Delft University of Technology

MASTER OF SCIENCE
in Chemical Engineering (track: process engineering)

MASTER OF SCIENCE
in Science Education & Communication (track: communication design for innovation)

Simulation of CO_2 capture and conversion into methanol using Aspen Plus and the design of an adaptive communication tool for the development of a shared vision within interdisciplinary virtual institutes

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by Jenke Anthea Tiesma

June 30, 2021

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Master Thesis June 2021

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Msc Chemical Engineering
Track: Process Engineering

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Track: Communication Design for Innovation

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Executive Summary

Climate change has been the topic of conversation in politics, society, university and industry for the past decades. As a society, we are slowly changing towards more environmentally friendly energy alternatives. However, besides our main source for energy, fossil fuels are currently also the primary feedstock for the chemical industry. In order to move towards a more sustainable future, there is a need for new methods of producing chemicals, without depending on fossil fuels. A promising method is the electrochemical conversion of CO_2 into chemicals, such as for example methanol. Therefore, the aim of this thesis is to find an optimal technological solution for the capture and of CO_2 and subsequent conversion of CO_2 to methanol with renewable based hydrogen, taking the socio-technological context into account.

This thesis is an integration between two master studies at the TU Delft: Chemical Engineering and Communication Design for Innovation. For the chemical engineering part of this research, the aim of the thesis is look at from a technological perspective. For the communication design for innovation part of this research, the aim of this thesis is viewed from a science communication perspective, focusing on the collaboration within research projects. Therefore are discussed in two separate summaries.

The research performed for chemical engineering part of this thesis fits within the activities of the e-Refinery institute. The communication part of this thesis uses the e-Refinery institute as a case study.

Chemical Engineering

The aim of the chemical engineering part of this thesis is to develop a process system model and performing simulation using a flow-sheeting package for conversion of CO_2 from a flue gas stream into methanol using hydrogen from a renewable source. The process has been simulated in Aspen Plus and a sensitivity analysis of the operating conditions (e.g. temperature and pressure) has been performed.

The process system model is simulated in three steps: (1) absorption, (2) stripping and (3) conversion. In the first step, CO_2 from a flue gas stream is absorbed into an aqueous mono-ethanolamine (MEA) solution with 30 wt% MEA using a 12-stage rate-based column. In the second step, CO_2 is stripped from the solvent using an identical 12-stage rate-based column. In the final step, CO_2 is converted to methanol, using H_2 in an adiabatic reactor with a length of 1.04 m and a diameter of 0.104 m. The flowsheet is finalized by integrated two recycle streams, a MEA recycle stream and a H_2 recycle stream.

The absorption step is simulated at a temperature of 40 °C and a pressure of 1 atm, resulting in 99.5% CO_2 absorption. The bottom stream of the absorber is led to a stripper, operating at 130 °C and 1.6 bar with a reboiler duty of 29.9kW, leading to 78.3% of the CO_2 being stripped from the solvent. The CO_2 pure stream leaving the stripper is compressed to 62 bar and mixed with H_2 in a mole-ratio of CO_2:H_2 of 1:4.2. Before the mixed stream enters the reactor, it is cooled to 68 °C. The CO_2 is converted into methanol with a yield of 37.9% and a selectivity of 99.9%.

A process system model has successfully been developed in this thesis, including the separation of CO_2 from a flue gas stream and the conversion of CO_2 into methanol, using H_2. The model has been finalized by integrating MEA and H_2 recycle streams. The final product is a methanol stream 83.4wt% methanol, 1.82wt% H_2O, 14.1wt% CO_2 and smaller amounts of N_2, H_2, CO and MEA.

Communication Design for Innovation

The aim of the communication part of the thesis is to develop a communication tool that aids research institutes, dealing with complex problems in uncertainty-rich projects, in the development of a shared vision.

In order to develop the communication tool, a systematic literature review has been performed around the drivers and barriers of the development of a shared vision. Furthermore, interviews with 9 members from the e-Refinery institute have been performed in order to find the particular drivers and barriers within this institute.

From the interviews, it is found that the design criteria for the development of a communication tool are (1) development of shared goals, (2) sharing of concerns and care for similar issues, (3) development of a shared vocabulary, (4) increasing interaction between members of the institute, (5) collective development of goals. An interactive virtual platform has been developed to aid in the development of a shared vision. The platform contains multiple features. The virtual platform includes a feature related to the sub-goals of individual researchers that are part of the institute Furthermore, concerns of the individual researchers can be added to the platform as well. The platform aids in the development of a shared vocabulary by integrating a language feature, where members are able to select unknown terms, jargon and equations, and other members can react to this by giving an explanation or an example, allowing the members of the e-Refinery institute to develop a shared vocabulary over time. The virtual platform is interactive in nature, meaning that members can react to each other and start discuss via the platform. The platform can also form the basis of new connections or new collaborations within the institute, which can be based on mutual goals, similar concerns or overlap in research methods.

The virtual platform is discussed and tested with two PhD students that are involved in the e-Refinery institute. Both were positive regarding the virtual platform, thinking it would be beneficial for the e-Refinery institute and fits the institute as well. The point of attention is the time needed to use the platform, it should not be too time consuming and fit in the daily work life of the researchers involved in the e-Refinery institute.

List of Abbreviations

Abbreviation	Explanation
CTM	CO_2 hydrogenation to methanol
DAC	Direct air capture
DEA	Diethanolamine
ENRTL	Electrolyte non-random two-liquid
EOS	Equation of state
FGD	Flue Gas Desulfurization
MEA	Monoethanolamine
MES	Microbial electrosynthesis system
MDEA	Methyldiethanolamine
MT	Metric tons
PBR	Packed-bed reactor
RK	Redlich-Kwong
RWGS	Reverse water-gas shift
SCR	Selective Catalytic Reduction
SNCR	Selective Noncatalytic Reduction

Abbreviation	Explanation
3mE	Mechanical, maritime and materials engineering
EEMCS	Electrical engineering, mathematics & computer science
NWO	Nederlandse organisatie voor Wetenschappelijk Onderzoek - Dutch Organization for Scientific Research
PI	Principal Investigator
TPM	Technology, policiy and management

List of symbols

Symbol	
α	Non-randomness factor
ϵ	Bed voidage
η_s	Dielectric constant of the solvent
$\lambda_i^{*,l}$	Thermal conductivity for liquid mixtures
λ_{solv}^l	Thermal conductivity for liquid solvent mixtures
μ	Fluid viscosity
ρ	Closest approach parameter
ρ	Fluid density
ϕ_s	Particle shape factor
τ_{ji}	Dimensionless interaction parameter
ω	Born coefficient
a_a	Reidel ionic coefficient
a_c	Reidel ionic coefficient
A_ϕ	Debye-Hückel parameter
D_P	Catalyst particle diameter
$\frac{dP}{dz}$	Change in pressure along reactor length
d_s	Density of the solvent
E	Reaction energy
G_f^0	Standard Gibbs free energy of formation of aqueous species
g_{ii}	Interaction energy between component i and i
g_{ji}	Interaction energy between component j and i
G_m^{*E}	Long range ion-ion interaction
$G_m^{*E,phd}$	Pitzer-Debye-Hückel contribution to the long range ion-ion interaction
$G_m^{*E,Born}$	Born contribution to the long range ion-ion interaction
$G_m^{*E,lc}$	Local interaction contribution to the long range ion-ion interaction
H_f^0	Standard enthalpy of formation of aqueous species
I_x	Ionic strength
k_0	Reaction constant
k	Boltzmann constant
$K_{a/b/c}$	Absorption constants
K_{pi}	Equilibrium constant of component i
k_i	Kinetic factor of component i
M_i	Molecular weight of component i
M_s	Molecular weight of the solvent
n	Reaction order
N_A	Avogadro's number
P	Pressure
P_C	Pressure at critical point
p_i	Partial pressure of component i
Q_e	Electron charge
R	Universal gas constant
r_i	Reaction rate of component i
r_i	Born radius of component i

S^0	Absolute entropy of aqueous species
T	Temperature
T_{bi}	Normal boiling point temperature of component i
T_C	Temperature at critical point
T_{Ci}	Critical temperature of component i
U	Superficial velocity
V	Volume
V_m^l	Apparent molar volume
x_{ca}^a	Mole fraction of the apparent electrolyte ca
x_i	Mole fraction of component i
z_i	Charge number of ion i

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I would like to thank Steven Flipse for supervising the communication part of my thesis. You were always available to help me, pushing me to do my best and a positive influence in times when I needed it. I would also like to thank Wiebren de Jong for the supervision of the chemical engineering part of my thesis. Helping me to think critically about my research and giving advice on how to improve. Furthermore, I would like to thank Caroline Wehrmann for being my second supervisor. You were a big help and motivator, giving me a boost of energy and inspiration after each meeting we had. Besides, my research would have been impossible without the aid and support of Hengameh Faramandazah. You were always there to help me with my research and the struggles I had in Aspen Plus. Thanks to you, I never felt like I had to solve it all alone, which helped me tremendously.

Furthermore, I would also like to thank all members of the e-Refinery institute, especially the ones that made time to be interviewed and to participate in my research. Not only did they help me to perform my research, all interactions were very inspiring and gave me much joy.

Finally, I was not able to finish this thesis without the support of my family and friends. I would like to thank them very much for listing to me, thinking with me and supporting me throughout the whole project.

Contents

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General introduction

In this general introduction, the context in which this research takes place is elaborated upon. This introduction first explains briefly the integrated aspect of this thesis. The rest of this research is split in two parts: part I Chemical Engineering, and part II Communication Design for Innovation. Both parts start with a more elaborate introduction to the research performed in each field. In part III, the integration between both fields is discussed.

This introduction gives a brief overview of the technological context of this thesis, including details about the basic chemical industry, as well as the methanol production industry. This is followed by a brief overview of the socio-technological context, which includes the concepts complex problems, uncertainty and adaptivity. Afterwards, the e-Refinery institute is presented. The research performed in the chemical engineering part of this thesis falls under goals of the e-Refinery institute. The science communication part of this research uses this institute as a case study. Finally, the overall problem description is given and this chapter wraps up with an overview of the structure of the rest of the report.

Integration of two fields

This thesis is the final research project that is performed to complete two masters at the Technological University of Delft: 1) MSc Chemical Engineering, with process as chosen track, and 2) MSc Communication Design for Innovation. This research integrates both fields of science communication and chemical engineering.

Technological Context

Climate change has been the topic of conversation in politics, society, universities and industry for the past decades. Society is slowly changing to more environmentally friendly alternatives. There has been plenty of research into greener alternatives for energy supply, such as wind energy or solar energy. Even though these forms of energy can decrease the need for oil, coal and natural gas, they cannot fully cover our dependency on fossil fuels. Fossil fuels are also the primary feedstock for the production of basic chemicals. In order to move towards a more sustainable future, there is a need for new methods of producing basic chemicals, without using fossil fuels as main feedstock.

Basic Chemicals

The chemical industry can be divided into three categories: basic chemicals, speciality chemicals and consumer chemicals. Basic chemicals are often intermediate products which are sold within the chemical industry or other industries for further processing before becoming products. The industry of basic chemicals is characterized by its enormous quantities (in the order of millions of tonnes). The industry of basic chemicals can roughly be divided into petrochemicals (chemicals derived from oil), polymers and basic inorganics. The industry of speciality chemicals is characterized by smaller quantities compared to the industry of basic chemicals (in the order of kilograms to tonnes), but with a higher value. Chemicals in this industry include amongst others pesticides, paints and inks. The industry of consumer chemicals is characterized by the direct sale to consumers, such as soaps and detergents [67].

The amount of sales (in %) in 2014 in Europe for each of these three categories is shown in Figure 1a. As can be seen, the industry of basic chemicals accounts for 60% of all sales, while the speciality chemicals and consumer chemicals only account for 28% and 12%, respectively [67]. Similar numbers can be seen for the sales in the United States.

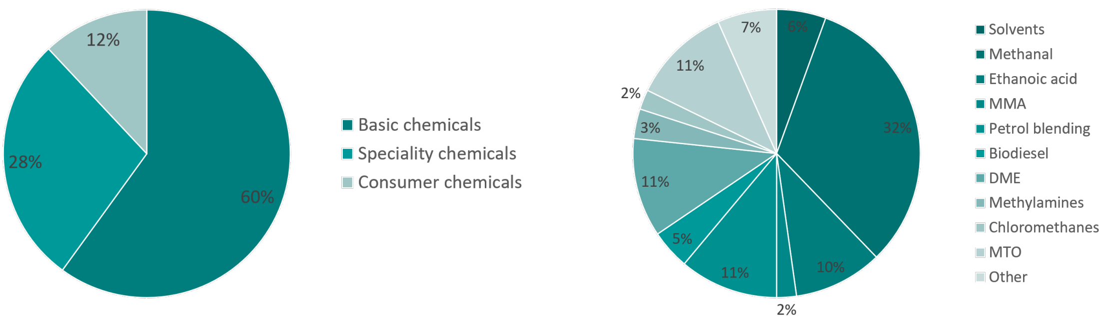
The basic chemical industry can be divided into seven sub-sectors: (1) industrial gases, (2) dyes and pigments, (3) other inorganic basic chemicals, (4) other organic basic chemicals, (5) fertilizers and nitrogen compounds, (6) plastics in primary forms, (7) synthetic rubber in primary forms. Of these seven sub-sectors, the two largest are "Other organic basic chemicals" and "plastic in primary forms" account together for 53.7% of the total amount of enterprises in Europe [90].

Basic chemicals are molecules based on mainly carbon, hydrogen, oxygen, nitrogen and sulfur atoms. The main raw material for the production of these chemicals is still petroleum. To give some ideas about the numbers, in Germany, crude oil accounts for roughly 75%, natural gas for 11% and coal for about 1%, while the amount of renewable raw materials has been stable for the past years at around 13% [92]. However, renewable sources are mainly used for the production of surfactants or everyday products such as plastics or additives, the share of renewable raw materials is still much lower for the production of chemicals [92]. In order to move towards a fossil free future and produce more sustainable basic chemicals, new, greener, raw materials have to be explored. The main bottleneck in producing basic chemicals in a sustainable manner, is on finding an alternative carbon source that is renewable and not depleting. Currently, the two most commonly mentioned carbon sources are biomass and CO_2. The research performed in this thesis focuses only on CO_2 as carbon source. The advantage of utilizing CO_2 is that CO_2 is a waste product and global emissions of CO_2 have been increased over the past decades. Turning CO_2 into valuable products is potentially both economically and environmentally beneficial, if the technology is coupled with renewable energy sources such as wind and solar power, or alternatively nuclear power.

Methanol as basic chemical

An important basic chemical is methanol. Methanol is an important intermediate for other bulk chemicals, including everyday products such as silicons, paints and plastics [1]. Furthermore, methanol is also a widely used solvent. The global production of methanol has been increasing over the past years, from 32 million metric tons (MT) in 2006 to a prediction of almost 100 MT in 2020 [39].

Currently, methanol is commercially produced from methane on a large scale [1]. So in order to move away from the fossil based society that we currently live in, other sources as raw materials have to be investigated and explored. A possible raw material for methanol production is CO_2. Possible sources of CO_2 would be CO_2 emitted from industrial plants, such as fossil fuel power plants or biogas power plants. Another possibility is to retrieve CO_2 directly from air (Direct Air Capture).



(a) (b)

Figure 1: (a) Sales (in %) per category of the chemical industry, adapted from the Essential chemical Industry [67], (b) Methanol uses, adapted from the Essential Chemical Industry [67]

Problem description

This thesis focuses on a way of producing basic chemicals in a more environmentally and greener way compared to the production of basic chemicals from oil.

This thesis focuses on the following overall goal:

> *Finding the optimal technical solution for the capture of CO_2 and subsequent conversion of CO_2 to methanol with renewable based H_2, taking the socio-technological context into account.*

This goals leads to the following overall research question:

> *How can technical solutions be developed for the capture of CO_2 and subsequent conversion of CO_2 into methanol with renewable based H_2, while managing uncertainty in the development of technical solutions?*

The e-Refinery institute

The research done for the chemical engineering part of this thesis falls within the research activities of the e-Refinery institute. The e-Refinery initiative was launched in may 2018 and has been growing rapidly since then [62]. Recently the initiative has grown into a research institute. This institute is a cross-disciplinary initiative, set-up by the TU Delft, collaborating with multiple industries with the main overall goal to move towards a more sustainable future that is not dependent on fossil fuels.

The e-Refinery institute is involved in the energy transition and focuses on the implications for the chemical industry. The institute brings researches and industrial partners together to develop the required technologies and human capital. The research that the e-Refinery initiative focuses on is the electrochemical conversion of sustainable electricity, water and air into fuels and chemical building blocks (e.g. basic chemicals), from a molecular scale to large-scale system integration. The e-Refinery faces three important societal challenges: CO_2 neutral fuels, seasonal energy storage and defossilization of the chemical industry [65].

The cross disciplinary approach

The e-Refinery institute consists of researchers from different backgrounds working together. This means that there is knowledge from different expertise, and this is integrated in different programs. The e-Refinery institute group is supported by the following faculties from Delft University of Technology: (1) Electrical Engineering, Mathematics and Computer Science, (2) Applied Sciences, (3) Mechanical, Maritime and Materials Engineering, (4) Technology, Policy and Management, (5) Aerospace Engineering.

Within these faculties, research is performed within the following disciplines: (1) power engineering, (2) catalysis, (3) electrochemistry, (4) material sciences, (5) transport phenomena, (6), reactor engineering, (7) process intensification, (8) process control, (9) separation technology, (10) energy technology & system engineering, and (11) process and system integration & societal embedding.

The institute consists of over 40 principal investigators and 50 postdoctoral researchers and doctoral researchers. Furthermore, the institute collaborates with different industries, research institutes, governments and academia.

Three-folded goals of the e-Refinery Institute

The institute is not only an institute for technological development and change, it has formulated goals on the technological, collaboration and education side of the project. These goals are shown in Figure 2, as formulated by the e-Refinery institute [64].

Figure 2: Three goals of e-Refinery institute (Adapted from e-Refinery [64])

Technological goals of e-Refinery

As shown in Figure 3, within the e-Refinery institute, research is performed at three different scales within different disciplines and two research lines (indirect and direct route). These scales are:

- Micro scale: In this scale, research is carried out on the fundamental basis, such as research related to catalysis, choice of electrode material, electrolyte and membrane. Choices that are made here, will impact how certain technologies will develop and whether they will be commercially viable.
- Meso scale: The main goal of this scale is to use insights from the micro scale in order to design, engineer and optimise new and existing technologies.
- Macro scale: The research related to this scale focuses more on the integration and societal embedding of the new technologies.

Furthermore, a distinction can be made between direct and indirect conversion of CO_2:

- Direct oxidative route: this route is used to produce short chain olefins (C_2H_2, C_3H_6), oxygenated products (CH_3OH, CH_2O, $HCOOH$) and hydrocarbons.
- Indirect oxidative route: this route is used to produce syngas, this syngas can be further processed into almost any kind of fuel or chemical.

The e-Refinery Institute - dynamics

As most research initiatives, the e-Refinery institute takes place in a larger network. As illustrated in Figure 4, different levels of the network can be distinguished. The largest rectangular layer represents the society in which projects take place. The smaller circles represent the different industries and research teams that work within the e-Refinery project, or are in some other ways involved with the project. The individual researchers within research teams or industries are represented by bold dots. Between the different parties, there are always key figures that facilitate cooperation and communication, which are represented by the bold rectangles on the

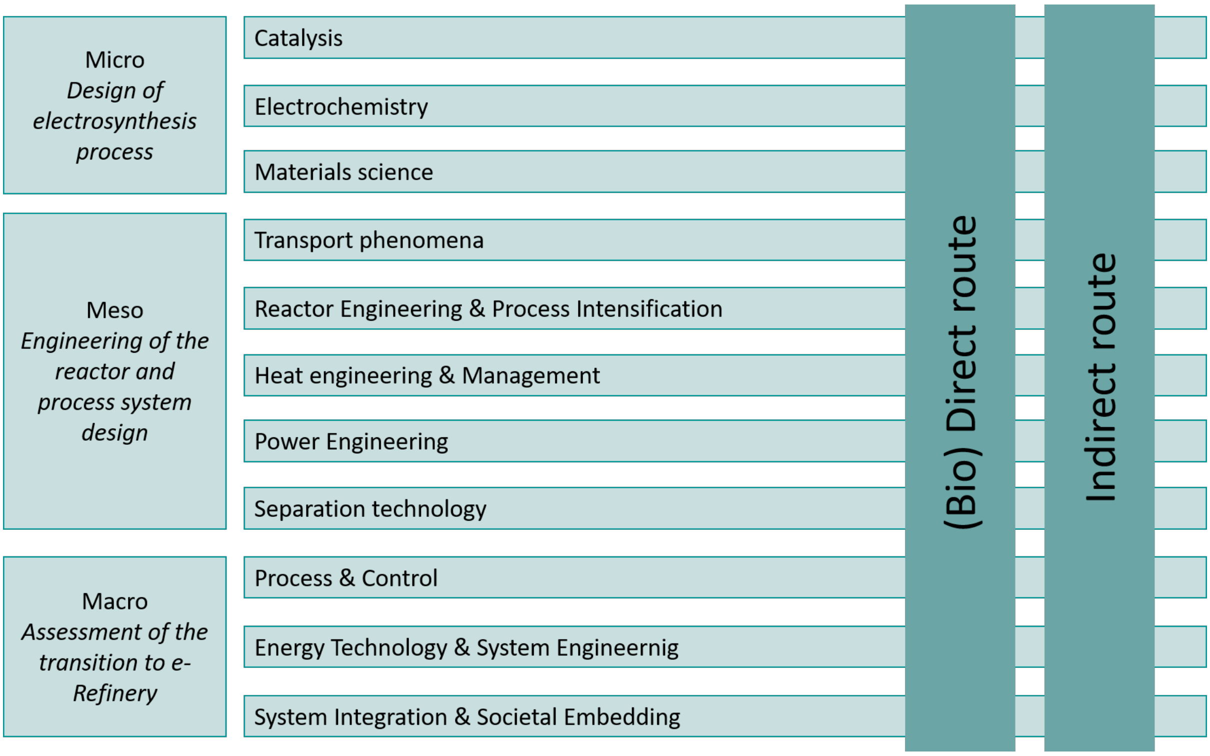


Figure 3: Overview of the disciplines, scales and research lines of the e-Refinery institute (adapted from the e-Refinery website [65])

interface of the link between the parties. The interaction and relations between the parties are shown with a dotted line.

The case study has an individual approach, focusing on researchers and key figures as an individual rather than focusing on cooperation links and the network itself.

