Chemicalprocess2 = opt_mod.addConstr((w_amount[waste[4]]== w_amount[waste[5]]* ratio_flyash_soil[0]), name ="Chemicalprocess2")
Chemicalprocess3 = opt_mod.addConstr((gp.quicksum(w_amount[f]*energy_waste[f] for f in fuel)>=
gp.quicksum(w_amount[s]*energy_slag[0] for s in slag)), name="Chemicalprocess3")

# 3. Capacity
Capacity1 = opt_mod.addRange(gp.quicksum(w_amount[w] for w in waste), capacity_min[0], capacity_max[0], name="capacity1")
Capacity2 = opt_mod.addConstrs ((w_amount[w] >= waste_min[w] for w in waste), name="capacity2" )
Capacity3 = opt_mod.addConstr ((w_amount[waste[2]]- m_number[machine[0]]
* capacity_machine[machine[0]] <= 0), name="capacity3")
Capacity4 = opt_mod.addConstr((gp.quicksum(w_amount[w] for w in waste) - m_number[machine[1]]*
capacity_machine[machine[1]] <= 0), name ="capacity4")
Capacity5 = opt_mod.addConstr((w_amount[waste[0]]<= maxpyro), name ="capacity5")

```

Appendix C: User manual for the decision support tool

Introduction

Dear reader, in this chapter a user manual is provided for the CORE Chemistry decision support tool (DST). The DST is designed using Microsoft Excel and programmed with Visual Basics for Applications and Python. For the mathematical Mixed-Integer Linear Programming Model please refer to Chapter 4: Model Development.

Overview

The decision support tool can be accessed by downloading the CORE_DST.xlsm document and enabling macros. It is possible to input parameter values to the MILP model through the overview sheet of the model, shown in Figure 12.

CORE Chemistry - Decision Support Tool

Waste Inputs								
Waste	Type	Storage	Energy	Density	Processing price	Minimum Process Amount	Maximum Process Amount	Drying
Pyroresidue	Fuel	Silo	11.84	0.5	200	8000	24000	no
Dusty	Fuel	Silo	21	0.244	85	8000	1000000	no
Sludge	Fuel	Tank	13.3	0.451	100	0	1000000	yes
Shredder	Fuel	Silo	29	1.1	120	0	1000000	no
Flyash	Slag	Silo		0.8	150	2000	1000000	no
Soil	Slag	Silo		1.5	60	8000	1000000	yes
Oil	Support	Tank		0.9	200	0	1000000	no

Start Optimization

Storage Constraints		Time (in days)
Daybunker storage		1
General Storage		7
Drying time		7

Machine Data					
Machinery	Investment cost	Salvage value	Salvage value present	Depreciation Cost	Capacity
Dryer	1600000	160000	97524.93928	60099	57600
Mixer	250000	25000	15238.27176	9390	48000

Storage Data		
Storage	Cost	Height
Silo	160	3
Shed	260	3
Tank	400	3
Daybunker	35	1.25

Operation Constraints		Time
Operation days in a year		320
Maximum Capacity (tons/year)		120000
Minimum Capacity (tons/year)		100000

Chemical constants		Value
Dusty/Oil ratio		0.01
Flyash/Soil ratio		4
Energy for Slag		5.5

Figure 12: Decision Support Tool for CORE Chemistry

It is possible to input waste data, storage data and machine data values into the MILP model and test different scenarios. In this documentation a step-by-step approach on how to use the DST is provided.

Instructions on installation

In this section instructions on how to install the DST is given. Initially, ensure that following documents are downloaded locally to the desired computer in use:

- CORE_operation_data.xlsx
- MILP_CORE.bat
- MILP_CORE.py
- CORE_DST.xlsm

CORE_DST.xlsm is the main file where inputs can be done, and the model can be run.

CORE_operation_data.xlsx is the excel database where all parameter inputs are stored. This file is linked to the main macro-enabled excel document and is updated automatically. MILP_CORE.py is the python code for the MILP model and reads the data from CORE_operation_data.xlsx. The python code is linked to CORE_DST.xlsm with VBA using the batch file, MILP_CORE.bat. The batch file first activates the Anaconda environment and then executes the python code.

When all the files are downloaded, the python code, batch file and the VBA code needs to be altered to specify the location of the files. Ensure that the files are saved into the same file directory for ease of use.

REMARK: Once every document is downloaded ensure to place them in the same folder. For initial configuration make sure to first open CORE_DST.xlsm and then open CORE_operation_data.xlsx. This way the link between two excel files are safely created. When running the decision support tool always ensure that CORE_operation_data.xlsx is **not open**.

In the python file MILP_CORE.py the following lines of code must be altered:

```
#Read excel file and data sheets
fuel_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                          sheet_name = "FuelData", index_col=0)
slag_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                          sheet_name = "SlagData", index_col=0)
waste_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                           sheet_name = "WasteData", index_col=0)
storage_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "StorageData", index_col=0)
daybunker_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                               sheet_name = "DayBunkerData", index_col=0)
machine_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "MachineData", index_col=0)
notank_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                            sheet_name = "NoTank", index_col=0)
noshed_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "NoShed", index_col=0)
nosilo_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "NoSilo", index_col=0)
operation_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                               sheet_name = "AdditionalData", index_col=0)
drying_data = pd.read_excel(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx',
                             sheet_name = "Drying", index_col=0)
```

The full folder path of the saved CORE_operation_data.xlsx must be switched with lines of code where at the moment there is C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\CORE_operation_data.xlsx. Ensure that the file is saved.

This must be repeated for fuel_data till drying_data.

In the batch file MILP_CORE.bat C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\MILP_CORE.py must be switched with the file path of the python code MILP_CORE.py. Ensure that the file is saved.

```
@echo OFF
set root = c:\Users\ekink\anaconda3
call %root%\Scripts\activate.bat %root%
call activate base
"C:\Users\ekink\anaconda3\python.exe" "C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\MILP_CORE.py"
pause
```

Finally the VBA code must be altered. This can be done by **Developer > Visual Basic** in CORE_DST.xlsm and altering the following lines of code:

```
Option Explicit

Sub PythonScript()

Dim strBatchName As String
strBatchName = """"C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\MILP_CORE.bat""""
Shell strBatchName

End Sub
```

C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\MILP_CORE.bat must be changed with the file path of the MILP_CORE.bat batch document. Ensure that the file is saved.

OptimizedAmounts.xlsx is the spreadsheet where the optimization results are recorded. This document is created after the optimization process and is not included in the given files. Finally, following file path must be altered in the python file MILP_CORE.py

```
x = []
y = []
myvars = opt_mod.getVars()

for v in myvars[0:7]:
    x.append(str(v.varName))
    y.append(v.X)

d = {'Waste type':x, 'Value':y}
df = pd.DataFrame(d)