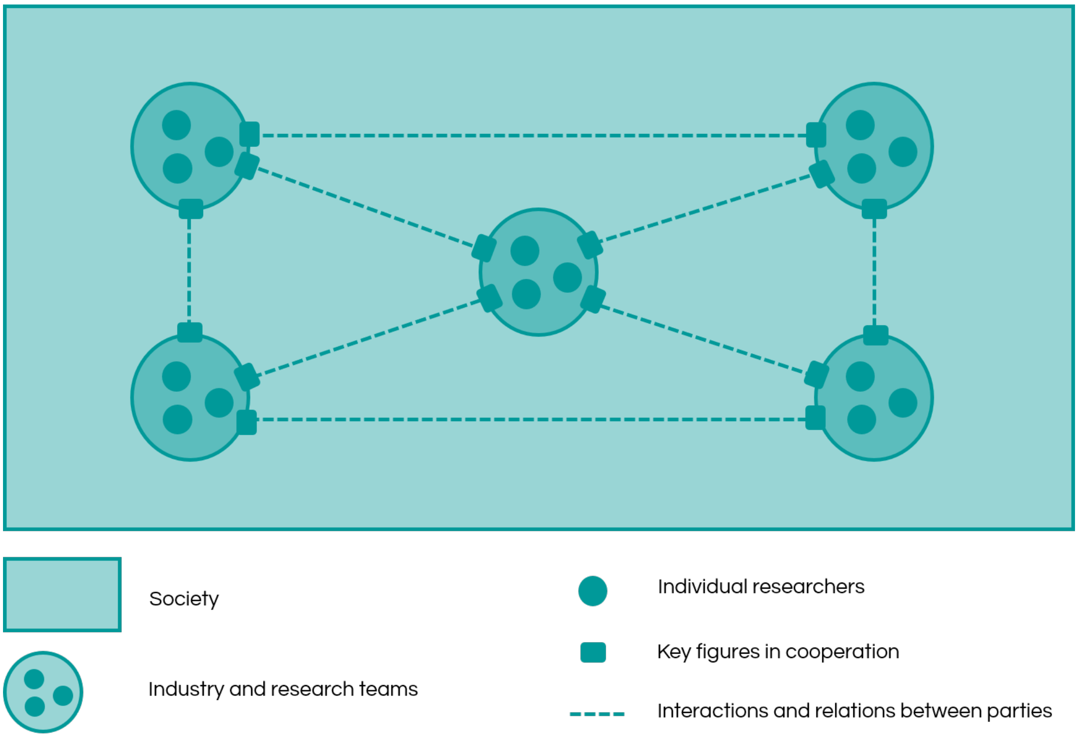


Figure 4: Levels of the network visualized for the e-Refinery institute.

Complex problems

Complex systems are characterized by Rauws (2017) by their openness, dynamics and non-linearity. By openness is meant that these systems exchange both information and energy with the environment, which makes the systems subjective to changes in the environment. Dynamics and non-linearity refers to the way a system responds to changes, meaning that small changes can possibly have large effect on the system, and large changes might only have a small effect [75].

Dorado and Ventresca (2013) use the concept of wicked problems to characterize complex problems, stating that complex problems can be defined by their absence of well-structured solutions and interconnectedness and circular causality; a sequence in which causes and effects lead back to the original cause, leading to a feedback loop [23]. To deal with this kind of complex problems, it is often needed to form a collaboration between multiple organizational sectors and different disciplines [44].

Based on the above given definitions, it can be argued that e-Refinery is also dealing with a complex system, working on complex problems.

Uncertainty

Uncertainty within a project cannot simply be defined as the lack of knowledge, since uncertainty can exist in situations in which plenty of information is available. Furthermore, additional information can both increase or decrease the level of uncertainty. Uncertainty is defined by Walker et al. (2003) as: *"any deviation from the unachievable ideal of complete deterministic knowledge of the relevant system"* [93].

Using this definition of Walker, uncertainty is inevitable in any project. In order to make the concept more tangible, the different facets of uncertainty must be explored and elaborated upon.

Uncertainty can manifest itself in different areas within a project, Ward and Chapman (2001) distinguish five different areas of uncertainty [95]:

1. Estimates of project parameters. This type of uncertainty is mainly concerned with the size of the project (e.g. time, cost, quality, etc.) and is possibly caused by lack of experience, clear requirements, complexity, limited analysis of processes involved and unforeseen events.

2. Basis of estimates of project parameters. This type of uncertainty is mainly caused by lack of objective or statistical data and an important source are assumptions.

3. Design and logistics. This type of uncertainty lies in the nature of the project deliverables and process of producing these. This uncertainty can be reduced by clearly specifying what is done, how, by whom and at what cost.

4. Objective and priorities. This uncertainty deals with clarity about project objectives, relative priorities between them and acceptable trade-offs.

5. Relationships between project parties. This uncertainty lies in the complex nature that might be present between various cooperating parties. This might introduce uncertainties in respect to specification of responsibilities, perception of roles, capabilities of parties, and communication across interfaces.

Besides the different areas in which uncertainty might play a role, Walker et al use different dimensions to clarify and specify uncertainty in projects. Three dimensions of uncertainty are distinguished by Walker et al. [93]:

- Location of uncertainty: in which parts of the system the uncertainty manifests itself.
- Level of uncertainty: determines how uncertainty a certain system is, ranging from deterministic knowledge to complete ignorance.
- Nature of uncertainty: the underlying phenomena that causes uncertainty in the system.

Engle (2011) argues that adaptivity is crucial when dealing with uncertainty, as it gives tools to anticipate or respond to perceived or current stresses. Thereby, adaptive capacity has an influence on the potential of implementing sustainable technologies [27]. Adaptivity can be defined in terms of flexible decision making and adjustment to uncertainties [103].

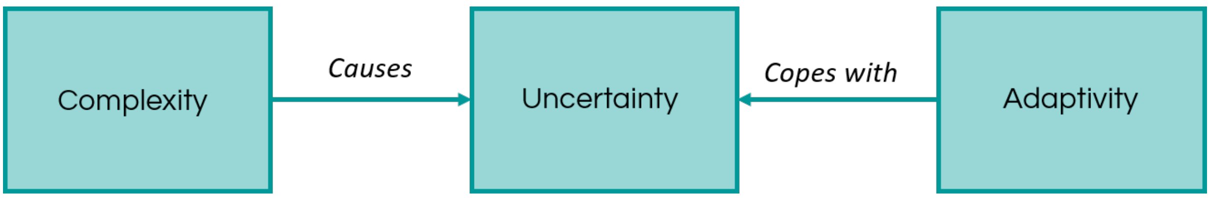


Figure 5: Relation between the concepts complexity, uncertainty and adaptivity (adapted from Vos (2020) [91])

The model by Vos (2020) in Figure 5 shows the relationship between the concepts complexity, uncertainty and adaptivity. Complexity is a cause and the nature of uncertainty within a project. The complex nature of a social-technological system makes it impossible to completely understand how the system reacts and responds to factors that are inherently part of the system, leading to an increased level of uncertainty [43]. Adaptivity is a way of coping with this uncertainty.

This research aims to use adaptivity as a concept to cope with uncertainty in the e-Refinery institute.

Structure

This report is divided into three parts: (I) chemical engineering, (II) science communication, and (III) integration between both fields. The first part takes a chemical engineering point of view to evaluate the research goal, while the second part uses a science communication approach. The report finalizes with an integration between both fields, showing the connection and synergy between the two fields.

The chemical engineering part of the report starts with an introduction to the problem from a technological perspective. Afterwards, an overview of the relevant background information is presented. This is followed by the methodology that is used in this research. Afterwards, the results are presented, followed by a discussion. The chemical engineering part wraps up with a conclusion and recommendations for future research.

The communication part of the report takes a science communication point of view to look at the problem. This parts start with a general introduction, which includes a more in-depth explanation of how the research is structured. This part of the research contains three phases: (1) discovery phase, (2) deepening phase, and (3) design phase. In the discovery phase, the problem is discovered by performing three interviews, leading to a problem direct. The deepening phase consists of two parts: a systematic literature review and interviews. In the last phase of this research, the design phase, a communication tool is designed and tested. Afterwards, the research methods and the results are discussed. This part finalizes with a conclusion.

In the third part of this research, a final note is given regarding the integration of the two fields.

Part I

Chemical Engineering

1 Introduction

The first part of this report focuses on the chemical engineering part of this research. In this part, a simulation is developed for the capture of CO_2 and the conversion of CO_2 into methanol (CH_3OH).

1.1 From CO_2 to valuable chemicals

There are five general techniques of conversion of CO_2 into valuable fuels or chemicals by using solar energy combined with water electrolysis for the production of hydrogen [60]:

1. Photochemical conversion: in this technique, sun light is used to reduce CO_2. The advantages of this method are the low temperatures of operation, small amount of energy input required, workable pressure, no negative impact on the environment. The main limitations are the low photocatalytic activity and selectivity.

2. Biochemical conversion: this comprises of solar energy conversion into chemicals through natural photosynthesis or enzymatic conversion in order to generate biofuels. The main limitations of this process are the high costs of enzymes, high sensitivity towards the environment, no straight-forwards scaling up methods, the reactions or co-factor dependent, which increases the price even more.

3. Electrochemical conversion: electricity is used to convert CO_2 into other chemicals. The main advantages are ability to control the process through reaction temperature and electrode potential. The main challenges are the slow kinetics of CO_2 reduction and small energy efficiencies.

4. Plasma chemical conversion: plasma is a gas that is (partially) ionized, consisting of electrons and neutral species, including different kinds of ions, radicals, molecules, and excited species. Plasma gas has the ability to split CO_2, however it is still not sufficiently energy efficient to produce plasma using electrical power.

5. Solar thermochemical conversion: CO_2 can also be reduced using direct solar energy, thermal conversion or quantum conversion. The main advantage is the direct utilization of sunlight in the conversion process. The main challenge for this technique lies in solving the thermal losses issues in the reactor.

1.2 Objectives, Goals and Research Questions

The overall goal of this part of the research is stated as follows:

> *The goal of this part of the research is developing a process system model and performing simulation using a flow-sheeting package for conversion of CO_2 from a flue gas stream into CH_3OH using H_2 from a renewable source.*

In order to develop the simulation, three main steps have to be taken:

- Separation of CO_2 from a flue gas stream
- Conversion of CO_2 into CH_3OH using H_2 from a renewable source
- Separation and upgrading of CH_3OH

1.2.1 Research Questions

The overall research question for this part of the research has been stated as followed:

> *What is the optimal process design and operating conditions for the production of CH_3OH from CO_2 from a flue gas stream using an aqueous amine solution?*

So for each step in the separation and conversion of CO_2, several sub-questions have been proposed.

Separation of CO_2 from flue gas:

1. Which techniques are available for the separation of CO_2 from a flue gas stream?
2. What are the optimal operating conditions (pressure, temperature and solvent wt%) for the separation of CO_2 from a flue gas stream using an aqueous amine solution?

Conversion of CO_2 to CH_3OH:

1. What are the possible techniques for the conversion of CO_2 into CH_3OH?
2. What are the optimal operating conditions (hydrogen input, pressure and temperature) for the conversion of CO_2 into CH_3OH

Regarding the separation and the upgrading of the methanol, the goal is to produce a methanol product with at least 85 wt% methanol. This includes a first step in the purification of the methanol to show that the process could lead to a valuable methanol product. In general, industrially sold methanol has a purity of 99.8% or higher. Since the focus of this thesis is on the optimization of the absorber, stripper and reactor, it is chosen to focus on these blocks and the further purification of methanol to an industrial grade is out of the scope of this thesis.

1.2.2 Methodology outline

The three steps (separation of CO_2 from a flue gas stream, conversion into CH_3OH and upgrading) are simulated in Aspen Plus V8.8. Each step is compared to available data in literature. The separation of CO_2 from a flue gas stream is simulated using a rate-based absorption and stripping model, RateSep. CO_2 is absorbed in an aqueous MEA solution. The conversion of CO_2 into CH_3OH is simulated with an adiabatic reactor. The methanol is upgraded using a distillation column. The process flowsheet is finalized by adding two recycle streams: a MEA recycle stream and a H_2 recycle stream

1.3 Structure of Part I

Part I of this report starts with an overview of the theory behind the processes that take place in the simulation. In this section, the different separation techniques to separate CO_2 from a flue gas stream are discussed, as well as the different techniques for the conversion of CO_2 into CH_3OH. Afterwards, the set up for the simulations is explained, including the theoretical background for the Aspen Plus simulations. Later, the separation and conversion steps in Aspen Plus are discussed, including a sensitivity analysis for the simulation. The results of the sensitivity analysis is discussed, concluding with an overall process design that includes recycle streams as well. The results are discussed in a discussion. This part of the research wraps up with a conclusion.

2 Theoretical background

This section gives an overview of the theoretical background of this research project. Section 2.1.1 provides information about the absorption and stripping process of CO_2. Section 2.3 describes the theoretical background behind the conversion of CO_2 into CH_3OH. In Section 2.4 the thermodynamic model that is used for the Aspen Plus simulations is elaborated upon.

2.0.1 CO_2 sources

One possible CO_2 source is flue gas. Gas turbines produce flue gas with around 3 mole% CO_2, for natural gas plants, this is around 5-6 mole% CO_2 and coal-fired power plans generate 10-12 mole% CO_2 [32]. For natural gas plants, the temperature of a flue gas is around 110-120 °C [46]. The input temperature for the absorber should be around 40 °C [69, 46]. In the flue gas, there are also NO_x, SO_x and other impurities present. These impurities have to be removed before the absorption, since the NO_x and SO_x can both react with amine solvents. Both impurities can irreversibly react to generate heat stable salts, which can not be reclaimed and thus leads to solvent lost [46]. NO_2 is the nitrogen-oxide that is responsible for the reaction and the level of NO_2 should be below 20 ppmv [46]. Most modern plants produce flue gas with a concentration already lower than 20 ppmv, so NO_2 generally forms no problem. Levels of SO_2 are recommended to be below 10 ppmv. In general,SO_x compounds are removed from the flue gas in desulfurisation processes, hereby it is a trade-off between costs required for desulfurisation and solvent makeup costs. [46]

The maximum recommended concentration of different impurities are summarized in Table 1.

Table 1: Maximum level of impurities in the flue gas stream before entering absorber [46]

Impurity	**Maximum recommended concentration**
NO_2	20 ppmv
SO_x	10 ppmv

Table 2 shows the composition of different flue gasses, including flue gasses form a coal fired plant and from a natural gas plant, given by the article from Desideri et al (2011), and the flue gas composition as specified by Plaza et al (2010) [22, 69].

Table 2: Flue gas compositions (Retrieved from Desideri et al (2011) and Plaza et al (2010) [22, 69])

Mole fraction	**Coal**	**Natural Gas**	**Plaza**
H_2O	0.062	0.174	0.066
CO_2	0.132	0.087	0.133
N_2	0.758	0.0721	0.81
O_2	0.048	0.017	-

2.1 CO_2 separation techniques

There are different techniques to separate CO_2 from a gas stream. The most common techniques are showing Figure 6.

2.1.1 Absorption

There are two main ways of absorbing CO_2 from a gas stream:

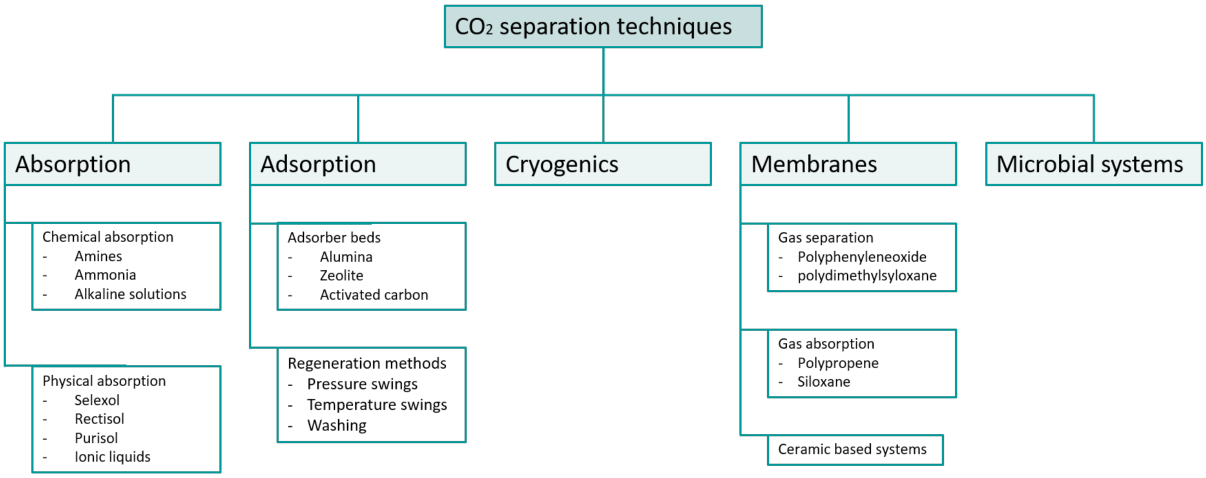


Figure 6: Techniques for the separation of CO_2 (adapted from Rao and Robin (2002) [73])

- Physical absorption
- Chemical absorption

In the physical absorption process, the CO_2 is physically absorbed into a solvent. The solubility of CO_2 follows Henry's law and the process is favoured by high pressure and low temperature operating conditions [79]. Ionic liquids can be used to physically or chemically absorb CO_2. For the physical absorption process, the CO_2 solubility in ionic liquids is influenced by the free volume and size of the ionic liquid, as well as the cation and anion. Generally speaking, the anion has a greater influence on the CO_2 solubility compared to the cation [105].

In the chemical absorption process, the CO_2 undergoes a (reversible) chemical reaction with the solvent, forming weakly bonded intermediates. Chemical absorption is in general more suitable for gas streams with low partial pressure of CO_2, such as air which has 413 ppm of CO_2 [8]. Aqueous amine solutions are traditionally a popular choice as solvent, since the absorption capacity is good, and the solvent is highly reactive and selective towards CO_2. Furthermore, aqueous amine solutions are economically beneficial due to their general low price. However, the disadvantages of using aqueous amine solutions are the relatively high energy needed for regeneration of the solvent, the volatility leading to a loss of solvent and the corrosive properties of the solvent [79]. Considering both the advantages and disadvantages, amines are still considered the most feasible option for the removal of CO_2 from flue gas from coal-fired or natural-gas fired power plants [69]. Regeneration is typically done at higher temperature of 100 - 130 °C and increased pressure of 1.5 to 2 bar [51]. Typical energy requirements vary between 4 and 5 GJ/tonCO_2 [51].

2.1.2 Adsorption

Adsorption is a physical process in which a gas or liquid attaches to solid surfaces, such as activated carbon, alumina, metallic oxides and zeolites [94]. The adsorbed compound can be regenerated by increasing the temperature (temperature swing adsorption) or by reduction of pressure (pressure swing adsorption), or a combination.

Adsorption is generally less suitable for gas streams with a low CO_2 concentration, since most adsorbents have a low selectivity and low adsorption capacity of CO_2. Furthermore, some adsorbents such as zeolites have a strong affinity for water vapour, making them less suitable for adsorption of CO_2 from flue gases. Due to the low adsorption capacity, it is generally more difficult to scale up, making it less suitable for large-scale power plant flue gas treatment [94].

2.1.3 Cryogenics

Cryogenic separation systems separate CO_2 from a gas stream by condensation. At a temperature of -56.6 °C and atmospheric pressure, the CO_2 condenses and can be separated from other compounds. This technique is more suitable for gas streams with higher CO_2 concentration, since the costs of refrigeration are relatively high [94].

2.1.4 Membrane-based separation and absorption

Membranes can be used in combination with gas absorption or gas separation processes. In gas absorption process, the membranes are located between the gas stream an the liquid solvent. In order to allow CO_2 transport across the membrane, it is required that the pressure of the liquid side and gas sides are equal. The efficiency of the separation process depends on the partial pressure of CO_2, which makes this process suitable for gas streams with high CO_2-concentration (concentration should be at least above 20 vol%) [94].

In gas separation processes, the CO_2 is separated from a gas stream by the selective membrane itself. This technique uses differences of permeation rates as basis of separation. Permeation rates are dependent on molecule size, diffusion coefficients and membrane material. The driving force of this type of separation is the difference in partial pressure of the components on both sides of the membrane. The main drawback of this type of separation is the low CO_2 capture capacity and the low purity of the captured CO_2. This can both be improved by using a multistage separation, however this does increase capital and operating costs [94]

2.1.5 Microbial systems

There are different types of microorganisms that are able to capture CO_2, including bacteria, cyanobacteria, algae, and archaea. In nature, these microorganisms are able to capture atmospheric CO_2 and convert it into other carbon-based products. The advantages and disadvantages of the different types of microorganisms are shown in Table 3.

2.1.6 Chosen separation technique

For the case of separating CO_2 from a flue gas stream, the separation technique should be able to handle the relatively low partial pressure of CO_2 in the flue gas stream. Therefore, it is decided to use a chemical absorption technique to separate the CO_2 from the flue gas stream.

Table 3: Advantages and disadvantages of different microorganisms (Retrieved and adapted from Kumar (2018) [49])

Microorganism	Advantage	Disadvantage
Bacteria	Easy grow under moderate nutrition conditions Simple and inexpensive cultivation	Temperature, pH, intensity of light affect productivity Require proper C:N ratio
Cyanobacteria	Easy cultivated Fast CO_2 utilization	Light (intensity, wavelength) and water requirement high phosphorous requirement
Algae	Aerobic microorganisms and easy cultivation Diverse carbon sources and carbon utilization pathways	Fermentation process under development High contamination changes
Archaea	CH_4 production	Fermentation process still under development Growth conditions difficult to maintain

2.1.7 Conversion route - overview

The process scheme for the conversion route that is proposed is shown in Figure 7. The first step in this route is the absorption of CO_2 from a CO_2 source. This is done in an absorption column with monoethanolamine (MEA) as solvent. In the second step, the absorbed CO_2 is sent to a stripper in which the CO_2 is desorbed. The solvent is regenerated and used again in the absorber. The remaining CO_2 is send to Reactor 1, in which the CO_2 reacts with hydrogen (H_2) into methanol (CH_3OH).

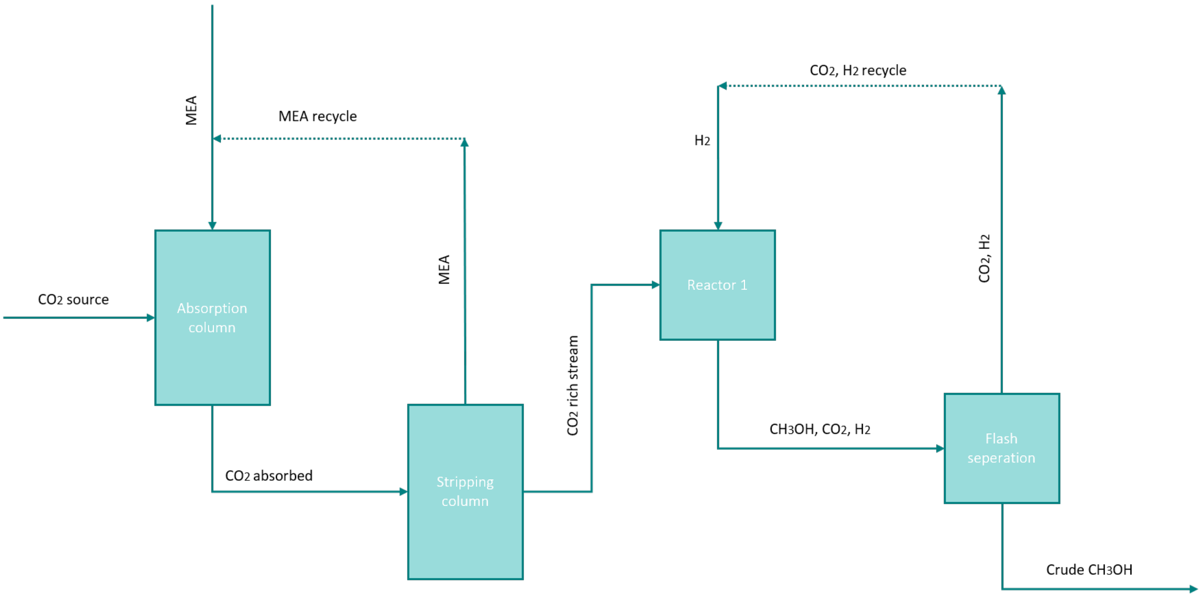


Figure 7: Block diagram for the capture of CO_2 and conversion into CH_3OH

2.2 Chemical absorption and stripping

The CO_2 is separated from a flue gas stream using a chemical absorption and stripping units.

2.2.1 Absorbing solvents

The most common amine based solvents for absorption of CO_2 are monoethanolamine (MEA), diethanolamine (DEA) and methyldiethanolamine (MDEA) [38]. The structures are shown in Figure 8.

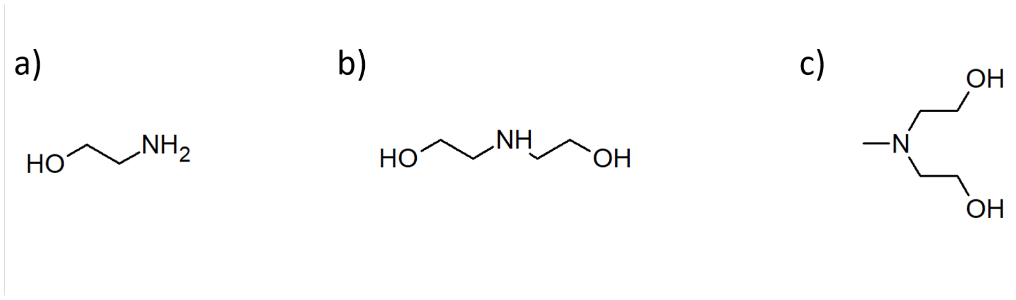


Figure 8: Molecular structures of (a) monoethanolamine (MEA), (b) diethanolamine (DEA), and (c) methyldiethanolamine (MDEA)

The main advantages and disadvantages of MEA, DEA and MDEA are shown in Table 4.

Table 4: Advantages and disadvantages of MEA, DEA, and MDEA (Retrieved from Singh (2011), Kim (2015), and Xue (2017) [84, 42, 104])

Amine	Advantage	Disadvantage
MEA	High reactivity Fast reaction kinetics Low solvent cost Ease of reclamation Low solvent costs Low adsorption of hydrocarbons	CO_2 loading limited to 0.5 mole of CO_2/mole amine High energy requirement for regeneration
DEA	Suitable for low pressure operations Lower heat of reaction with CO_2 Fast reaction kinetics Low solvent costs Less reactive to sulphur components	High energy requirement for regeneration
MDEA	High loading capacity (1.0 mol of CO_2/mole of amine) Low enthalpy of reaction with acid gases Lower regeneration energy requirements Suitable for gas streams containing both CO_2 and H_2S	Slower reaction rate of CO_2 absorption

Primary and secondary amines, such as MEA and DEA, are able to react directly to CO_2 and form a carbamate ion. The reaction mechanism is based on the formation of a zwitterion, followed by the removal of the proton by a base B. The general reactions are shown in Equation 1 and Equation 2 [84]. R_1 and R_2 represent the substituted groups attached to the amine group and B represents a base molecule, which may be a hydroxyl ion or water.

$$\mathrm{CO_2 + R_1R_2NH \rightleftharpoons R_1R_2NH^{+}COO^{-}} \tag{1}$$

$$\mathrm{R_1R_2NH^{+}COO^{-} + B \rightleftharpoons R_1R_2NCOO^{-} + BH^{+}} \tag{2}$$

The zwitterion is the intermediate species in this reaction and is likely to be very unstable. Therefore the zwitterion may be an transition state or it may be a very short-lived species [84]. Therefore, the reaction is often given as a single step, Equation 3.

$$\mathrm{CO_2 + R_1R_2NH + B \rightleftharpoons R_1R_2NCOO^{-} + BH^{+}} \tag{3}$$

The reaction mechanism for this reaction is shown in Figure 9.

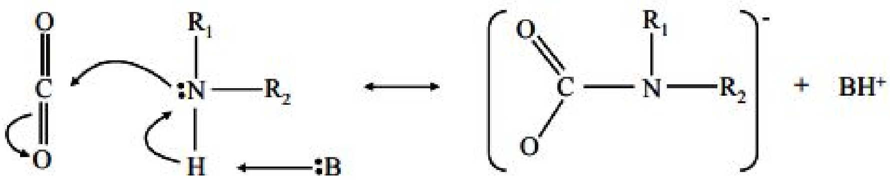


Figure 9: Reaction mechanism for CO_2 reacting with primary or secondary amines (retrieved from Singh (2011) [84])

Tertiary amines, such as MDEA, cannot directly reactor with CO_2 to form a carbamate ion due to the lack a free proton. The reaction mechanism for tertiary amines is given in Equation 4 5 and 6 [84].

$$\mathrm{CO_2\,(aq) + H_2O \rightleftharpoons H_2CO_3} \tag{4}$$

$$\mathrm{CO_2\,(aq) + OH^{-} \rightleftharpoons HCO_3{}^{-}} \tag{5}$$

$$\mathrm{CO_2 + R_1R_2R_3N + H_2O \rightleftharpoons R_1R_2R_3N^{+}H + HCO_3{}^{-}} \tag{6}$$

Using a $MEA - H_2O$ solution has as advantage that MEA is highly reactive with CO_2, a high limit load (0.5:1 mole CO_2:MEA) and relatively low molecular weight. The main drawback is the great stability of the carbamate ion. Due to the stability of the carbamate ion, more heat is required for the regeneration [22].

2.2.2 Reaction mechanism

In the chemical absorption process, the CO_2 reacts with the solvent (MEA). In the MEA-CO_2-H_2O-system, there are several equilibrium reactions taking place, Equation 7 to 11.

$$2\,\mathrm{H_2O} \rightleftharpoons \mathrm{H_3O^+} + \mathrm{OH^-} \tag{7}$$

$$\mathrm{CO_2} + 2\,\mathrm{H_2O} \rightleftharpoons \mathrm{HCO_3{}^-} + \mathrm{H_3O^+} \tag{8}$$

$$\mathrm{HCO_3{}^-} + \mathrm{H_2O} \rightleftharpoons \mathrm{CO_3{}^{2-}} + \mathrm{H_3O^+} \tag{9}$$

$$\mathrm{MEAH^+} + \mathrm{H_2O} \rightleftharpoons \mathrm{MEA} + \mathrm{H_3O^+} \tag{10}$$

$$\mathrm{MEACOO^-} + \mathrm{H_2O} \rightleftharpoons \mathrm{MEA} + \mathrm{HCO_3{}^-} \tag{11}$$

In the absorption process of absorbing CO_2 into MEA, three equilibrium and two kinetic reactions take place [55, 106]. The Equilibrium reactions are shown in Equation 7, 9 and 10. The two kinetic reactions are shown in Equation 12 and 13.

$$\mathrm{CO_2} + \mathrm{OH^-} \rightleftharpoons \mathrm{HCO_3{}^-} \tag{12}$$

$$\mathrm{H_2O} + \mathrm{MEA} + \mathrm{CO_2} \rightleftharpoons \mathrm{MEACOO^-} + \mathrm{H_3O^+} \tag{13}$$

The kinetic data for reaction 12 and 13 are given in the form of the Arrhenius Equation, given in Equation 14.

$$\text{Kinetic factor} = k_0 T^n e^{-E/RT} \tag{14}$$

In which k_0 is the reaction constant, T the temperature in K, n the reaction order, E the reaction energy in J/mol and R the gas constant in $J/(\mathrm{mol} \cdot K)$. The values for the reaction constants and the reaction energies are retrieved from Aspen Technology Inc. (2006) and shown in Table 5 [4]. In the table it can be seen that for the backward reaction 13 two different values for the reaction constant and the reaction energy are provided, one for the absorption process and different values for the stripping process. These values have been compensated for the temperature difference in the process.

Table 5: Reaction kinetic data for the absorption and stripping reactions (retrieved from Aspen Technology Inc. (2008) [4])

	k_0 (kmol/(m^3·s))	E (cal/mol)
Reaction 12 *forward*	$1.33 \cdot 10^{17}$	13,249
Reaction 12 *backward*	$6.63 \cdot 10^{16}$	25,656
Reaction 13 *forward*	$3.02 \cdot 10^{14}$	9,855.8
Reaction 13 *backward, absorption*	$5.52 \cdot 10^{23}$	16,518
Reaction 13 *backward, stripping*	$6.50 \cdot 10^{27}$	22,782

The molecular structures for MEA, $MEACOO^-$ and $MEAH^+$ are shown in Figure 10.

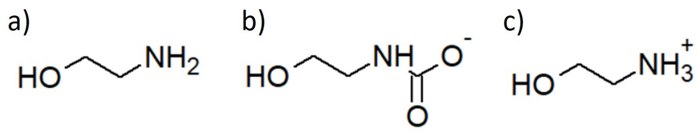


Figure 10: Molecular structure for a) MEA, b) $MEACOO^-$ and c) $MEAH^+$

2.2.3 Regeneration

In order to strip the CO_2 from the amines, the temperature should be increased to free the CO_2. In the regeneration process, the temperature is increased between 100 and 140 °C [84]. Usually, steam is provided to the system to provide the heat of reaction and enable the transport of CO_2 out of the system. At increased temperatures, the chemical kinetics of regeneration increases and the reaction equilibrium shifts in order to release CO_2. The top stream leaving the stripper consists of the released CO_2 and remaining H_2O. In a condenser, the H_2O is separated from the CO_2, leading to a CO_2 rich stream.

The energy consumption in the stripper reboiler is a significant number in the process of CO_2 removal. It is estimated to be 15-30% of the energy requirement for 90% CO_2 removal [84]. Typical energy requirements for the reboiler vary between 4 and 5 GJ/tonCO_2 for the MEA recovery process [51].

2.3 Conversion of CO_2

After the CO_2 is absorbed and stripped from the flue gas stream, the CO_2 stream is used for further processing and converted towards methanol.

2.3.1 Conversion reactions in the methanol reactor

The reactions for the production of methanol from carbon dioxide and carbon monoxide are shown in Equation 15 and 16, respectively [89, 33]. Both reactions are exothermic since the reaction enthalpy of both reactions is negative.

$$\mathrm{CO_2 + 3\,H_2 \rightleftharpoons CH_3OH + H_2O}\ \Delta\mathrm{H_{298K}} = -49\,\mathrm{kJ/mol} \tag{15}$$

$$\mathrm{CO + 2\,H_2 \rightleftharpoons CH_3OH}\ \Delta\mathrm{H_{298K}} = -91\,\mathrm{kJ/mol} \tag{16}$$

Another reaction that takes place when mixing carbon dioxide with hydrogen, is the reverse water gas shift (RWGS) reaction, shown in Equation 17, which is an endothermic reaction.

$$\mathrm{CO_2 + H_2 \rightleftharpoons CO + H_2O}\ \Delta\mathrm{H_{298K}} = +\,41\,\mathrm{kJ/mol} \tag{17}$$

The the reaction rate expression for the formation of methanol from CO_2 is shown in Equation 18. The reaction rate equation for the reverse water gas shift is shown in Equation 19. Both are retrieved from Vanden Bussche and Froment (1996) [89].

$$r_{CH_3OH} = k_{CH_3OH}\frac{(p_{CO_2}p_{H_2}) - (1/K_{pCH_3OH})(p_{CH_3OH}p_{H_2O}/p_{H_2}^2)}{(1 + K_a(p_{H_2O}/p_{H_2} + K_b\sqrt{p_{H_2}} + K_c p_{H_2O})^3} \tag{18}$$

$$r_{RWGS} = k_{RWGS} \frac{p_{CO_2} - (1/K_{pRWGS})(p_{CO}p_{H_2O}/p_{H2})}{(1 + K_a(p_{H_2O}/p_{H2}) + K_b\sqrt{p_{H2}} + K_c p_{H_2O})} \tag{19}$$

In which:

- r_i = reaction rate in [$\text{mol} \cdot \text{kg}_{cat}^{-1} \cdot \text{s}^{-1}$]
- k_i = kinetic factor in [$\text{kmol} \cdot \text{kg}_{cat}^{-1} \cdot \text{s}^{-1} \cdot \text{bar}^{-1}$] or [$\text{kmol} \cdot \text{kg}_{cat}^{-1} \cdot \text{s}^{-1} \cdot bar^{-2}$]
- p_i = partial pressure [bar]
- K_{pi} = equilibrium constant in [$-$] or [bar^{-2}]
- $K_{a/b/c}$ = adsorption constants [bar^n]

The values for the reaction rates are given in Table 6. The values must be presented in the form of Equation 20, which shows the Arrhenius Equation. In this equation, A_i* represents the pre-exponential factor and B_i* represents either the activation energy (E) or the reaction enthalpy (-ΔH). The values are retrieved from Vanden Bussche and Froment (1996) [89].

$$k_i \text{ or } K_i = A_i^* exp\left(\frac{-B_i^*}{RT}\right) \tag{20}$$

Table 6: Values for the reaction rate in the form of Equation 20, retrieved from Vanden Bussche and Froment (1996) [89].

Variable (Unit)	A_i^*	B_i^* (J/mol)
k_{CH_3OH} ($\text{mol} \cdot \text{kg}_{cat}^{-1} \cdot \text{s}^{-2} \cdot \text{bar}^{-2}$)	1.07 $\text{mol} \cdot \text{kg}_{cat}^{-1} \cdot \text{s}^{-2} \cdot \text{bar}^{-2}$	36,696
k_{RWGS} ($\text{mol} \cdot \text{kg}_{cat}^{-1} \cdot \text{bar}^{-1}$)	$1.22 \cdot 10^{10}$ $\text{mol} \cdot \text{kg}_{cat}^{-1} \cdot \text{bar}^{-1}$	-94,765
K_a (-)	3453.38	-
K_b ($\text{bar}^{-0.5}$)	0.499 $\text{bar}^{-0.5}$	17,197
K_c (bar^{-1})	$6.62 \cdot 10^{-11}$ bar^{-1}	124,119

The equilibrium constants based on the partial pressure of each component, K_{pi} are retrieved from Graaf et al. [33]. The Equations for the equilibrium constants for the formation of methanol and the RWGS reaction are given by Equation 21 and 22, respectively.

$$lnK_{pCH_3OH} = \frac{7059.73}{T} - 47.415 \tag{21}$$

$$lnK_{pRWGS} = \frac{-4773.26}{T} - 4.672 \tag{22}$$

In order to plug the kinetic data into Aspen Plus, the constants of the kinetic pre-factor have to be rewritten in the form of equation 23, the other terms have to be rewritten to the form of Equation 24. The constants are rewritten by changing the units of pressure from bar to Pascal and the unit mol is rewritten to kmol.

$$k_i = k_{i,0} exp\left(-\frac{E_i}{RT}\right) \tag{23}$$

$$ln(K_i) = A_i + \frac{B_i}{T} \tag{24}$$

The adjusted values are given in Table 7 and Table 8, adjusted to the form of Equation 23 and Equation 24 respectively.

Table 7: Adjusted values for simulation of the reactor kinetics in the form of Equation 23

Variable	$k_{i,0}$	E_i
k_{CH_3OH}	$1.07 \cdot 10^{-13}$ kmol $\cdot$ kg$^{-1} \cdot$ s$^{-1} \cdot$ Pa^{-2}	$-36,696$ kJ $\cdot$ kmol^{-1}
k_{RWGS}	$1.22 \cdot 10^{2}$ kmol $\cdot$ kg$_{cat}^{-}1 \cdot$ s$^{-1} \cdot$ Pa^{-1}	$94,765$ kJ $\cdot$ kmol^{-1}

Table 8: Adjusted values for simulation of the reactor kinetics in the form of Equation 24

Variable	A_i	B_i
$ln(\frac{1}{K_{pCH_3OH}})$	47.415	-7059.73
$ln(\frac{1}{K_{pRWGS}})$	-4.672	4773.26
$ln(K_a)$	8.1471	-
$ln(K_b)$	-6.4522	2068.44
$ln(K_c)$	-34.9526	14,928.92

2.3.2 Side-reactions

Besides the methanol reactions, there are also some impurities generated when hydrogen can react to the produced carbonmonoxide. These impurities include ethanol, formic acid, and 1-propanol. The reactions for these impurities are shown in Equation 25, Equation 26 and Equation 27 [12].

$$2\,CO + 4\,H_2 \rightleftharpoons CH_2CH_3OH + H_2O \tag{25}$$

$$3\,CO + 2\,H_2 \rightleftharpoons HCOOCH_3 \tag{26}$$

$$3\,CO + 6\,H_2 \rightleftharpoons C_3H_7OH + 2\,H_2O \tag{27}$$

For the simulation of the conversion of CO_2 into methanol using H_2, the side-reactions are assumed to be negligible compared to the conversion reactions described in the section above. This assumption is rooted in the fact that there is very little CO available in the reactor, and therefore, only a very limited amount of ethanol, formic acid, or 1-propanol could theoretically be produced.

2.3.3 Reactor choice

There are multiple reactors available for the conversion of CO_2 into CH_3OH. For the scope of this thesis, three options are evaluated:

- Adiabatic reactor

- Water cooled reactor
- Gas cooled reactor

For the conversion of CO_2 hydrogenation to methanol (CTM), reactors are generally operated at a pressure of 50 - 100 bar and a temperature of 200 - 300 °C. The reactor choice can generally be divided into two main types: (1) adiabatic reactors, or (2) isothermal (internal cooled) reactors. The latter type can be either water cool reactors or gas cooled reactors. These three types of reactor are shown in Figure 11.

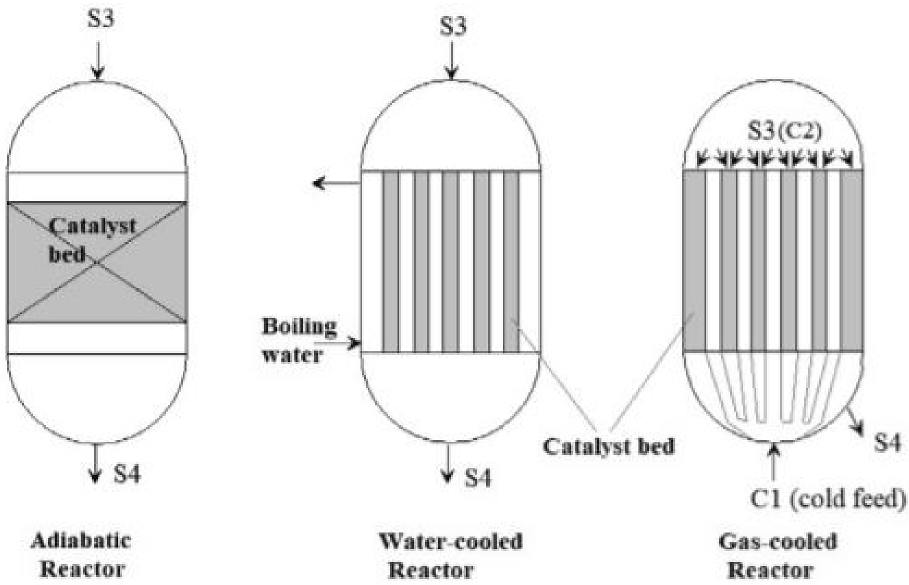


Figure 11: Three reactor types for the conversion of CO_2 to methanol (retrieved from Cui and Kaer [16])

An adiabatic reactor is a vessel that is insulated to such an extend that the heat transfer is minimized. Therefore, the temperature of the inlet stream is increased or decreased over the length of the reactor solely due to the heat of the reaction, dependent on whether the reactions are exothermic or endothermic [31]. Adiabatic reactors usually have multiple catalyst beds and use cooling methods such as injecting of a cold gas after each catalyst bed, this is in order to avoid hot-spots. Having local hot-spots can result in deactivation of the catalyst or sintering of the catalyst, the process in which a catalyst forms a coherent solid mass due to heat or pressure without melting [99]. The heat release in the reactor is due to the exothermic RWGS (reactions 15 and 16). The main reaction (reaction 17) is endothermic. When reaction 15 (the main reaction) dominates, the heat release in the reactor is lower.

A water cooled-reactor is a reaction with a shell-tube structure in order to remove heat from the exothermic process. The boiling water in the shell removes heat from the reactor [16].

A gas-cooled reactor is another form of a shell-tube reactor and in this case a cold gas in the tube side of the reactor cools the catalyst bed in the shell side of the reactor. This type of shell-tube reactor is less complex compared to the water cooled-reactor since it does not have the additional water stream [16].

The main difference between the three types of reactors is the cooling method used. The main concern is to avoid hot-spots of a temperature above 280 °C, while still having a reasonable methanol yield, which is dependent on the temperature and the reaction rate (per volume catalyst) [16]. All reactors show potentials for the CTM process. Traditional processes with a high CO content in the inlet stream, ask for a more robust cooling system and hot-spot reduction, making the water-cooled reactor the most feasible option. However, process streams being CO_2-rich at the inlet exhibit less hot-spots temperatures compared to CO-rich inlet streams. This makes the gas-cooled and adiabatic reactors also feasible options for these type of processes [16].