writer = pd.ExcelWriter(r'C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\OptimizedAmounts.xlsx')
df.to_excel(writer)
print('Optimized amounts are written successfully to excel file OptimizedAmounts.xlsx')
writer.save()
```

C:\Users\ekink\OneDrive - Universiteit Twente\Desktop\Bachelor Thesis\OptimizedAmounts.xlsx must be changed to the desired location where the final excel file should be saved. It is suggested to use the same folder as the previous files.

Running the model

Once the initial configurations with the file paths are made, the model can be run from the decision support tool document CORE_DST.xlsm. Open the file and ensure that all related files previously downloaded (especially CORE_operation_data.xlsm) are closed.

CORE_DST.xlsm initially contains the parameter values discussed in the thesis. If nothing is changed and the button **“Start Optimization”** is pressed the model will run with these values.

Inputs to the model can be easily changed by altering the numerical values in each table.

Waste Inputs								
Waste	Type	Storage	Energy	Density	Processing price	Minimum Process Amount	Maximum Process Amount	Drying
Pyroresidue	Fuel	Silo	11.84	0.5	200	8000	24000	no
Dusty	Fuel	Silo	21	0.244	85	8000	1000000	no
Sludge	Fuel	Tank	13.3	0.451	100	0	1000000	yes
Shredder	Fuel	Silo	29	1.1	120	0	1000000	no
Flyash	Slag	Silo		0.8	150	2000	1000000	no
Soil	Slag	Silo		1.5	60	8000	1000000	yes
Oil	Support	Tank		0.9	200	0	1000000	no

Table 13: Table for inputting waste values

The waste streams can be changed by altering the **“Waste”** column shown in Table 13. The type can be altered from the **“Type”** column and all the other different parameters can be altered from their respective columns. All columns of the waste table are available for inputting values.

Machine Data					
Machinery	Investment cost	Salvage value	Salvage value present	Depreciation Cost	Capacity
Dryer	1600000	160000	97524.93928	60099	57600
Mixer	250000	25000	15238.27176	9390	48000

Table 14: Table for inputting machine values

The machine parameter values can be input from Table 13. The only necessary input columns are the **“Investment cost”** and the **“Salvage value”**. From this **“Salvage value present”** and **“Depreciation Cost”** are automatically calculated. These values cannot be altered by the user directly. **“Capacity”** can be altered by the user.

The other values in Table 15 and Table 16 can be all altered by the user.

Once all the values are entered, the model can be run by pressing the “**Start Optimization**” button as shown in Figure **Error! Reference source not found.**

Storage Constraints	Time (in days)
Daybunker storage	1
General Storage	7
Drying time	7

Operation Constraints	Time
Operation days in a year	320
Maximum Capacity (tons/year)	120000
Minimum Capacity (tons/year)	100000

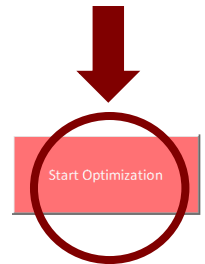
Chemical constants	Value
Dusty/Oil ratio	0.01
Flyash/Soil ratio	4
Energy for Slag	5.5

Table 15: Table for inputting storage values

Table 16: Other constraints

REMARK: If any parameter value is changed in the file CORE_DST.xlsm, open CORE_operation_data.xlsx and ensure that it is saved with the new parameter values. Then close the file CORE_operation_data.xlsx and then run the model from CORE_DST.xlsm by pressing the button as shown in Figure .

CORE Chemistry - Decision Support Tool



Waste Inputs								
Waste	Type	Storage	Energy	Density	Processing price	Minimum Process Amount	Maximum Process Amount	Drying
Pyroresidue	Fuel	Silo	11.84	0.5	200	8000	24000	no
Dusty	Fuel	Silo	21	0.244	85	8000	1000000	no
Sludge	Fuel	Tank	13.3	0.451	100	0	1000000	yes
Shredder	Fuel	Silo	29	1.1	120	0	1000000	no
Flyash	Slag	Silo		0.8	150	2000	1000000	no
Soil	Slag	Silo		1.5	60	8000	1000000	yes
Oil	Support	Tank		0.9	200	0	1000000	no

Storage Constraints	Time (in days)
Daybunker storage	1
General Storage	7
Drying time	7

Operation Constraints	Time
Operation days in a year	320
Maximum Capacity (tons/year)	120000
Minimum Capacity (tons/year)	100000

Chemical constants	Value
Dusty/Oil ratio	0.01
Flyash/Soil ratio	4
Energy for Slag	5.5

Machine Data					
Machinery	Investment cost	Salvage value	Salvage value present	Depreciation Cost	Capacity
Dryer	1600000	160000	97524.93928	60099	57600
Mixer	250000	25000	15238.27176	9390	48000

Storage Data		
Storage	Cost	Height
Silo	160	3
Shed	260	3
Tank	400	3
Daybunker	35	1.25

Figure 13: DST screenshot

Once the button is clicked the Command Window will open. In some cases, even though it is open, it does not appear on the screen, and it might be necessary to click on the icon on the task bar as indicated in Figure 14.



Figure 14: Taskbar

Once clicked following window will appear on the screen:

```
Academic license - for non-commercial use only - expires 2021-08-13
Using license file C:\Users\ekink\gurobi.lic
Gurobi Optimizer version 9.1.2 build v9.1.2rc0 (win64)
Thread count: 6 physical cores, 12 logical processors, using up to 12 threads
Optimize a model with 116 rows, 115 columns and 278 nonzeros
Model fingerprint: 0xae65fc7
Variable types: 92 continuous, 23 integer (21 binary)
Coefficient statistics:
  Matrix range      [7e-03, 1e+15]
  Objective range   [4e+01, 6e+04]
  Bounds range      [1e+00, 2e+04]
  RHS range         [1e+00, 1e+15]
Warning: Model contains large matrix coefficient range
Warning: Model contains large rhs
        Consider reformulating model or setting NumericFocus parameter
        to avoid numerical issues.
Found heuristic solution: objective 1.231194e+07
Presolve removed 105 rows and 94 columns
Presolve time: 0.00s
Presolved: 11 rows, 21 columns, 39 nonzeros
Found heuristic solution: objective 1.233460e+07
Variable types: 17 continuous, 4 integer (3 binary)
Root relaxation: objective 1.669817e+07, 8 iterations, 0.00 seconds
```

Figure 13: Optimization results shown from the Command Window

When scrolled down, the values of the decision values are visible. These values are also saved into a separate excel file called OptimizedAmounts.xlsx and text “Optimized amounts are successfully written to OptimizedAmounts.xlsx” must be visible from the Command Window at the very bottom.