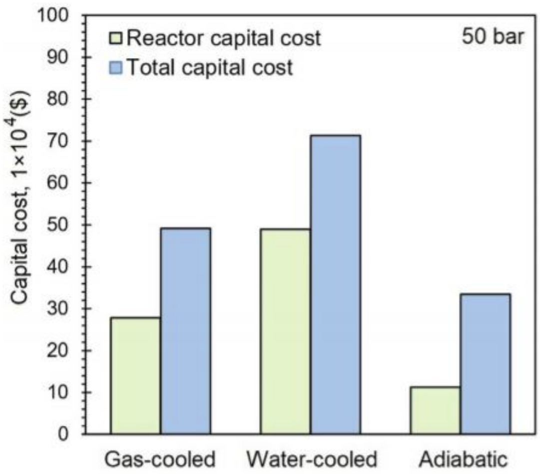


Figure 12: Capital costs of the three different methanol conversion reactors at an operating pressure of 50 bar (retrieved from Cui and Kaer [16])

Figure 12 shows the capital costs for three different conversion reactors at an operating pressure of 50 bar. From this figure, it can be seen that the adiabatic reactor has the lowest capital costs and the lowest operating costs. This is one of the main advantages of the adiabatic reactor.

Due to the CO_2-rich inlet stream, and therefore decreased demand for a robust cooling system, and the advantage of low capital costs, it is chosen to simulate the process with an adiabatic packed bed reactor.

2.3.4 Pressure drop within the reactor

The pressure drop in a packed bed reactor (PBR) is generally calculated with the Ergun Equation. The Ergun equation, as specified by the Aspen Plus help guide, is shown in Equation 28.

$$-\frac{dP}{dz} = 150\frac{(1-\epsilon)^2}{\epsilon^2}\frac{\mu U}{\phi_s^2 D_p^2} + 1.75\frac{1-\epsilon}{\epsilon^2}\frac{\rho U^2}{\phi_s^2 D_p^2} \tag{28}$$

In which $\frac{dP}{dz}$ is the change in pressure (dP) along the length of the reactor (dz) in $Pa \cdot m^{-1}$, ϵ the bed voidage, ϕ_s the particle shape factor, D_P the diameter of the particle in m, μ the viscosity of the fluid in $Pa \cdot s$, ρ the density of the fluid in $kg \cdot m^{-3}$ and U the superficial velocity in $m \cdot s^{-1}$.

In order to simulate the pressure drop in the PBR in Aspen Plus, the diameter, shape factor and void fraction of the catalyst is needed

2.3.5 Catalyst simulation in Aspen Plus

It is chosen to simulate the CO_2 to methanol conversion process using a commercially available $Cu/ZnO/Al_2O_3$ catalyst. This catalyst is well established for this process and a large number of kinetic equations are available [89]. The catalyst is packed in vertical tubes, which are placed in a shell.

The rate-basis for both reactions is simulated in Aspen Plus as catalyst based. The catalyst is specified in Aspen Plus in the reactor block. The data for the catalyst are retrieved from Chen et al (2011) and shown in Table 9 [10].

Table 9: Catalyst data (Retrieved from Chen et al (2011) [10])

Parameter	**Value**
Specifications	
Bed voidage	0.285 $m^3 \cdot m^{-3}$
Particle density	1190 $kg \cdot cum^{-1}$
Particle Geometry	
Diameter	5 mm
Shape factor	1

2.3.6 Hydrogen production

Hydrogen is needed in order to produce methanol from CO_2. Industrially, the synthesis of ammonia and methanol are the largest hydrogen consumption industries [47]. There are several methods of producing hydrogen, including steam reforming and electrolysis of water. Currently around 4% of the hydrogen produced worldwide is produced using water electrolysis [74].

In the steam reforming process, natural gas is most commonly used as feed. Heavier hydrocarbons, up to naphtha, can also be used. The production of hydrogen takes two steps, shown in Equation 29 and 30 [47]. The process is carried out at temperatures between 970-1100K and at a pressure up to 3.5 Mpa. Even though this process is the most commonly used process of hydrogen production, it has big disadvantages, especially regarding sustainability. Besides the production of hydrogen, CO_2 is also produced in this process. Furthermore, this process is dependent on fossil fuels, both for the manufacturing process as well as for the heat source [47]. Therefore, this process is also not renewable.

$$\mathrm{C}_n\mathrm{H}_m + n\,\mathrm{H_2O} \longrightarrow n\,\mathrm{CO} + (n + {}^1\!/\!{}_2 m)\,\mathrm{H_2} \tag{29}$$

$$\mathrm{CO} + \mathrm{H_2O} \longrightarrow \mathrm{CO_2} + \mathrm{H_2} \tag{30}$$

Another method of producing hydrogen is via water electrolysis. In this process, electricity is used to split water into oxygen and hydrogen. The reaction for this process is shown in Equation 31.

$$\mathrm{H_2O} \longrightarrow 2\,\mathrm{H_2} + \mathrm{O_2} \tag{31}$$

This currently is the only process of producing hydrogen without needing fossil fuels. Other advantages are the high product purity and the feasibility on small and large scales. The reaction requires electricity, when using renewable energy sources such as solar energy or wind energy, the total CO_2 emissions for the hydrogen production process can be considerably reduced [47]. However, the main drawback of using solar energy is the low efficiency and the main drawback of wind energy is the intermittence and mismatch with demand. The energy requirement for conventional industrial electrolyzers is on average between 4.5- 5 $kWh \cdot m^{-3}$ H_2 [74].

2.4 Thermodynamic Model

The property method decides which collection of methods and models is used by Aspen Plus to compute thermodynamic and transport properties. The thermodynamic properties are: fugacity coefficients, enthalpy, entropy, Gibbs free energy and volume. The transport properties are: viscosity, thermal conductivity, diffusion coefficient and surface tension for the liquid phase.

The Electrolyte Non-Random Two Liquid (ENRTL) model has been used as a thermodynamic model in this study for the non-ideal liquid phase, with the Redlich-Kwong (RK) equation of state. According to the Aspen Plus help environment, the property method uses the following:

- The Redlich-Kwong equation of state for vapor phase properties
- The unsymmetric reference state for ionic species
- Henry's law for solubility of supercritical gases in a liquid phase
- Unsymmetrical Electrolyte NRLT method for handling zwitterions

2.4.1 Electrolyte Non-Random Two Liquid (ENRTL)

The Electrolyte Non-Random Two-Liquid (ENRTL) model is an extended version of the NRTL model proposed by Chen et al. to fit aqueous electrolyte solutions as well [9]. Later the model was extended by Mock et al. to describe mixed solvent electrolyte systems as well [57].

The model is based on two fundamental assumptions [9, 57]:

1. **Like-ion Repulsion Assumption**. It is assumed that repulsive forces between same charged particles are extremely large. As result, there are no cations located right next to other cations, as well as no anions located next to other anions.

2. **Local Electroneutrality Assumption**. It is assumed that the distribution of cations and anions around a solvent molecules leads to a net local charge of zero.

The excess Gibbs energy in the ENRTL model consists of two contributions: (1) long-range ion-ion interaction and (2) short-range local interactions as a result of short-range and long-range interaction between neighbouring species. The short range interactions include ion-molecule, ion-ion, and molecule-molecule interactions [46]. The expression for the long-range ion-ion interaction consists of a contribution given by the Pitzer-Debye-Hückel ($G_m^{*E,pdh}$) equation as well as a contribution from the Born ($G_m^{*E,Born}$) equation. The expression for the local interactions ($G_m^{*E,lc}$) is derived from the NRTL equation. This yields a total excess Gibbs energy provided by Equation 32 [37].

$$\frac{G_m^{*E}}{RT} = \frac{G_m^{*E,pdh}}{RT} + \frac{G_m^{*E,Born}}{RT} + \frac{G_m^{*E,lc}}{RT} \tag{32}$$

The contribution to the electrostatics excess Gibbs energy for long-range interaction is provided by Equation 33.

$$\frac{G_m^{*E,pdh}}{RT} = -\left(\sum_i x_i\right)\left(\frac{1000}{M_s}\right)^{1/2}\left(\frac{4A_\phi I_x}{\rho}\right) ln\left(1+\rho I_x^{1/2}\right) \tag{33}$$

In which $G_m^{*E,pdh}$ is the contribution to the electrostatic excess Gibbs energy from the Pitzer-Debye-Hückel formula, R universal gas constant, T temperature, x_i the mole fraction of component i, M_s the molecular weight of the solvent, A_ϕ the Debye-Hückel parameter, I_x the ionic strength, and ρ the so called "closest approach"parameter. The Debye-Hückel parameter is proveded by Equation 34 and the ionic strength is provided by Equation 35. The value for ρ depends on both the electrolyte and the expression used for short range forces.

$$A_\phi = \frac{1}{3}\left(\frac{2\pi N_A d_s}{1000}\right)^{1/2}\left(\frac{Q_e^2}{\epsilon_s kT}\right)^{3/2} \tag{34}$$

In which N_A is Avogadro's number, d_s is the density of the solvent, Q_e the electron charge, ϵ_s the dielectric constant of the solvent, and k the Boltzmann constant.

$$I_x = \frac{1}{2}\sum_i x_i z_i^2 \tag{35}$$

In which z_i is the charge number of ion i.

Besides the Pitzer-Debye-Hückel formula for the long range excess Gibbs energy, also the Born equation is taken into account. This equation is provided by Equation 36.

$$\frac{G_m^{*E,Born}}{RT} = \frac{Q_e^2}{2kT}\left(\frac{1}{\epsilon} - \frac{1}{\epsilon_w}\right)\left(\frac{\sum_i x_i z_i^2}{r_i}\right)10^{-2} \tag{36}$$

In which r_i is the Born radius of species i.

The contribution of the short-range interaction is provided by the NRTL approach. The main assumption in the NRTL model is that the heat of mixing is much larger compared to the non-ideal entropy of mixing, which holds for electrolyte systems as well [9].

The ratio between the local mole fractions x_{ji} and x_{ii} in short-range of a central species i is given by Equation 37.

$$\frac{x_{ji}}{x_{ii}} = \frac{x_j}{x_i}G_{ji} \tag{37}$$

In which x_j and x_i are the mole fractions of species j and i respectively and G_{ji} is given by Equation 38

$$G_{ji} = exp(-\alpha\tau_{ji}) \tag{38}$$

In which α is the non-randomness factor and τ_{ji} is the dimensionless interaction parameter, provided by Equation 39

$$\tau_{ji} = \frac{g_{ji} - g_{ii}}{RT} \tag{39}$$

In which g_{ji} and g_{ii} are the interaction energies between species j and i, and between i and i, respectively. These energies are inherently symmetrical, meaning that $g_{ji} = g_{ij}$.

2.4.2 Redlich-Kwong Equation of state

The Redlich-Kwong equation of state has been postulated by O. Redlich and J.N.S. Kwong in 1949 [76], shown in Equation 40. The equation has an empirical nature and relates the pressure of a gas to the temperature and the volume of the gas.

$$P = \frac{RT}{V - b} - \frac{a}{\sqrt{T}V(V + b)} \tag{40}$$

In which P is the gas pressure, R the universal gas constants, T temperature and V the volume. The constants a is a correction factor for the attractive potential of molecules and b is a correction factor for the volume. The constants a and b depend on the gas that is being evaluated, and can be obtained from critical point data of the gas. The equations for constants a and b are given by Equation 41 and Equation 42 respectively.

$$a = 0.42748\frac{R^2 T_C^{2.5}}{P_C} \tag{41}$$

$$b = 0.08664\frac{RT_C}{P_C} \tag{42}$$

In which T_C is the temperature at the critical point and P_C the pressure at the critical point.

2.4.3 ESPSAFT - Vapor Equation Of State

The modification section in Aspen Plus allows to modify the base method. The possible modifications are shown in Table 10.

Table 10: Modifications of the thermodynamic model in Aspen Plus

Parameter	**Explanation**
Vapor EOS	Allows to select an equation of state for all vapor phase properties
Liquid gamma	Selection of an activity coefficient model
Data set	specification of a parameter data set number in order to calculate EOS or liquid gamma model
Liquid enthalpy	route to calculate liquid mixture enthalpy
Liquid volume	route to calculate liquid mixture volume
Poynting correction	specify whether or not Poynting correction is sued when calculating liquid fugacity coefficients
heat of mixing	Specify whether or not heat of mixing is included in liquid mixture enthalpy

2.4.4 Thermal Conductivity - Riedel Electrolyte Model

The thermal conductivity is a measure for the ability to conduct heat in a material. The thermal conductivity is used in order to evaluate the heat transfer coefficients and it determines the rate of heat transfer. The thermal conductivity of liquid mixtures for pure species ($\lambda_i^{*,l}$) is calculated in Aspen Plus by the Sato-Riedel model, given in Equation 43.

$$\lambda_i^{*,l} = \frac{1.1053152}{M_i^{1/2}} \left(\frac{3 + 20(1 - T_{ri})^{2/3}}{3 + 20(1 - T_{bri})^{2/3}} \right) \tag{43}$$

In which T_{ri} and T_{bri} are given by Equation 44 and 45.

$$T_{ri} = \frac{T}{T_{ci}} \tag{44}$$

$$T_{bri} = \frac{T_{bi}}{T_{ci}} \tag{45}$$

In which M_i is the molecular weight of species i, T_{bi} the normal boiling point and T_{ci} the critical temperature. The Vredeveld mixing rule gives the thermal conductivity for liquid solvent mixtures (λ_{solv}^l), shown in Equation 46.

$$\left(\lambda_{solv}^l\right)^{-2} = \sum_i w_i \left(\lambda_i^{*,l}\right)^{-2} \tag{46}$$

The correction to the liquid mixture thermal conductivity due to the presence of electrolytes ($\lambda^l(T)$) is also given by the Riedel model in Equation 47.

$$\lambda^l(T) = \left[\lambda_{solv}^l(T = 293K) + \sum_{ca}(a_c + a_a)\frac{x_{ca}^a}{V_m^l}\right] \frac{\lambda_{solv}^l(T)}{\lambda_{solv}^l(T = 293K)} \tag{47}$$

In which x_{ca}^a is the mole fraction of the apparent electrolyte ca, a_c and a_a are the Riedel ionic coefficients and V_m^l the apparent molar volume, which is computed by the Clarke density model.

2.5 Flow models

In Aspen Plus, several flow models can be used in order to simulate the flow inside a column. Aspen Plus uses the temperature, pressure and composition and determine the bulk properties. All models are based on the model of a stage, shown in Figure 13. The flow models determine the bulk properties, which are used in calculating mass and heat transfer and the reaction rates. These models include mixed flow, counter-current flow, VPlug flow, Lplug, and Vplug-Pavg flow.

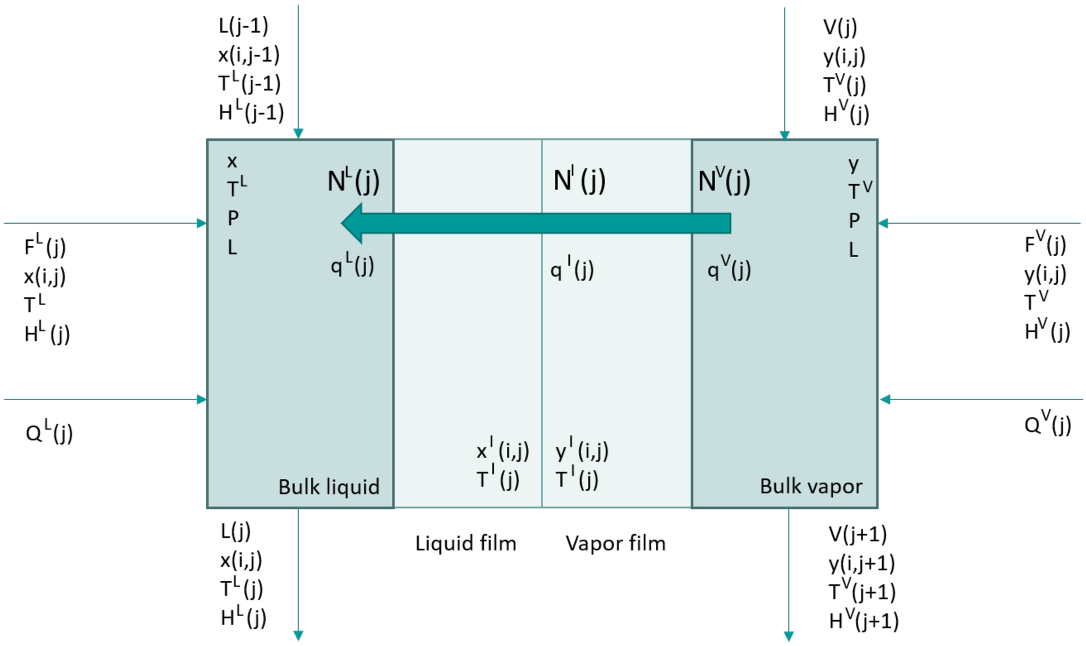


Figure 13: Model of a stage in Aspen Plus (adapted from Aspen Plus help guide [3])

2.5.1 Mixed flow

In the mixed flow, the bulk properties for each phase are considered to be the same as the outlet conditions for each phase leaving the stage. Meaning that each phase is considered to be completely mixed [46]. The mixed flow model is shown in Figure 14.

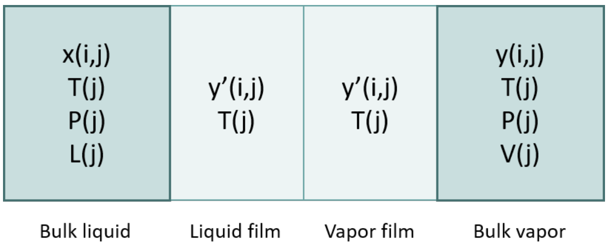


Figure 14: Mixed flow model in Aspen Plus RateSep (adapted from Aspen Plus help guide [3])

2.5.2 Counter-current flow

In the counter-current flow model, the bulk properties for each phase are calculated by taking an average of the inlet and outlet properties [46].

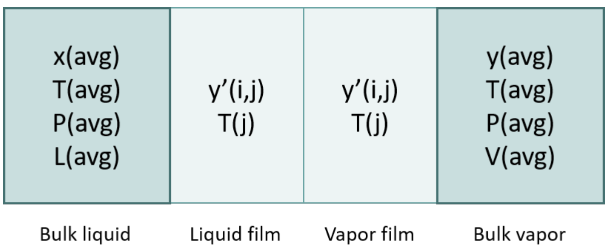


Figure 15: Counter-current flow model in Aspen Plus RateSep (adapted from Aspen Plus help guide [3])

2.5.3 Vplug flow

In the VPlug flow model, the bulk properties of the liquid phase are considered to be the same as the outlet conditions leaving the stage. For the vapor phase, an average of the inlet and outlet properties is taken, similar to the counter-current model. Furthermore, the pressure is assumed to be the same as the outlet pressure [46].

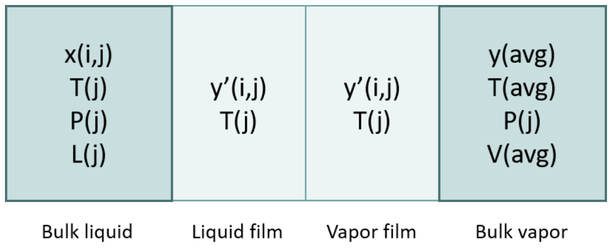


Figure 16: Vplug flow model in Aspen Plus RateSep (adapted from Aspen Plus help guide [3])

2.5.4 Lplug flow

The Lplug flow model calculates the bulk properties for the vapor phase by considering them to be the same as the outlet conditions leaving the stage. For the liquid phase an average of the inlet and outlet properties is taken, similar to the counter-current model. Again, the pressure is assumed to be the same as the outlet pressure [46].

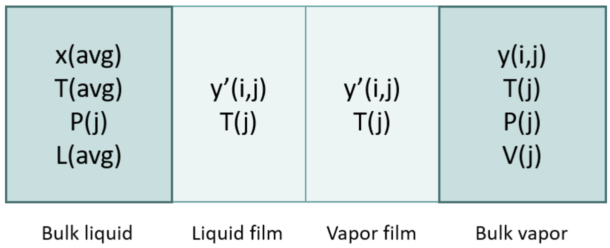


Figure 17: Lplug flow model in Aspen Plus RateSep (adapted from Aspen Plus help guide [3])

2.5.5 Vplug-Pavg flow

The Vplug-Pavg flow model is similar to the Vplug flow model. The only difference is that in this case the pressure is not assumed to be the same as the outlet pressure, but the pressure is assumed to be the same as the average pressure [46].

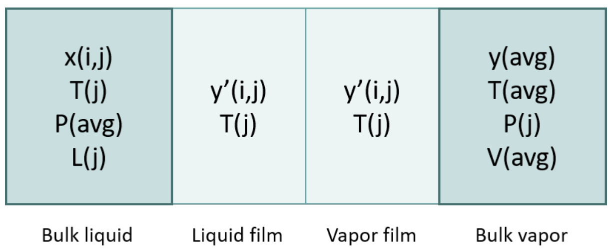


Figure 18: Vplug-Pavg flow model in Aspen Plus RateSep (adapted from Aspen Plus help guide [3])

3 Methodology - simulation set-up

This section starts with the basis of design, giving an overview of the design criteria and the assumptions that are made in this section. Afterwards, the simulation set-up is explained. The simulation set-up consists of two parts: (1) the properties set-up, and (2) the process simulation set-up. The simulation set-up is defined in the three main blocks: (1) absorption block, (2) stripping block, and (3) conversion block. Other blocks needed to run the simulation, such as pumps and heaters, are also discussed.

3.1 Basis of design

The goal is to develop a simulation for the conversion of CO_2 into CH_3OH.

3.1.1 Design criteria

The following criteria were made for the final product:

- The purity of the methanol should be at least 85 mole%
- The desired production volume is at least 200 kg per day

3.1.2 Assumptions

In simulating the absorption and stripping process, a few initial assumptions have been made in order to simplify the process:

- The CO_2 source is flue gas with no pollutants such as NOx and SOx.
- Henry's law can be used to estimate mass transfer for gas to liquid phase for CO_2, O_2 and N_2.
- The absorption process is adiabatic

This is the same set of assumptions as made by Desideri and Paulucci [22]. The presence of NOx and SOx should be avoided since they react with amines, which prevents regeneration and raises the MEA make-up, leading to additional losses of the solvent.

For the conversion step, the following set of assumptions have been made:

- A pure hydrogen feed stream can be used for the conversion of CO_2 into H_2
- The conversion can be simulated using an adiabatic reactor

3.2 Properties environment

The first step in the simulation of the reactive absorption-stripping process of CO_2 is the set up of the properties environment. In the properties environment, all the components specified, the thermodynamic models are chosen, and the interaction between species is specified as well.

3.2.1 Components

The components involved in the absorption process are listed in Table 11.

Henry's law is used for non-condensable components [25]. The components CO_2, N_2 and O_2 are specified in as Henry's components. This set of components is further referred to as HC-1.

Table 11: List of components

Component	Molecule	Type
Nitrogen	N_2	Conventional
Oxygen	O_2	Conventional
Hydrogen	H_2	Conventional
Carbon dioxide	CO_2	Conventional
Carbonate	CO_3^{2-}	Conventional
Hydrogen carbonate	HCO_3^-	Conventional
Water	H_2O	Conventional
Hydronium	H_3O^+	Conventional
Hydroxide	OH^-	Conventional
Monoethanolamine (MEA)	C_2H_7NO	Conventional
$MEACOO^-$	$C_3H_8NO_3^-$	Conventional
$MEAH^+$	$C_2H_8NO^+$	Conventional
Methanol	CH_3OH	Conventional
Carbon monoxide	CO	Conventional

3.2.2 Method's Specification

The Electrolyte Non-Random Two Liquid (ENRTL) thermodynamic model is used as a base method for the simulation of the absorption and stripping step. This method is used in significant numbers of work that model CO_2 absorption in MEA and is said to be the most suitable model for describing the electrolytic interactions present in the $CO_2 - MEA - H_2O$ system [55, 69]. For the computation of non-idealities of the vapor/gas phase, the Redlich-Kwong Equation of State is used, which is also mentioned by a number of papers [55, 69].

The method specifications are summarized in Table 12.

3.2.3 Estimated Parameters

Missing parameters are estimated by Aspen Plus. For the components $MEACOO^-$, $MEAH^+$ and H_3O^+, the standard Gibbs free energy of formation of aqueous species (G_f^0 or DGAQHG), standard enthalpy of formation of aqueous species (H_f^0 or DHAQHG), absolute entropy of aqueous species (S^0 or S25HG) and Born coefficient (ω or OMEGHG) are estimated.

The standard Gibbs free energy of formation is defined as the change in Gibbs free energy during the formation of 1 mole of compound from the constituent elements in their standard state [101]. The standard enthalpy of formation is defined as the change in enthalpy during the formation of 1 mole of a compound from the constituent elements in their standard state [100]. The absolute entropy is the increase in entropy as a result of heating a substance from a temperature of zero Kelvin to a certain temperature [26]. The Born coefficient is used to describe the solvation properties of an ionic species in a certain substance [21]. The estimated values for these parameters are given in Table 13.

Table 12: Method specifications

Parameter	
Property methods and options	
Method Filter	COMMON
Base method	ENRTL-RK
Henry Components	HC-1
Petroleum calculation options	
Free-water method	STEAM-TA
Water solubility	3
Electrolyte calculation options	
Chemistry ID	ABS
Use true components	yes
Modifications	
Vapor EOS	ESPSAFT
Data set	1
Liquid gamma	GMENRTLQ
Data set	1
Liquid molar enthalpy	HLMX0Q
Liquid molar volume	VLMX0Q
Heat of mixing	-
Poynting correction	yes
Use liquid reference state enthalpy	-

Table 13: Estimated parameters in Aspen Plus

	Unit	$MEACOO^-$	$MEAH^+$	H_3O^+	**Method**
G_f^0	J/kmol	$-6.22155 \cdot 10^8$	$-3.05415 \cdot 10^8$	$-2.37129 \cdot 10^8$	AQU-EST1
H_f^0	J/kmol	$-6.887 \cdot 10^8$	$-3.375 \cdot 10^8$	$-2.8583 \cdot 10^8$	AQU-DATA
S^0	J/kmol-K	$6.58957 \cdot 10^5$	$5.59627 \cdot 10^5$	$6.9910 \cdot 10^4$	AQU-EST2
ω	J/kmol	$-3.1906 \cdot 10^8$	$-3.1906 \cdot 10^8$	$1.21946 \cdot 10^8$	HELGESON

3.2.4 Chemistry

Under the chemistry tab, the equilibrium reactions 7 to 11 are specified.

3.3 Absorption set-up

The first step in the conversion route is the absorption of CO_2. In order to model this process, 30wt% aqueous monoethanolamine (MEA) is chosen as a solvent. For the simulation of the absorption step, the articles Aspen Technology (2008), Errico et al. (2016), Maddedu et al. (2019), Plaza et al. (2009), and Zhang et al. (2011) are reviewed and used [4, 28, 55, 69, 106].

In order to model the process in Aspen Plus, it is important to consider which phenomena are involved in the absorption and stripping process of CO_2. These are shown in Figure 19 [55].

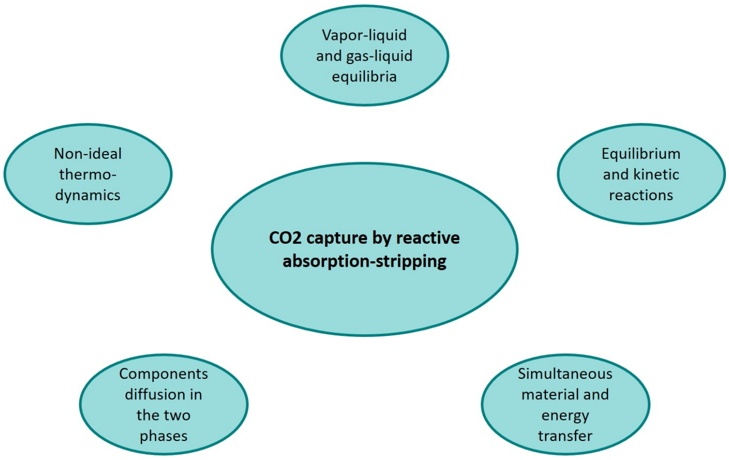


Figure 19: Phenomena involved in the absorption and stripping process of CO_2 (Adapted from Madeddu et al (2019) [55])

3.3.1 Flowsheet

The first step in the simulation of the absorption process of CO_2 into MEA is the setup of the flowsheet. The Aspen Plus flowsheet for the absorption block is shown in Figure 20.

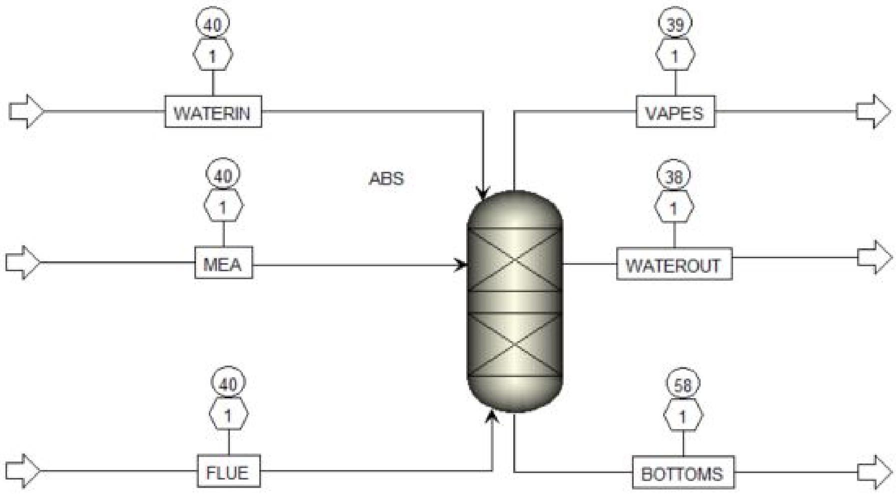


Figure 20: Flowsheet design in Aspen Plus for the absorption process.

3.3.2 Streams Input

The parameters of the streams entering the absorption block are specified in Table 14. The same input data is used as in the paper by Plaza et al. (2009) [69]. However, the inflow is changed from the units kmol/s to the units kmol/hr, since the kmol/s units lead to abnormal stream velocities and flooding in the column. Furthermore, an additional water stream, added as a water wash section, is added to the design, as proposed by Aspen Technology Inc. This stream aids in maintaining the mass balance and aids convergence [4].

Table 14: Input of the absober block

Stream ID	Parameter	Value
MEA		
	Total flow rate	57.6 kmol/hr
	H_2O	51.124 kmol/hr
	MEA	6.452 kmol/hr
	Pressure	1.013 bar
	Temperature	40 °C
$FLUE$		
	Total flow rate	6.1 kmol/hr
	H_2O	0.366 kmol/hr
	N_2	4.941 kmol/hr
	CO_2	0.793 kmol/hr
	Pressure	1.013 bar
	Temperature	40 °C
$WATERIN$		
	Total flow rate	4 kmol/hr
	H_2O	4 kmol/hr
	Pressure	1.013 bar
	Temperature	40 °C

The absorber column is split up in two segments: the water washing section and the absorbing section. The stream WATERIN enters the column from the top at stage 1 and leaves at stage 2. The stream MEA enters at stage 3 and FLUE at stage 12. The VAPES stream leaves at stage 1 and the BOTTOMS at stage 12. Figure 21 shows the two segments of the absorption column and the entering streams.

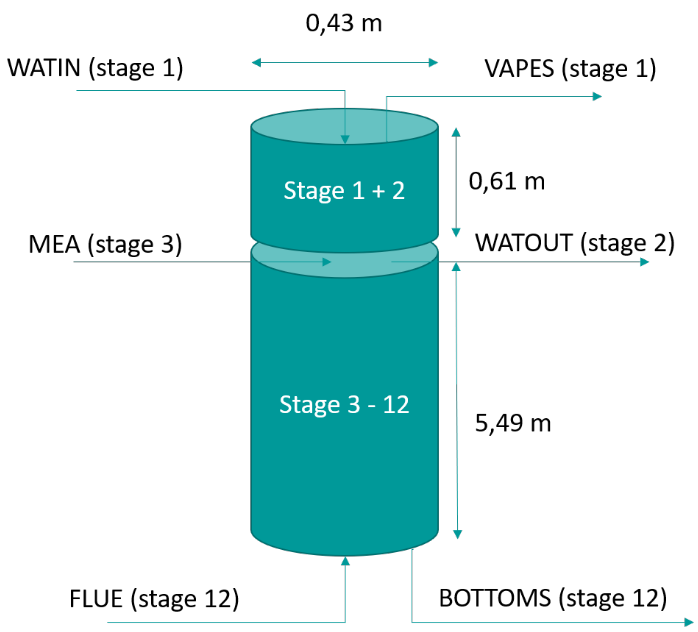


Figure 21: Absorption column segments and inlet and output sterams

The data for the inlet and outlet streams of the absorption block are shown in Table 15.

Table 15: Data of the streams entering and leaving the absorption block

	Stage	**Convention/phase**
Inlet stream ID		
FLUE	12	Vapor
MEA	3	Liquid
WATERIN	1	On-stage
Outlet stream ID		
BOTTOMS	12	liquid
WATEROUT	2	liquid, 3.5 kmol/hr
VAPES	1	vapor

3.3.3 Rate-based RADFRAC Absorption block

The absorption process is modeled in Aspen plus using a rate-based RADFRAC with 12 stages and no condenser or reboiler. Vapor and liquid are classified as valid phases. The setup of the RADFRAC is shown in Table 16.

Table 16: Setup of the rate-based RADRAC absorption block in Aspen Plus

	Aspen Plus
Calculation type	Rate-based
Number of stages	12
Condenser	none
Reboiler	none
Valid phases	vapour-liquid
Convergence	Standard

3.3.4 Absorption Trays and Material Data

The data for the trays and packing are retrieved from Plaza [69]. The height ratio between the two sections are based on the data from Aspen Technology Inc., in which the height of the first section is 0.10 times the total height. The parameters used for the trays and packing are shown in Table 17.

Table 17: Parameters and values for the trays and packing of the absorption block in Aspen Plus.

Packing rating	
Section 1	
Starting stage	1
Ending stage	2
Packing material	FLEXIPAC 250Y
Packing factor	92.19 1/m
Section diameter	0.43 m
Section packed height	0.61 m
Section 2	
Starting stage	3
Ending stage	12
Packing material	FLEXIPAC 250Y
Packing factor	92.19 1/m
Section diameter	0.43 m
Section packed height	5.49 m

3.3.5 Rate-based modelling

The absorption process is simulated as a rate-based process. The packing-rate is the rate dependent step in the absorption process. Therefore, both sections of the absorber block are simulated as rate-based. The liquid film discretization parameter is activated and simulated with 5 discretization points, which is determined by Madeddu et al. [55] and in agreement with the work of Kucka et al. and Li et al. [48, 51]. The calculation parameters are listed in Table 18.

Table 18: Calculation parameters for the packing rate-based modelling

Parameter	
Calculation Parameters	
Flow model	VPlug [4]
Interfacial area factor	1
Heat transfer factor	1
Liquid mass transfer coefficient factor	1
Vapor mass transfer coefficient factor	1
Film resistance	
Liquid phase	Discrxn [55, 51]
Vapor phase	Film [51]
Film non-ideality correction	
Liquid phase	yes [4]
Vapor phase	yes [4]

In order to run the rate-based modelling, certain correlations should be chosen in order to evaluate the rate-based model parameters, as followed [55]:

- Wetted surface area: the wetted surface available per m^2 packing material. This value determines the area available for contact and exchange between the gas phase (the flue gas with CO_2) and the liquid phase (the solution of MEA and water).

- Material and energy transfer coefficient: the material transfer coefficient is defined as the ratio between the diffusion coefficients. The energy transfer coefficient is defined as the ratio between the thermal conductivity and the film thickness. These coefficients are used to evaluate the flow rate of the transfer between the phases.
- Fractional liquid hold-up: this parameter is defined as the percentage of free-volume that is occupied by the liquid (thus the MEA-water solution).

The correlations for mass and heat transfer are retrieved from Madeddu [55]. The correlation for the interfacial area method is left to default setting of Aspen Plus. The correlations are shown in Table 19. The correlations are further explained in Appendix B.

Table 19: Correlations used for the mass transfer coefficient, heat transfer coefficient and interfacial area

	Correlation	**Explenation**
Mass transfer coefficient method	Bravo et al. (1985) [55, 51]	Predicts mass transfer coefficients for structured packing
Heat transfer coefficient method	Chilton and Colburn [55, 51]	Calculates heat transfer coefficients from the binary mass transfer coefficients
Interfacial area method	Bravo et al (1985) [51]	Predicts interfacial area for structured packing
Hold up method	Stichlmair et al (1989)	Predicts liquid holdup in all kinds of packing

In the rate-based setup section of Aspen Plus, the reaction condition factor is changed to 0.9 as explained by Madeddu et al. [55] and in agreement with Zhang et al. [106]. As quoted by Madeddu et al. [55]: *"Setting the reaction rate to 0.9 gives more weight to the bulk conditions in the evaluation of the film reaction rates, due to the fast reactions in the liquid film."* The set-up for the rate-based modelling is given in Table 20. An explanation of the parameters is given in Appendix C.

Table 20: Global set up of rate based modelling

Parameter	Value
Chilton-Colburn	0.0001
Transfer condition	0.5
Reaction condition	0.9 [55]
Film discretization option	Geometric
Film discretization ration	10 [55]
Flow model condition factor top	0.5
Flow model condition factor bottom	0.5
Flow model transfer factor	0.2
Mixed model on internal feed stages	no

3.4 Stripping

The second step in the process is the stripping of the CO_2 from the MEA. This step involves the same reaction as specified in Section 2.2.2.

3.4.1 Flowsheet

The setup of the flowsheet for the stripping process is shown in Figure 22.

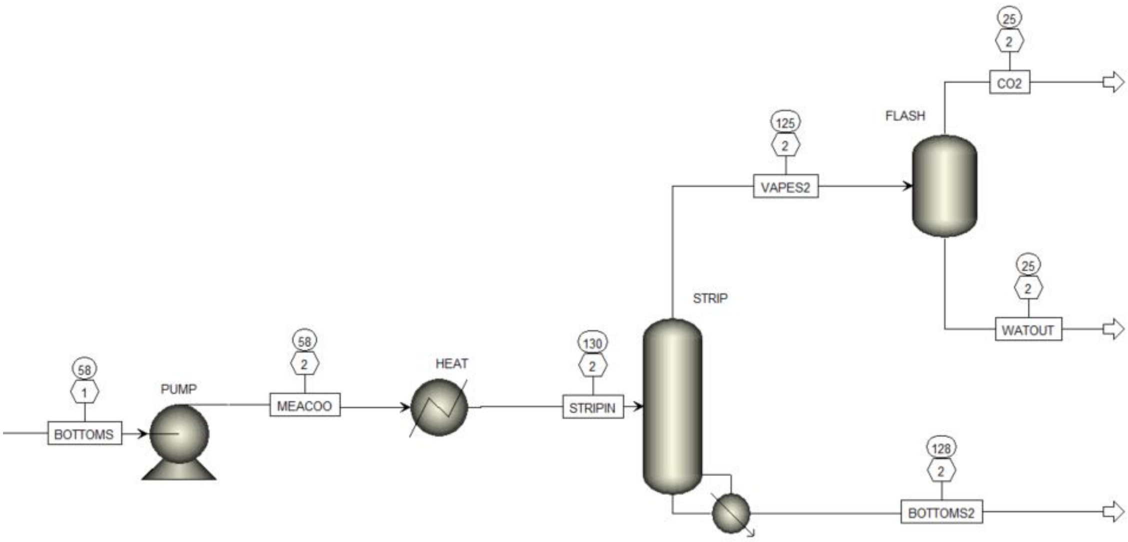


Figure 22: Flowsheet design in Aspen Plus for the stripping process

3.4.2 Pressure and temperature change

Before entering the stripper, the bottom stream of the absorber is first lead through a pump and through a heat exchanger in order to increase the pressure and temperature of the stream. The pump is called 'PUMP' in the Aspen Plus simulation and is used to increase the pressure from 1.01 bar to 1.6 bar. The net work required for this pump is 0.07615 kW. The heating unit, called 'HEAT' in the Aspen Plus simulation, is used to increase the temperature from 58.3 °C to 130 °C. The heat duty of the heater is 526.025 kW.

3.4.3 RATEFRAC stripper block

The stripper process is simulated in Aspen Plus using a rate-based RADFRAC block with 12 stages, no condenser and a kettle reboiler. The vapor stream leaving the stripper is lead to a separate condenser. The reboiler duty is matched to the amount of CO_2 that is desorbed from the MEA. The data for the setup of the stripper block is shown in Table 21.

The reboiler duty of the stripper is set to 29.9 kW, which corresponds to an energy requirement of 4 GJ/ton CO_2. In literature, an energy requirement of 3.24-4.20 GJ/ton CO_2 is mentioned as industrial numbers [87].

Table 21: Setup of the RATEFRAC stripping block in Aspen Plus

	Aspen Plus
Calculation type	Rate-based
Number of stages	12
Condenser	none
Reboiler	none
Valid phases	vapour-liquid
Convergence	Standard
Reboiler duty	29.9 kW
Free water reflux ratio	-
Stage-one pressure	1.6 bar
Column pressure drop	10 Pa

The bottom stream of the absorber enters the stripper, after passing through a pump and heat-exchanger, on-stage at stage 1. The two product streams, labeled BOTTOMS2 leaves the stripper at the bottom of the stripper at stage 12 and the vapor stream, labeled VAPES2, leaves the stripper at the top at stage 1. The data for the inlet and outlet streams of the stripper block is shown in Table 22.

Table 22: Data of the streams entering and leaving the stripper block

	Stage	**Convention/phase**
Feed Streams		
STRIPIN	1	On-stage
Product streams		
BOTTOMS2	12	Liquid
VAPES2	1	Vapor

3.4.4 Stripping Trays and Material data

For the stripper, both trays and packing are specified in the simulation of the stripping of CO_2 from MEA. The stripper is similar to the absorber. The parameters used for the packing rating are shown in Table 23.

Table 23: Parameters and values for the trays and packing of the stripping block in Aspen Plus.

Packing rating	
Starting stage	1
Ending stage	2
Packing material	FLEXIPAC 250Y
Packing factor	92.19 1/m
Section diameter	0.43 m
section packed height	6.1 m

3.4.5 Rate-based modelling

The stripping process is simulated as a rate-based process. The packing-rate is the rate dependent step in the stripping process. The liquid film discretization parameter is activated and simulated with 5 discretization points, determined by Maddedu et al [55] and in agreement with the work of Kucka et al [48] and Li et al [51]. The calculation parameters are listed in Table 24.

Table 24: Calculation parameters for the packing rate-based modelling

Parameter	
Calculation Parameters	
Flow model	VPlug
Interfacial area factor	1
Heat transfer factor	1
Liquid mass transfer coefficient factor	1
Vapor mass transfer coefficient factor	1
Film resistance	
Liquid phase	Discrxn
Vapor phase	Film
Film non-ideality correction	
Liquid phase	no
Vapor phase	no

The global set-up of the rate-based modelling is shown in Table 25.

Table 25: Global set up of rate-based modelling of the stripper

Parameter	**Value**
Chilton-Colburn average parameter	0.0001
Transfer condition factor	0.5
Reaction condition factor	0.9
Film discretization option	geometric
Film discretization ratio	10
Film model condition factor (top)	0.5
Film model condition factor (bottom)	0.5
Flow model transition factor	0.2
Mixed model on internal feed stages	no

The correlations for the mass transfer coefficient method, heat transfer coefficient method and interfacial area method are the same as for the absorber and described in Section 3.3.5.

3.4.6 Condenser

The condenser is simulated as a separate FLASH2 block in the Aspen Plus simulation. The condenser is set on a temperature of 24.85 °C, and a pressure of 1.6 bar. The net heat duty for the condenser equals -526.168 kW.

3.5 Conversion

The next step is the conversion of CO_2 into CH_3OH with H_2. The flowsheet for the conversion is shown in Figure 23.

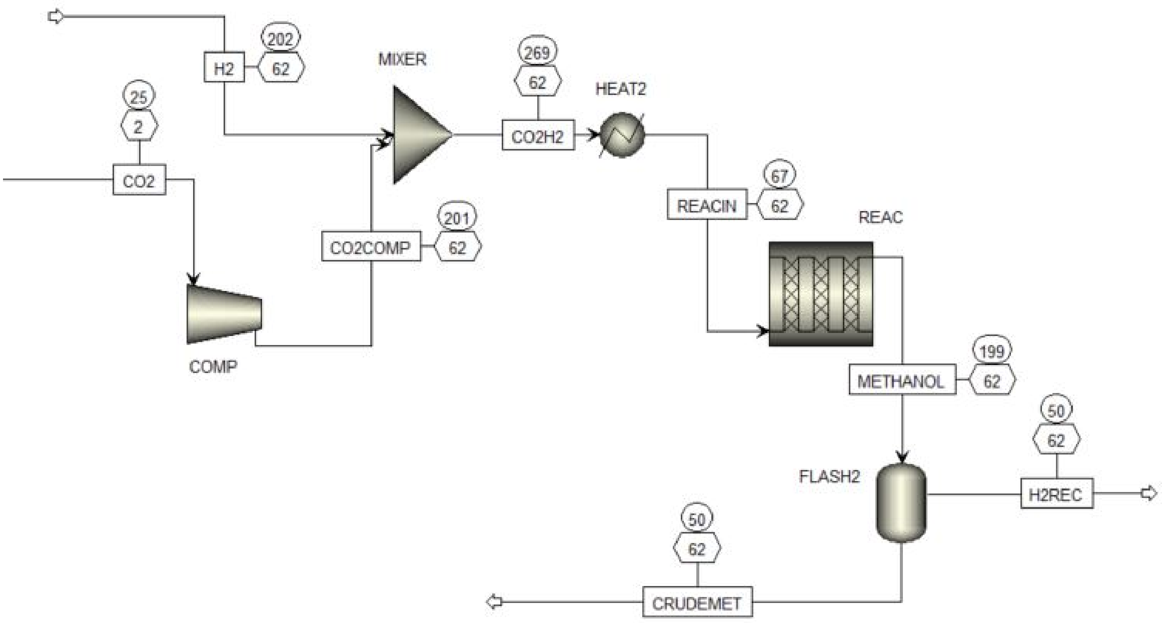


Figure 23: Flowsheet design in Aspen Plus for the conversion process

3.5.1 Pressure change

The stream leaving previous unit, the flash condenser, is lead to a compressor to increase the pressure from 1.6 bar to 62 bar, labeled COMP in the simulation. The compressor is simulated as isentropic compressor. The net work required for the compressor is 3.124 kW and has an efficiency of 0.72. The data of the streams entering and leaving the compressor are shown in Table 26.

Table 26: Data of streams entering and leaving the compressor

Stream ID	**Temperature (°C)**	**Pressure (bar)**
CO2	25 C	1.6
CO2COMP	201.169 C	62

3.5.2 Mixer

In the next block, the CO_2 stream is mixed with the H_2 stream. The ratio of H_2:CO_2 is set to be 2:1 mole. The inlet and outlet stream data of the H_2 stream is shown in Table 27. The streams with stream ID $H2$ and $CO2COMP$ are inlet streams, the stream with stream ID CO_2H_2 is the outlet stream.

Table 27: Input and output of the mixer block

Stream ID	Parameter	Value
$H2$		
	Total flow rate	2.5 kmol/hr
	Pressure	62 bar
	Temperature	25 °C
$CO2COMP$		
	Total flow rate	0.65 kmol/hr
	H_2O	0.013 kmol/hr
	N_2	0.048 kmol/hr
	CO_2	0.589 kmol/hr
	Pressure	62 bar
	Temperature	201.2 °C
$CO2H2$		
	Total flow rate	3.15 kmol/hr
	H_2O	0.013 kmol/hr
	N_2	0.048 kmol/hr
	CO_2	0.589 kmol/hr
	H_2	2.5 kmol/hr
	Pressure	62 bar
	Temperature	142.7 °C

3.5.3 Heater

The mixed CO_2 and H_2 stream flows to the heater, that brings the stream to the desired temperature for inlet of the reactor, which if further explained in Section 4.3. The heater, labeled HEAT2 in the simulation, is set to have an outlet temperature of 68 °C. This is the inlet temperature for the reactor. In general, a temperature of 200 °C or higher is used for the methanol formation reaction. In this thesis, it is decided to use an inlet temperature of 68 °C and let the temperature increase inside the reactor to reach temperatures of 200 °C and higher. Using an inlet temperature of 68 °C yielded the highest methanol conversion numbers, which is further explained in the results. The net duty for this heater is -2.093 kW.

3.5.4 Reactor

The stream is let to an adiabatic reactor. The reactor has a length of 1.04 m and a diameter of 0.104 m. The dimensions of the reactor are based on a similar reactor used by VanBussche et al. (1996). The calculations are shown in Appendix **??**. The process stream is set on vapor-only. The pressure drop is calculated using the Ergun correlation for the pressure drop in a packed bed reactor, as explained in Section 2.3.4, using the catalyst data provided in Section 2.3.5.

3.6 MEA recycle stream

The bottom stream from the stripper, the lean CO_2 stream, is recycled to the absorber. The recycle stream consists of the following units: purger, heating unit, pressure changer, mixer, and another heating unit.

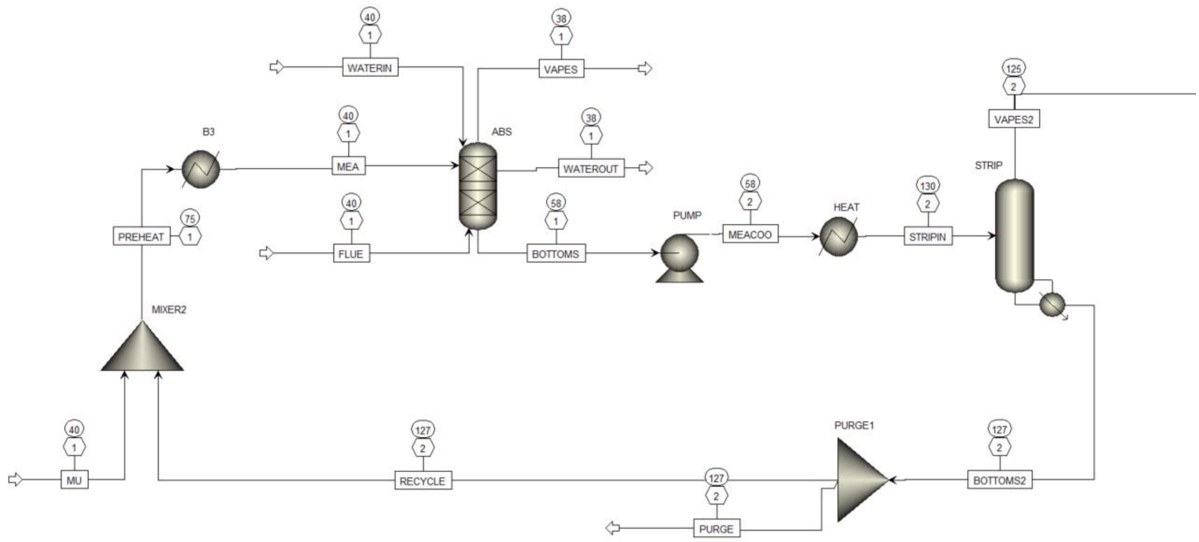


Figure 24: MEA recycle stream

3.6.1 Purger

The bottom stream from the stripper is first lead to a purger in order to avoid accumulation of materials in the recycle stream. The purger removes 10% of the bottoms stream in order to purge the gases.

3.6.2 Mixer

The resulting stream is lead to a mixing unit and mixed with a makeup stream to compensate for the MEA and water loss. The amount in the makeup stream is calculated using the calculator option in Aspen Plus.

3.6.3 Heating unit

The resulting stream is heated up to 40 °C before entering the absorber column. The net duty required for the heater equals -47.4301 kW.

3.6.4 MEA Make-up stream

The amount in the make-up stream is calculated using the calculator function in Aspen Plus. The calculations of the calculator block are shown in Appendix A

3.7 Hydrogen recycle stream

The methanol stream leaving the reactor is send to a FLASH2 separator where the methanol is separated from the remaining hydrogen and CO_2. The methanol stream, crudemeth, can be further processed towards higher quality methanol. The CO_2 and H_2 are send back to the reactor as a recycle stream. The flowsheet for the recycle stream is shown in Figure 25.

3.7.1 Flash separation

The flash separation separates the H_2 and CO_2 from the methanol. The flash block operates at 50 °C and 62 bar.

3.7.2 Purger

The purger splits the stream in order to avoid accumulation in the recycle stream. The purger removes 30% of the H2REC stream.

3.7.3 H_2 Makeup stream

The H_2 makeup stream make-ups for the H_2 that is used in the reaction or lost in the process. The H_2 input into the reactor is kept constant at 2.5 kmol/hr.

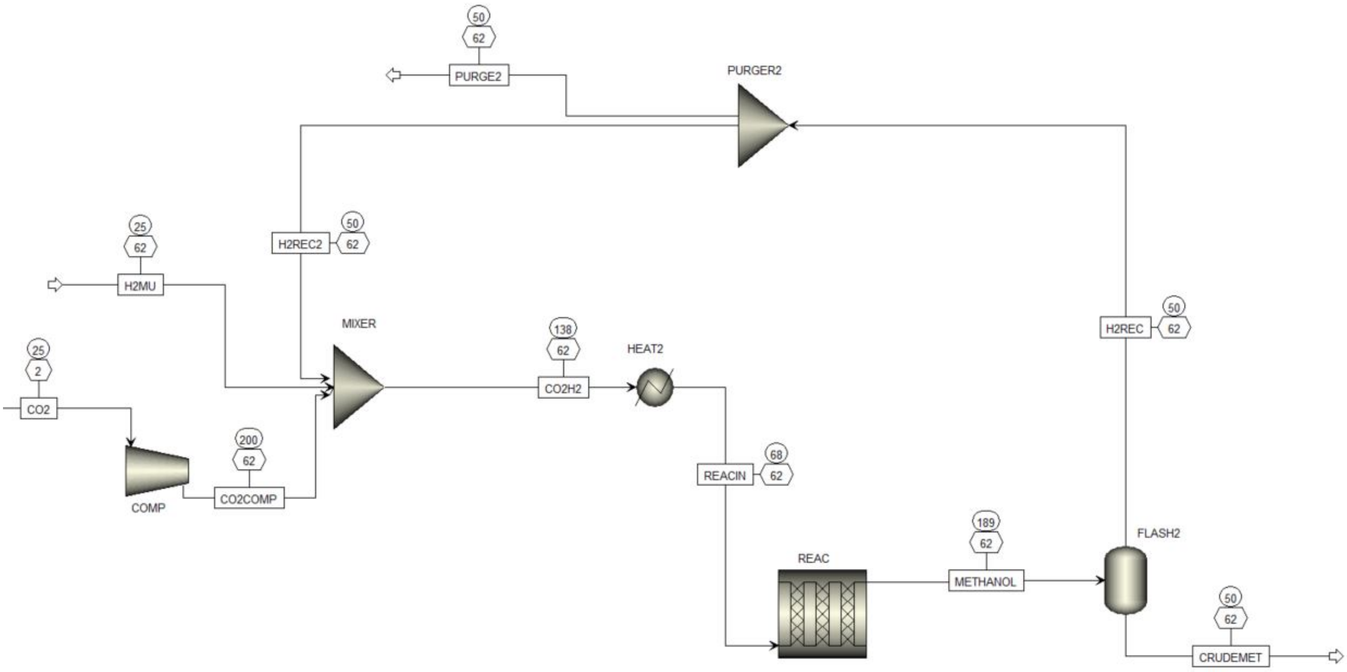


Figure 25: H_2 recycle stream

3.8 Methanol purification

The last step in this simulation is the work-up of the methanol. The crude methanol stream leaving the flash block is decompressed in three subsequent compressors and afterwards cooled to 25 °C. This stream enters a distillation column in order to purify the methanol from the crude methanol stream. The flowsheet for the purification step is shown in Figure 26

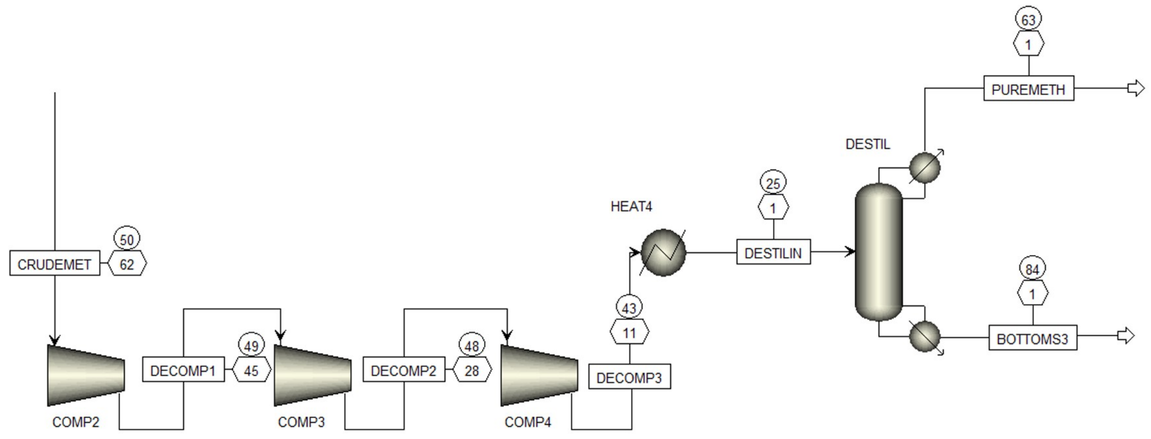


Figure 26: Flow sheet of the methanol distillation step

3.8.1 Compressors and heating unit

The crude methanol stream is decompressed in three subsequent compressors, labeled COMP2, COMP3, and COMP4 in the simulation. The first compressor has an outlet pressure of 45 bar, the second 28 bar and the third 11 bar. The net work required for the first compressor, COMP2, equals -6.578 Watt, for the second compressor, COMP3, this is -7.782 Watt and for the third compressor, COMP4, it equals -14.039 Watt. All compressors have an efficiency of 0.72. The stream is further decompressed and cooled in the heating block, labeled HEAT4 in the simulation. The stream leaving the heating block is 25 °C and 1 bar. The net duty of the heater equals -240.977 Watt.

3.8.2 Distillation

The methanol-water distillation is simulated using an equilibrium RADFRAC column. The distillation process is simulated with 30 numbers of stage, a partial-vapor condenser and a kettle reboiler. The reflux ratio and distillate to feed ratio are both specified at 0.1 (mole basis). However, both these variables are manipulated making use of the design specification option in Aspen Plus in order to reach the desired methanol recovery and purity. The set-up of the column are shown in Table 28.

Table 28: Setup of the RADFRAC distillation block in Aspen Plus

	Aspen Plus
Calculation type	Equilibrium
Number of stages	30
Condenser	Partial-vapor
Reboiler	Kettle
Valid phases	vapour-liquid
Convergence	Standard
Reflux ratio	0.1 (mole-based)
Distillate to feed ratio	0.1 (mole-based)
Free water reflux ratio	-
Stage-one pressure	1 bar

After the crude methanol stream is decompressed and cooled to 25 °C, the stream enters the distillation column, above-stage at stage 15. The two product streams, labeled BOTTOMS3 and PUREMETH, leave the distillation column. The BOTTOMS3 stream is the water-rich stream, leaving the distillation column at the bottom. The PUREMETH stream is the methanol-rich product stream, leaving the distillation column at the top. The data for the inlet and outlet streams of the distillation column are shown in Table 29

Table 29: Data of the streams entering and leaving the distillation block

	Stage	**Convention/phase**
Feed Streams		
DESTILIN	15	Above-stage
Product streams		
BOTTOMS3	30	Liquid
PUREMETH	1	Vapor

The design specifications are used to reach the desired mole purity of 85% methanol in the PUREMETH stream. The mole recovery is set to be 80%. The reflux ratio is marked as adjustable variable, with a lower bound of 0.01 and an upper bound of 20, running the simulation results in a reflux ratio of 0.56. The distillate to feed ratio is also marked as adjustable variable, with a lower bound of 0.01 and an upper bound of 1, running the simulation results in a distillate to feed ratio of 0.43.

4 Results

This section presents the results from the simulation. First, the results of the absorption step are presented, including a sensitivity analysis of the temperature and solvent concentration. Afterwards the stripper results are show, including a sensitivity analysis of the pressure and temperature. Afterwards, the reactor results are presented. The optimum hydrogen input, reactor pressure and inlet temperature are found using a sensitivity analysis. This section wraps up with showing the results after integrating both the MEA and H_2 recycle stream.

4.1 Absorption results

The results of this absorption simulation are shown in Table 30. This table shows the stream data of both inlet streams (FLUE and MEA) and both outlet streams (BOTTOMS and VAPES).

The amount of CO_2 absorbed is calculated using Equation 48 and equals 99.5%.

$$CO_2 \text{ Absorbed} = \frac{MEACOO \text{ out}}{CO_2 \text{ in}} \cdot 100\% = \frac{0.789}{0.793} \cdot 100\% = 99.5\% \tag{48}$$

Figure 27a shows the temperature of the of the liquid and vapor along the absorber column. Figure 27b shows the reaction rates of CO_2 and $MEACOO^-$ along the absorber column. It can be seen that the temperature increases over the stage number, leading to a hotter temperatures at the bottom of the absorber column. From Figure 27b it can be seen that the reaction rate is the highest between stage 7 and 8, meaning that most of the CO_2 is absorbed in these stages. Due to the exothermic nature of the absorption reaction, the temperature also increases in these stages, which explains the higher temperatures at the bottom of the column.

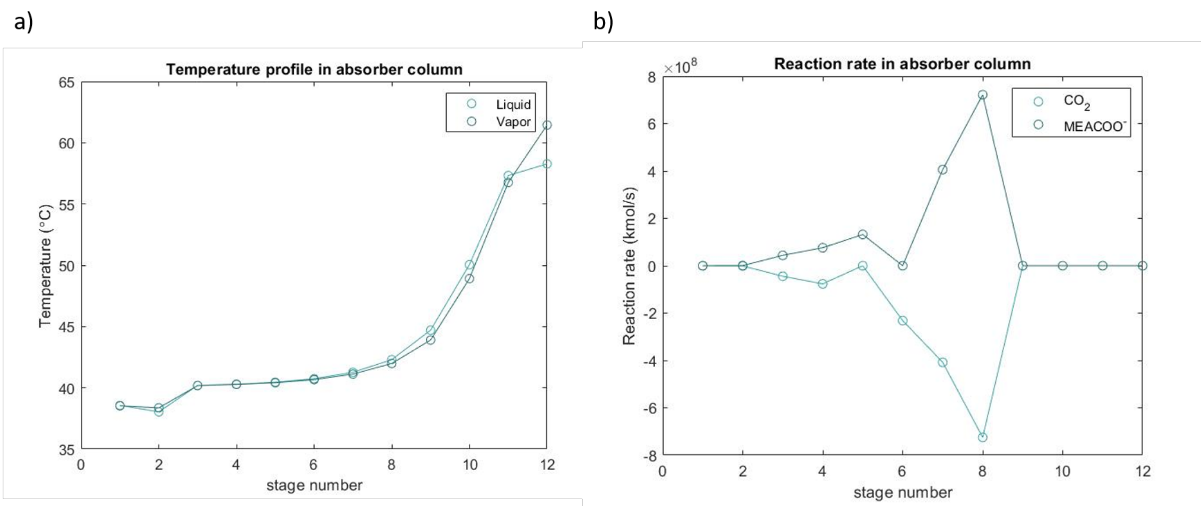


Figure 27: a) temperature of the liquid and vapor along the absorber column, b) reaction rate of CO_2 and $MEACOO^-$ along the absorber column

Figure 28a shows the liquid temperature as a function of stage number on the left axis and the reaction rate of CO_2 in the right axis. Figure 28b shows the liquid temperature as a function of stage number on the left axis and the $MEACOO^-$ composition on the right axis.

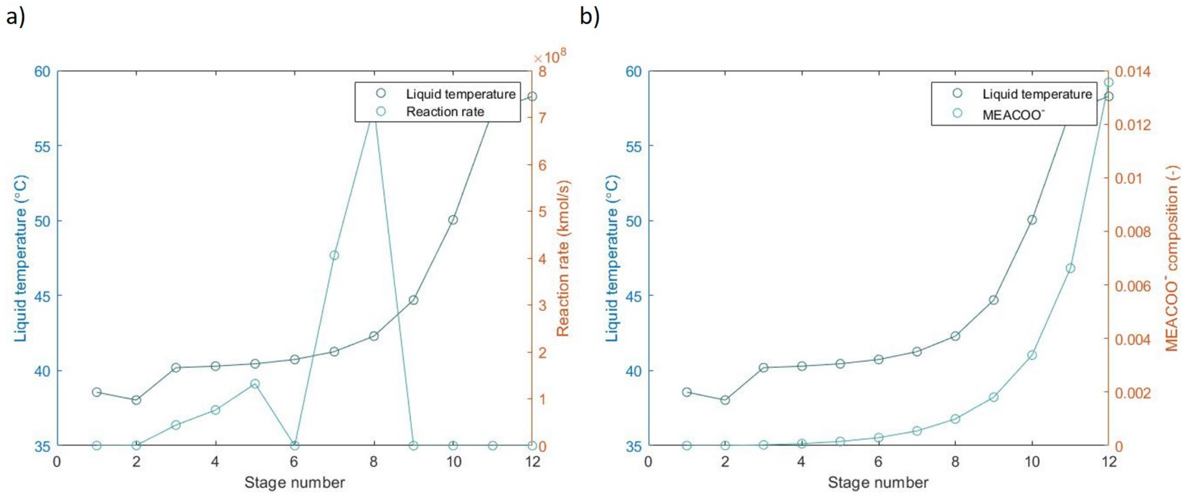


Figure 28: a) Liquid temperature along the absorber column on the right axis and reaction rate of $MEACCO^-$ along the absorber column on the left axis, b) liquid temperature along the absorber column on the right axis and $MEACOO^-$ composition along the absorber column on the left axis.

Table 30: Stream results of the absorption block

	FLUE	MEA	WATERIN	BOTTOMS	WATEROUT	VAPES
Temperature (°C)	40	40	40	58.3	38	61.4
Pressure (bar)	1.013	1.013	1.013	1.013	1.013	1.013
Vapor frac	1	0	0	0	0	1
Solid frac	0	0	0	0	0	0
Mole flow (kmol/hr)	6.1	57.6	4.0	58.166	3.5	5.423
Mass flow (kg/hr)	179.908	1316.05	72.061	1361.59	63.109	143.32
Enthalpy (Gcal/hr)	-0.095	-3.889	-0.272	-3.997	-0.238	-0.02
Mass Flow (kg/hr)						
H_2O	6.594	921.022	72.061	930.389	62.974	6.477
MEA	0	394.084	0	298.193	0.013	0.003
N_2	138.415	0	0	1.522	0.115	136.747
CO_2	34.9	0	0	< 0.001	< 0.001	0.092
$MEACOO^-$	0	0	0	82.098	0.002	0
H_3O^+	0	trace	trace	trace	trace	0
OH^-	0	0.204	trace	0.015	<0.001	0
HCO_3^-	0	0	0	0.065	0.002	0
$MEAH^+$	0	0.744	0	49.222	0.004	
Mole Flow (kmole/hr)						
H_2O	0.366	51.124	4	51.644	3.496	0.36
MEA	0	6.452	0	4.882	<0.001	0
N_2	4.941	0	0	0.055	0.004	4.881
CO_2	0.793	0	0	trace	trace	0.002
$MEACOO^-$	0	0	0	0.789	< 0.001	0
H_3O^+	0	trace	trace	trace	trace	0
OH^-	0	0.012	trace	0.001	trace	0
HCO_3^-	0	0	0	0.001	<0.001	0
$MEAH^+$	0	0.012	0	0.793	<0.001	0

4.1.1 Sensitivity Analysis

The following section shows the results of the sensitivity analysis performed for the absorption block. Both the temperature and MEA wt% in the inlet stream used to perform the sensitivity analysis.

The absorption process is simulated with different stream inlet temperatures. The inlet temperature is varied between 30 °C and 50 °C with a step-size of 1 °C. Increasing the temperature of the inlet stream decreases the driving force of absorption, however, it increases the reaction rate and the diffusivity rate. Therefore, a sensitivity analysis is performed to find the optimum temperature for CO_2 absorption. The bottoms and vapor distillate temperature, as well as the % absorbed CO_2 is shown as a result of the change in inlet temperature.

The results of the sensitivity analysis regarding the inlet temperature are shown in Figure 29. Figure 29a shows the change in CO_2 as a function of temperature of the inlet streams. Figure 29b shows the change temperature of the bottom and vapor stream as a function of temperature of the inlet streams. As can be seen from Figure 29a) the amount of CO_2 absorbed increases when the inlet temperature is increased. Subsequently, the temperature of both outlet streams, the vapes and bottom stream, also increase as the inlet temperature is increased. An optimum temperature is around 46 °C and 48 °C, after which the amount of CO_2 absorbed decreases again. The optimum temperature for the absorption process is a trade-off between amount of CO_2 absorbed and temperature of the outlet streams. Hotter outlet streams also increase the energy requirement in the process later on. Therefore it is decided to use 40 °C for the further development of the simulation.

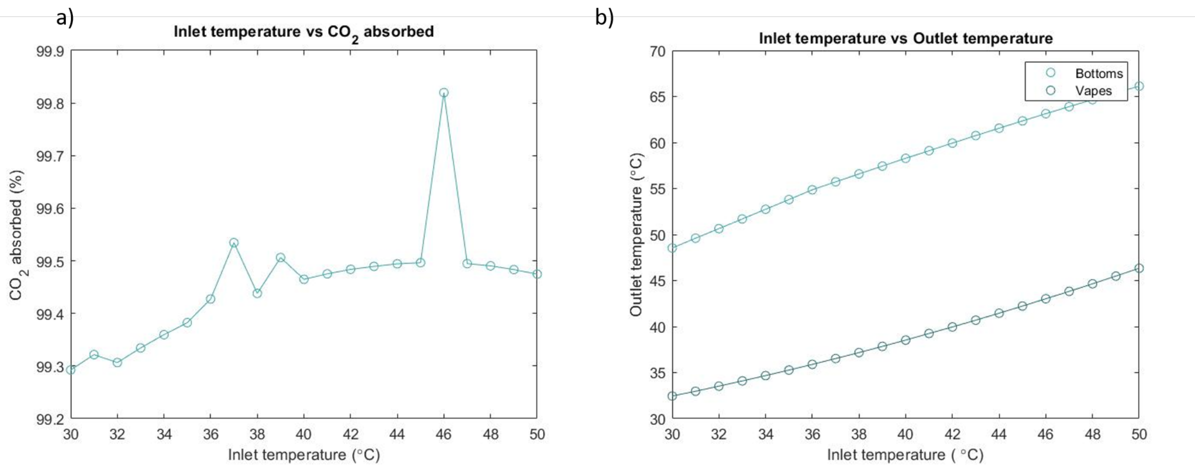


Figure 29: Figure a) shows the change in CO_2 absorbed as a function of inlet temperature of the inlet stream, figure b) shows the temperature of the vapor and bottom outlet stream as a function of temperature of the inlet stream

The absorption process is simulated with different wt% of MEA in the solvent stream. The wt% of MEA is varied between 25 wt% and 35 wt% with a step-size of 5 wt%. The bottoms and vapor distillate temperature, as well as the % absorbed CO_2 is shown as a result of the change in MEA wt%.

Figure 30 shows the results of the sensitivity analysis regarding the wt% of MEA in the inlet stream. As can be seen from Figure 30a the amount of CO_2 absorbed decreases when the wt% of MEA in the solvent is increased. Figure 30b shows that also the temperatures of both output streams decreases with increasing wt% MEA in the input stream. For the rest of the simulation it is decided to use 30 wt% MEA as solvent.

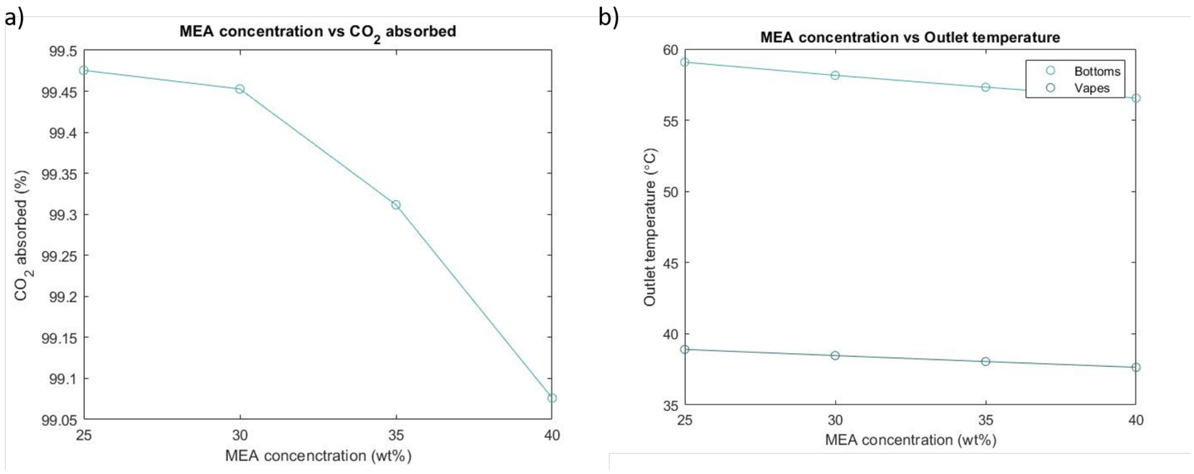


Figure 30: Figure a) shows the change in CO_2 absorbed as a function of wt% MEA in the solvent inlet stream, figure b) shows the temperature of the vapor and bottom outlet stream as a function of wt% in the solvent inlet stream

Table 31 shows the amount of CO_2 absorbed from the flue gas stream for the different flow models. Dependent on the flow model, the absorption ranges between 98.6% and 99.5%.

Table 31: Amount of CO_2 absorbed from the flue gas stream for the different flow models.

Flow model	$MEACOO^-$ **(kmol/hr)**	CO_2 **absorbed (%)**
VPlug	0.789	99.5
Mixed	0.783	98.7
Countercurrent	0.788	99.3
Vplug-Pavg	0.789	99.5
Lpug	0.782	98.6

4.1.2 Comparison with literature

Desideri and Paolucci (1999) report a CO_2 removal of 90.4% for their natural gas fired power plant and 90.0% for the coal fired power plant, after integrating CO_2 recovery [22]. Errico et al. (2011) report absorption numbers between 98.4% and 99.1% depending on some changes in the model. Maddedu et al. (2019) report CO_2 removal numbers ranging between 99.1 % up to 99.6%, depending on the number of segments used in the model. The absorption numbers presented in this thesis, ranging between 98.6% and 99.5% are comparable to the numbers presented by Errico et al. (2011) and Maddeddu et al. (2019).

Oi et al. (2007) show that increasing the gas and liquid inlet temperature of the absorption column yield lower CO_2 absorption results. However, in this case the trend is simulated for absorption at equilibrium. Higher temperatures will also give higher absorption rates due to higher reactions rates, this effect is not seen when simulating the process as equilibrium [66].

Kothandaraman mention a similar profile for the increase of the solvent temperature as shown in Figure 29a. With increasing temperature, the driving force of the absorption decreases. However, the rate of the reaction and the diffusivity increases as temperature increases [46]. Furthermore, they mention a temperature bulge at the top of the column since a significant amount of the reaction occurs at the top, where the liquid enters the column, and since the reaction is exothermic, this leads to a temperature increase [46]. However, this profile is not seen in the simulations done in this thesis, see Figure 27a. Here, the temperature increases over the stage numbers and the highest temperatures are seen at the bottom of the column. This suggest that in the simulation, the reaction does not occur significantly more at the top of the column, hence not having a temperature bulge at the top of the column. In the Figure 27a, it can also be seen that the reaction rate spikes at stage 8, which further explains the increase in temperature at the bottom of the column. Maddedu et al. (2019) provide some more insight in temperature profiles that are often seen in absorption column. In general, three situations can be distinguished:

- L/V < 5 : the temperature bulge is located at the top of the column;
- $5 <$ L/V < 6 : the temperature bulge is located in the middle of the column;
- L/V > 6 : the temperature bulge is located at the bottom of the column.

In this simulations, it was seen that the temperature bulge is located at the bottom of the column, suggesting L/G > 6. The location of the temperature bulge generally depends on the type of packing that is used in the simulation, where structured packing often shows a bulge at the top of the column. When random packing is considered, a higher L/G is required, hence showing a temperature bulge at the middle or bottom of the column. The packing material used in the simulations of this thesis, FLEXIPAC 250Y, is considered to be a structured packing. Therefore, it is expected to see a temperature bulge located at the top of the column, which is not seen in the temperature profile. Figure 31 shows the liquid temperature profile inside the column for a column with random packing. This profile shows a similar trend as Figure 27a.

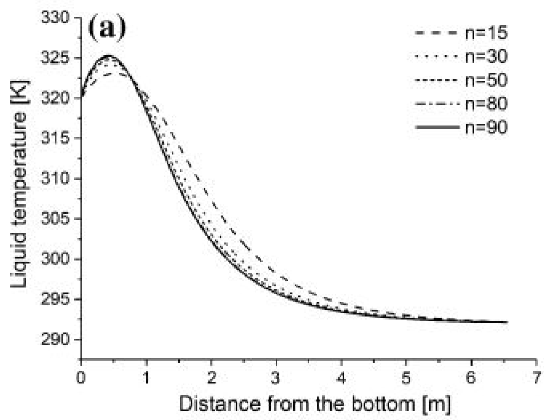


Figure 31: Liquid temperature in the absorption column (Retrieved from Maddedu et al (2019) [55])

4.2 Stripping Results

The results of the stripper block are shown in Table 32. The table show the data of the inlet stream (STRIPIN) and both outlet streams (BOTTOMS2 and VAPES2). The amount of CO_2 stripped from the $MEACOO^-$ stream is calculated in Equation 49 and equals 78.3 %.

$$CO_2 \text{ stripped} = \frac{CO_2 \text{ out}}{MEACOO^- \text{ in}} \cdot 100\% = \frac{0.618}{0.789} \cdot 100\% = 78.3\% \tag{49}$$

The amount of CO_2 stripped compared to the amount of CO_2 entering the process in the flue gas stream, is calculated in Equation 50 and equals 77.9 %.

$$CO_2 \text{ recovered} = \frac{CO_2 \text{ out}}{CO_2 \text{ in}} \cdot 100\% = \frac{0.618}{0.793} \cdot 100\% = 77.9\% \tag{50}$$

Table 32: Stream results of the stripper block

	STRIPIN	**BOTTOMS2**	**VAPES2**
Temperature (°C)	130	128.1	125.2
Pressure (bar)	1.621	1.6	1.6
Vapor frac	0.66	0	1
Solid frac	0	0	0
Mole flow (kmol/hr	58.166	18.674	40.111
Mass flow (kg/hr)	1361.59	585.123	776.471
Enthalpy (Gcal/hr)	-3.545	-1.223	-2.296
Mass flow (kg/hr)			
H_2O	930.389	235.501	694.887
MEA	298.193	321.004	52.823
N_2	1.522	trace	1.552
CO_2	<0.001	trace	27.21
$MEACOO^-$	82.089	17.703	0
H_3O^+	trace	trace	0
OH^-	0.015	0.008	0
HCO_3^-	0.065	0.144	0
CO_3^{2-}	0.062	0.008	0
$MEAH^+$	49.222	10.755	0
Mole flow (kmol/hr)			
H_2O	51.644	13.072	38.572
MEA	4.882	5.255	0.865
N_2	0.055	trace	0.0555
CO_2	trace	trace	0.618
$MEACOO^-$	0.789	0.17	0
H_3O^+	trace	trace	0
OH^-	0.001	<0.001	0
HCO_3^-	0.001	0.002	0
CO_3^{2-}	0.001	<0.001	0
$MEAH^+$	0.793	0.173	0

Figure 32a shows the temperature profile of the liquid and vapor stream in the stripper column. Figure 32b shows the reaction rate of CO_2 and $MEACOO^-$ along the stripper column.

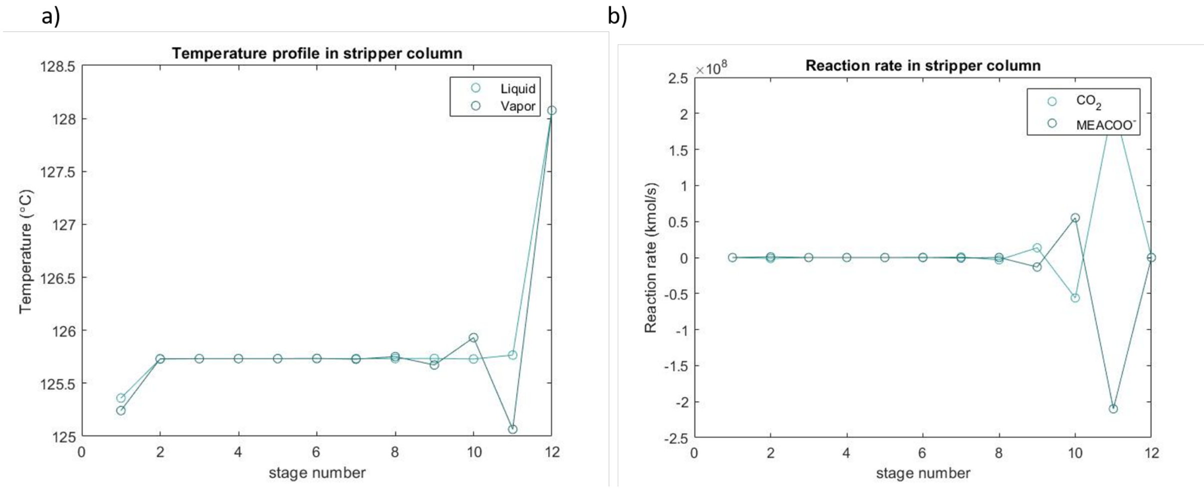


Figure 32: a) vapor and liquid temperature along the stripper column, b) reaction rate of CO_2 and $MEACOO^-$ along the stripper column

Figure 33a shows the liquid temperature along the stripper column on the left y-axis and the reaction rate of $MEACOO^-$ on the right y-axis. Figure 33b shows the liquid temperature along the stripper column on the left y-axis and the CO_2 composition along the stripper column on the right y-axis.

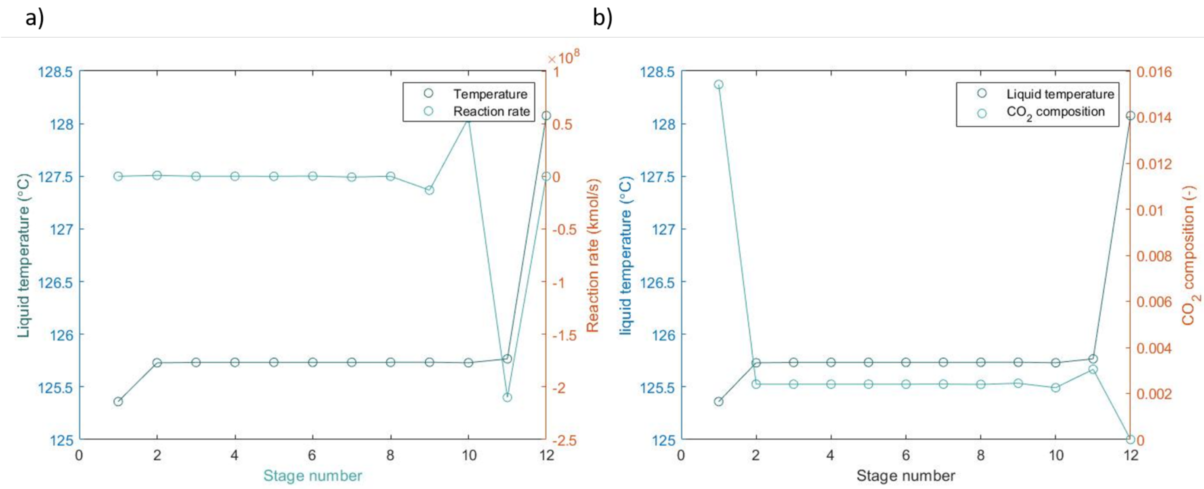


Figure 33: a) liquid temperature along the stripper column on the left y-axis and $MEACOO^-$ reaction rate along the right y-axis b) liquid temperature along the stripper column on the left y-axis and CO_2 composition on the right y-axis.

The results of the condenser block are shown in Table 33. The stream with stream ID VAPES2 enters the condenser block. The stream with stream ID CO2 leaves the condenser block at the top and is the CO_2 rich stream, used for the further processing and conversion into methanol. The stream WATOUT contains the remaining MEA and water and leaves the condensor block at the bottom as waste stream. Table 33 shows the data of the inlet stream (VAPES2) and both outlet streams (CO2 and WATOUT).

The amount of CO_2 recovered after the condenser block is shown in Equation 51 and equals 74.7%.

$$CO_2 \text{ stripped} = \frac{CO_2 \text{ out}}{MEACOO^- \text{ in}} \cdot 100\% = \frac{0.589}{0.789} \cdot 100\% = 74.7\% \tag{51}$$

The amount of CO_2 recovered from the flue gas stream is shown in Equation 52 and equals 74.3%.

$$CO_2 \text{ stripped} = \frac{CO_2 \text{ out}}{MEACOO^- \text{ in}} \cdot 100\% = \frac{0.589}{0.93} \cdot 100\% = 74.3\% \tag{52}$$

The condenser is able to separate 95.3% of the CO_2 entering the condenser block, having less than 5% CO_2 loss in this block. The resulting CO_2 rich stream contains 90.6% CO_2, 7.4% N_2, 2.0% H_2O and trace amounts of MEA.

Table 33: Stream results of the condenser block

	VAPES2	**CO2**	**WATOUT**
Temperature (˚C)	125.2	24.9	24.9
Pressure (bar)	1.6	1.6	1.6
Vapor frac	1	1	0
Solid frac	0	0	0
Mole flow (kmol/hr	40.111	0.65	39.46
Mass flow (kg/hr)	776.471	27.52	748.951
Enthalpy (Gcal/hr)	-2.296	-0.056	-2.692
Mass flow (kg/hr)			
H_2O	694.887	0.233	694.654
MEA	52.823	<0.001	52.823
N_2	1.522	1.343	0.209
CO_2	27.21.6	25.943	1.266
Mole flow (kmol/hr)			
H_2O	38.572	0.013	38.559
MEA	0.865	trace	0.865
N_2	0.055	0.048	0.007
CO_2	0.618	0.589	0.029

As can be seen from Figure 34a, increasing the reboiler duty of the stripper also increases the amount of CO_2 stripped from the inlet stream. It is chosen to use a reboiler duty of 29.9 kW, which corresponds to an energy requirement of 4 GJ/tonCO_2. In Figure 34b, it can be seen that the BOTTOMS temperature also increases with increasing reboiler duty. The VAPES stream temperature stays constant with increasing temperature.

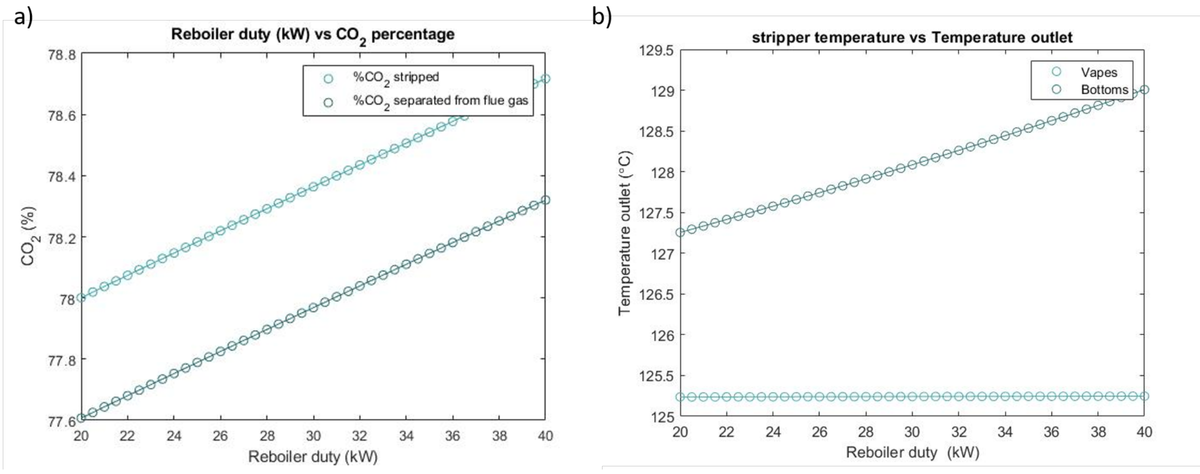


Figure 34: a) CO_2 stripped from the $MEACOO^-$ stream and flue gas stream as a function of reboiler duty, b) Stripper VAPOR and BOTTOMS outlet temperature as a function of stripper duty

4.2.1 Sensitivity analysis

Figure 35a shows the amount of CO_2 descorbed from the $MEACOO^-$ stream and from the flue gas stream as a function of stripper temperature. Higher temperatures yield higher desorption rates. At a temperature of 120 °C only around 45% of the CO_2 is desorbed, while at 130 °C 78.3% of the CO_2 is desorbed. Figure 35b shows the temperatures of the outlet streams as a function of stripper temperature. When the stripper temperature is increased, both temperatures of the outlet stream also increase.

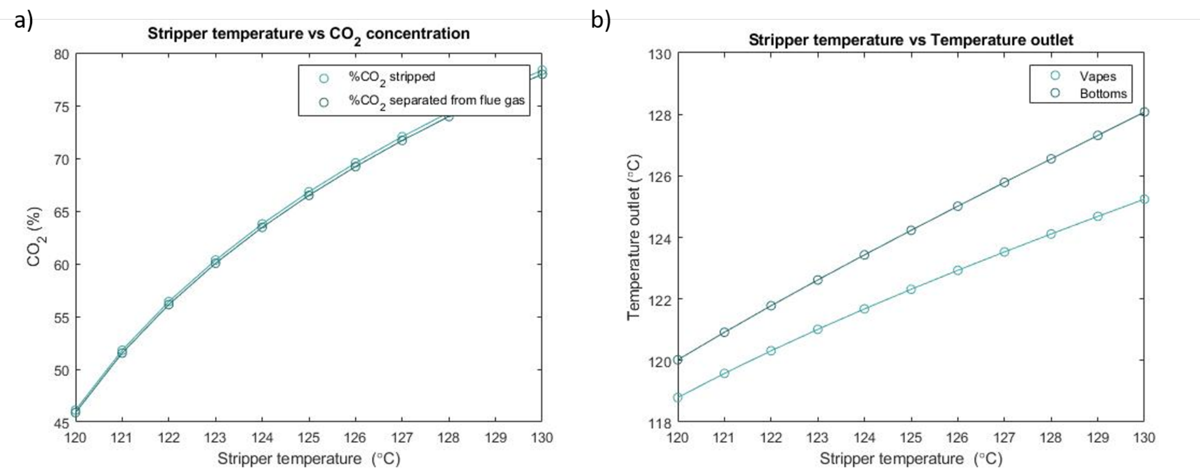


Figure 35: a) CO_2 stripped from the $MEACOO^-$ stream and flue gas stream as a function of stripper temperature, b) VAPOR and BOTTOMS temperature as a function of stripper temperature.

4.2.2 Comparison with literature

The Aspen Technology Inc. file present a total CO_2 removal of 79.1% for their simulations [4]. In this thesis a CO_2 removal of 77.9% was found, which is slightly lower compared to the Aspen Technology Inc. file.

Oi et al (2007) mention convergence issues in the stripper with regards to the sensitivity analysis for the pressure [66]. Oi et al (2007) mention an increased CO_2 removal efficiency at higher stripper temperatures, showing a similar trend as presented in this thesis.

Kothandaraman mentions reboiler duties of 4.25 GJ/tonCO_2 for coal power plants and 4.5 GJ/tonCO_2 for natural gas power plants. The natural gas power plants often have a slightly higher reboiler duty due to a lower rich loading [46]. Kothandaraman report CO_2 capture numbers of 85% at a temperature of 125 °C, while in this thesis at 125°C the amount of CO_2 captures is slightly above 65 %.

Increasing the temperature of the system leads to favoured CO_2 transfer to the gas phase [46]. Therefore, operating the stripper at higher temperature is favorable and leads to higher CO_2 desorption numbers. he sensitivity analysis performed in this thesis showed this profile for the temperature, increased temperature lead to higher CO_2 desorption rates. Eventually, the temperature in the stripper is limited by the degradation of MEA, since higher temperatures also accelerate the degradation rate. It is suggested in literature to not use temperatures above 125 °C in order to limit degradation [46].

As a final note, it should be noted that the CO_2 recovery after the stripper is too some extend arbitrary, since it can easily be increased by increasing the reboiler duty. A compromise between the energy requirement and the desired CO_2 recovery should always be found.

4.3 Conversion Results

The results of the conversion block are discussed in this section. The stream data of the inlet stream (REACIN) and the outlet stream (METHANOL) are shown in Table 34.

The amount of CO_2 converted into CH_3OH is calculated using Equation 53 and equals 37.9%.

$$CH_3OH \text{ conversion} = \frac{CH_3OH \text{ out}}{CO_2 \text{ in}} \cdot 100\% = \frac{0.223}{0.589} \cdot 100\% = 37.9\% \tag{53}$$

Besides the conversion of CO_2 into CH_3OH, CO is also formed. The selectivity towards CH_3OH is calculated using equation 54 and equals 99.9 %.

$$CH_3OH \text{ selectivity} = \frac{CH_3OH \text{ out}}{CH_3OH \text{ in} + CO \text{ out}} \cdot 100\% = \frac{7.15}{7.15 + 0.007} \cdot 100\% = 99.9\% \tag{54}$$

Table 34: Stream results of the conversion block

	REACIN	**METHANOL**
Temperature ˚C	67	198.7
Pressure (bar)	62	61.993
Vapor frac	1	1
Solid frac	0	0
Mole flow (kmol/hr	3.15	2.704
Mass flow (kg/hr)	32.56	32.56
Enthalpy (Gcal/hr)	-0.055	-0.055
Mass flow (kg/hr)		
H_2O	0.233	4.258
MEA	<0.001	<0.001
N_2	1.343	1.343
CO_2	25.943	16.111
H_2	5.04	3.69
CH_3OH	0	7.15
CO	0	0.007
Mole flow (kmol/hr)		
H_2O	0.013	0.236
MEA	trace	trace
N_2	0.048	0.048
CO_2	0.589	0.366
H_2	2.5	1.83
CH_3OH	0	0.223
CO	0	<0.001

Figure 36a shows the methanol percentage in the outlet stream as a function of H_2 inlet amount, ranging from 0.5 kmol/hr to 3 kmol/hr. As can be seen in the graph, the highest yield is found at an input of 2.5 kmol/hr of hydrogen. This corresponds to a mole ratio of CO_2:H_2 of 1:4.2. Figure 36b shows the methanol percentage in the outlet stream as a function of pressure. The amount of methanol produced increases as the pressure increases.

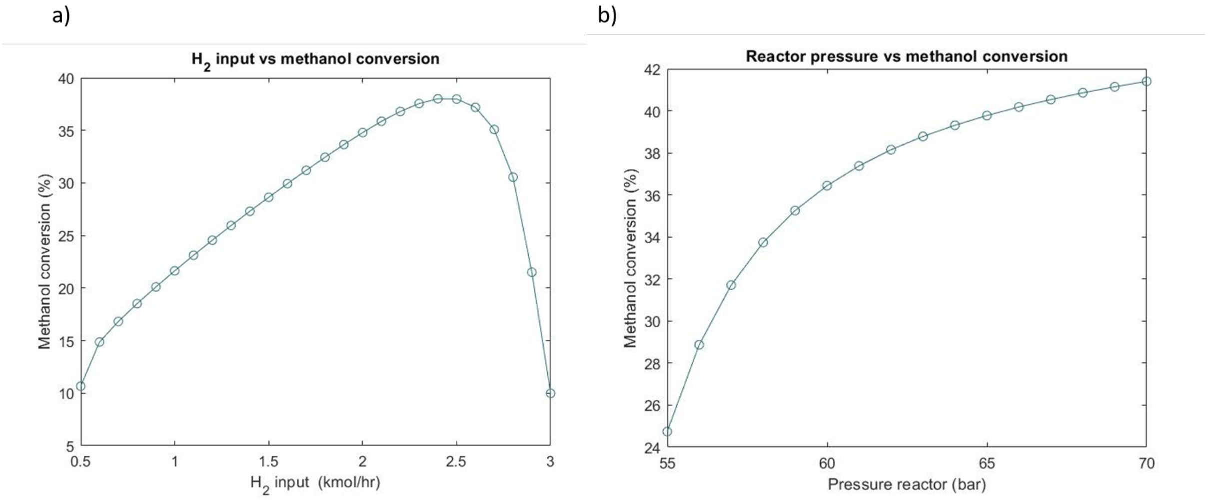


Figure 36: a) methanol conversion as a function of amount of H_2 in the inlet stream, b) methanol conversion as a function of reactor pressure

Figure 37a shows the methanol percentage in the outlet stream of the reactor as a function of temperature of the inlet stream between the 20 °C and 250 °C, Figure 37b zooms in between 60 °C and 70 °C. As can been seen in the graphs, the highest amount of methanol is produced at a temperature of 68 °C. According to literature methanol conversion starts to take place at temperatures around 200 °C.

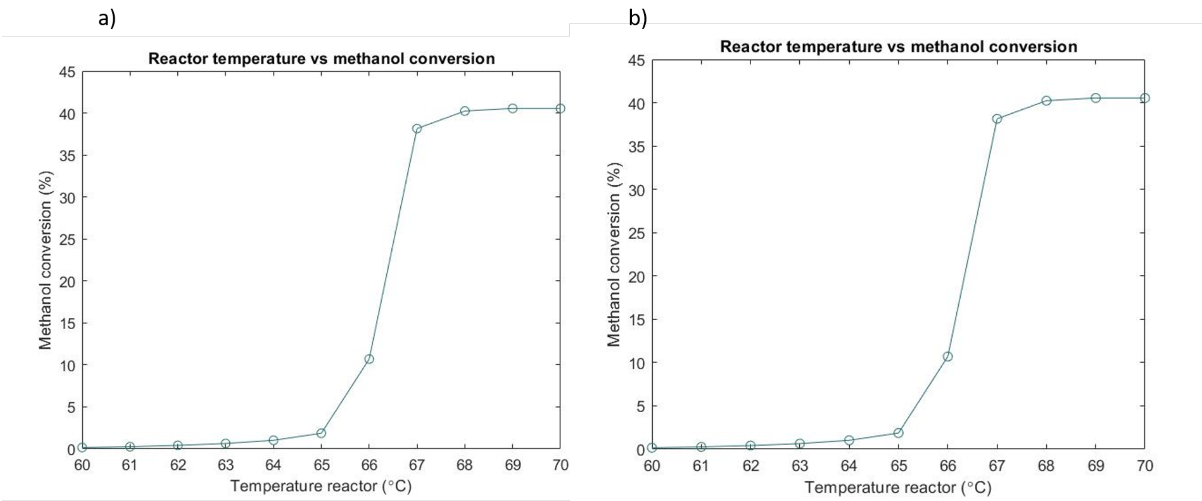


Figure 37: a) methanol conversion as a function of reactor inlet temperature between 20 °C and 250 °C, b) methanol conversion as a function of reactor inlet temperature between 60 °C and 70 °C.

To further investigate the temperature profile, a temperature profile within the reactor is also plotted. Figure 38a shows the temperature inside the reactor as a function of reactor length, with an inlet temperature of 68 °C. As can be seen in this graph, the temperature inside the reactor increases to around 200 °C. The methanol production also takes place in the reactor parts where the temperature is around 200 °C, in agreement with literature on methanol production. Figure 38 shows the residence time as a function of reactor length, showing a linear trend.

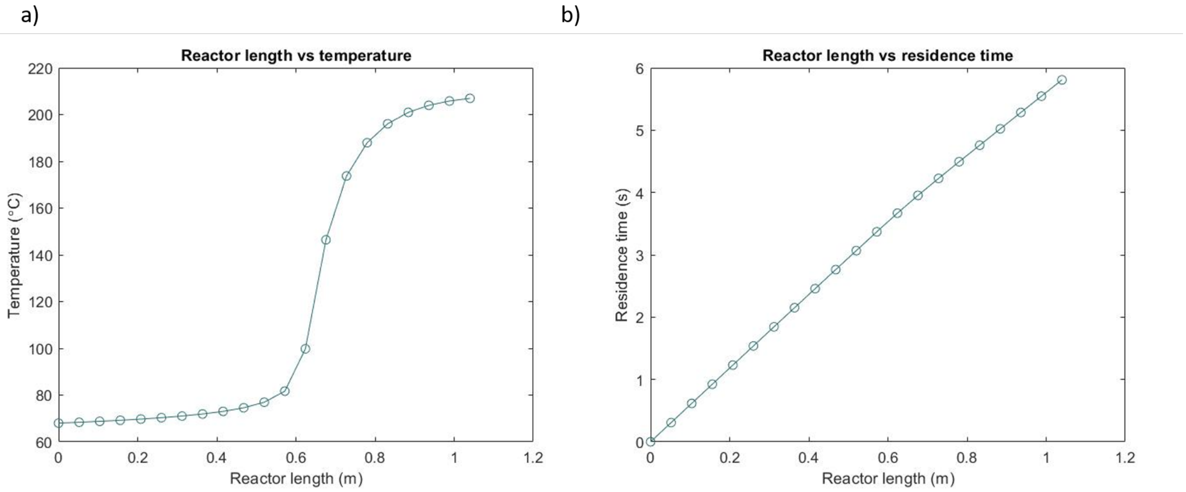


Figure 38: a) Temperature inside the reactor b) residence time as a function of reactor length

Figure 39a shows the reactor composition for CO_2, H_2, CH_3OH and CO over the reactor length. Figure 39b shows the composition of CH_3OH over the reactor length. As can be seen here, the CO_2 and H_2 are converted into methanol in the reactor part where the temperature increases up to 200 °C.

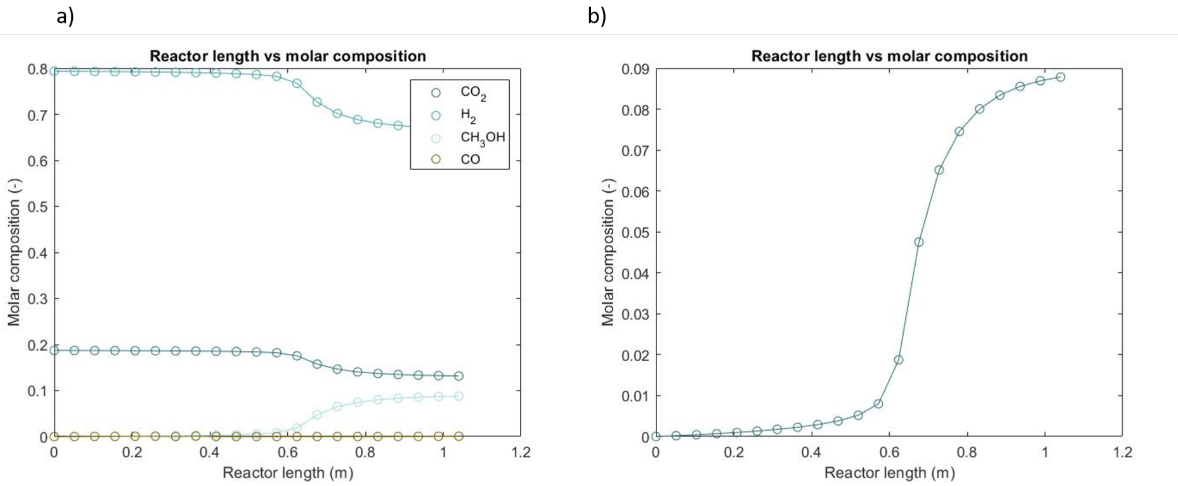


Figure 39: a) molar compositions of CO_2, H_2, CH_3OH and CO inside the reactor, b) molar composition of CH_3OH inside the reactor

4.3.1 Comparison with literature

In literature, the highest conversion rates are mentioned at inlet temperatures above 200°C. Chen et al. (2011) show an optimum inlet temperature of 228 °C, where the methanol production reaches it's maximum [10]. It is further explained that higher temperatures impede methanol formation once a thermodynamic equilibrium is reached, due to the exothermic nature of the reaction. Higher temperatures lead to higher reaction rates, which results in faster reaching of thermodynamic equilibrium, often before the bed outlet, i.e. often a large amount of the catalyst bed is not used. When the temperature is too low, thermodynamic equilibrium cannot be reached before the bed outlet [10]. From Figure 39a it can be seen that in the simulation thermodynamic equilibrium is also reached before the bed outlet. In the simulation, a significantly lower inlet temperature (68 °C) is used compared to the article by Chen et al. In the article by Chen et al. a reactor with inter-cooling is used, while in this thesis, the conversion is simulated using an adiabatic reactor. Due to the choice of an adiabatic reactor, the temperature inside the reactor increases rapidly when inlet streams of above 200 °C are used, and therefore thermodynamic equilibrium is reached extremely fast, leading to lower methanol production rates. Therefore, it is chosen to use a lower inlet temperature and let the temperature increase over the length of the reactor, as shown in Figure 37a.

4.4 Recycle streams

This section shows the results after the MEA recycle stream and the H_2 recycle stream are added to the flowsheet.

4.4.1 MEA recycle stream

The MEA recycle stream is first presented. This recycle stream includes a purger and a mixer.

4.4.2 Purger

The purger removes 10% of the BOTTOMS stream and separates the stream into a PURGE and RECYCLE stream. The inlet streams and outlet streams of the purger are shown in Table 38

Table 35: Stream results of the purger block

	BOTTOMS2	RECYCLE	PURGE
Temperature (°C)	127.5	127.5	127.5
Pressure (bar)	1.6	1.6	1.6
Vapor frac	0	<0.001	<0.001
Solid frac	0	0	0
Mole flow (kmol/hr	20.905	18.815	2.091
Mass flow (kg/hr)	646.563	581.906	64.656
Enthalpy (Gcal/hr)	-1.374	-1.236	-0.137
Mass flow (kg/hr)			
H_2O	267.53	240.777	26.753
MEA	343.903	309.512	34.39
N_2	trace	trace	trace
CO_2	trace	trace	trace
$MEACOO^-$	21.729	19.556	2.173
H_3O^+	trace	trace	trace
OH^-	0.008	0.007	0.001
HCO_3^-	0.183	0.164	0.018
CO_3^{2-}	0.011	0.009	0.001
$MEAH^+$	13.2	11.88	1.32
Mole flow (kmol/hr)			
H_2O	14.85	13.365	1.485
MEA	5.63	5.067	0.563
N_2	trace	trace	trace
CO_2	trace	trace	trace
$MEACOO^-$	0.209	0.188	0.021
H_3O^+	trace	trace	trace
OH^-	<0.001	<0.001	<0.001
HCO_3^-	0.003	0.003	<0.001
CO_3^{2-}	<0.001	<0.001	<0.001
$MEAH^+$	0.213	0.191	0.021

4.4.3 MEA Make-up stream

The stream data of the MEA make-up stream is given in Table 36

Table 36: Stream data of the MEA make-up stream

	MU
Temperature (°C)	40
Pressure (bar)	1.013
Vapor frac	0
Solid frac	0
Mole flow (kmol/hr)	39.144
Mass flow (kg/hr)	764.817
Enthalpy (Gcal/hr)	-2.657
Mass flow (kg/hr)	
H_2O	680.245
MEA	84.572
Mole flow (kmol/hr)	
H_2O	37.759
MEA	1.385

The new stream data of the absorbed block including the recycle stream is shown in Table 37

Table 37: Stream results of the absorption block with the recycle stream

	FLUE	**MEA**	**WATERIN**	**BOTTOMS**	**WATEROUT**	**VAPES**
Temperature (°C)	40	40	40	57.7	37.6	61.4
Pressure (bar)	1.013	1.013	1.013	1.013	1.013	1.013
Vapor frac	1	0	0	0	0	1
Solid frac	0	0	0	0	0	0
Mole flow (kmol/hr)	6.1	57.959	4.0	58.532	3.5	5.236
Mass flow (kg/hr)	179.908	1346.72	72.061	1392.39	63.11	143.197
Enthalpy (Gcal/hr)	-0.095	-3.934	-0.272	-4.043	-0.238	-0.02
Mass Flow (kg/hr)						
H_2O	6.594	921.022	72.061	927.222	62.973	6.347
MEA	0	394.084	0	305.822	0.012	0.003
N_2	138.415	trace	0	1.554	0.116	136.744
CO_2	34.9	trace	0	< 0.001	< 0.001	0.102
$MEACOO^-$	0	19.556	0	83.718	0.002	0
H_3O^+	0	trace	trace	trace	trace	0
OH^-	0	0.007	trace	0.003	<0.001	0
HCO_3^-	0	0.164	0	8.488	0.002	0
$MEAH^+$	0	11.88	0	63.302	0.004	0
Mole Flow (kmole/hr)						
H_2O	0.366	51.124	4	51.469	3.496	0.352
MEA	0	6.452	0	5.007	<0.001	<0.001
N_2	4.941	trace	0	0.055	0.004	4.881
CO_2	0.793	trace	0	trace	trace	0.002
$MEACOO^-$	0	0.188	0	0.804	<0.001	0
H_3O^+	0	trace	trace	trace	trace	0
OH^-	0	<0.001	trace	<0.001	trace	0
HCO_3^-	0	0.003	0	0.139	<0.001	0
$MEAH^+$	0	0.191	0	1.019	<0.001	0

4.4.4 H_2 recycle stream

The H_2 recycle stream is presented in this section. The recycle stream includes a FLASH separation block, a purger and a mixer.

4.4.5 FLASH

In the FLASH block, the METHANOL stream leaving the reactor is cooled to 50 °C to separate the methanol from the remaining CO_2 and H_2. The bottom stream involves the crude methanol and the vapor stream

Table 38: Stream results of the flash block

	METHANOL	**CRUDEMET**	**H2REC**
Temperature (°C)	189.1	50	50
Pressure (bar)	61.978	62	62
Vapor frac	1	0	1
Solid frac	0	0	0
Mole flow (kmol/hr	3.53	0.631	2.899
Mass flow (kg/hr)	85.258	16.162	69.096
Enthalpy (Gcal/hr)	-0.162	-0.04	-0.132
Mass flow (kg/hr)			
H_2O	5.683	5.59	0.092
MEA	<0.001	<0.001	trace
N_2	4.499	0.055	4.443
CO_2	62.434	1.251	61.181
H_2	2.669	0.003	2.667
CH_3OH	9.896	9.26	0.636
CO	0.078	<0.001	0.078
Mole flow (kmol/hr)			
H_2O	0.315	0.31	0.005
MEA	trace	trace	trace
N_2	0.161	0.002	0.159
CO_2	1.419	0.028	1.39
H_2	1.324	0.001	1.323
CH_3OH	0.309	0.289	0.02
CO	0.003	trace	trace

4.4.6 Purger

The purger splits 30% of the recycle stream into a purge stream. The purge stream is relatively large in order to aid in the convergence. Since the recycle stream is large compared to the reactor input stream, Aspen Plus has difficulties with converging the mass balances of the mixer block before the reactor. Therefore, it is decided to use a larger purge stream and therefore a smaller recycle stream. This facilitated the convergence of the mass balances.

4.4.7 H_2 make-up stream

The H_2 make-up stream keeps the inflow of H_2 to the reactor at a constant of 2.5 kmol/hr. The data of the H_2 make-up stream is shown in Table 39.

Table 39: Stream data of the MEA make-up stream

	MU
Temperature (°C)	25
Pressure (bar)	62
Vapor frac	1
Solid frac	0
Mole flow (kmol/hr)	1.284
Mass flow (kg/hr)	2.588
Enthalpy (Gcal/hr)	<0.001
Mass flow (kg/hr)	
H_2	2.588
Mole flow (kmol/hr)	
H_2	1.284

4.4.8 Reactor

The reactor input and output streams after the addition of the H_2 recylce stream is shown in Table 40.

Table 40: Stream results of the conversion block

	REACIN	**METHANOL**
Temperature ˚C	68	189.1
Pressure (bar)	62	61.978
Vapor frac	1	1
Solid frac	0	0
Mole flow (kmol/hr	4.121	3.513
Mass flow (kg/hr)	85.261	85.261
Enthalpy (Gcal/hr)	-0.162	-0.162
Mass flow (kg/hr)		
H_2O	0.354	5.683
MEA	<0.001	<0.001
N_2	4.498	4.498
CO_2	75.455	62.436
H_2	4.455	2.669
CH_3OH	0.445	9.896
CO	0.054	0.078
Mole flow (kmol/hr)		
H_2O	0.002	0.315
MEA	trace	trace
N_2	0.161	0.161
CO_2	1.714	1.419
H_2	2.21	1.324
CH_3OH	0.014	0.309
CO	0.002	0.003

4.5 Methanol purification

The stream results of the distillation block are shown in Table 41.

Table 41: Stream results of the distillation block

	DESTILIN	**BOTTOMS3**	**PUREMETH**
Temperature (°C)	25	83.8	62.6
Pressure (bar)	1	1	1
Vapor frac	0.053	0	1
Solid frac	0	0	0
Mole flow (kmol/hr	0.631	0.359	0.272
Mass flow (kg/hr)	16.162	7.282	8.881
Enthalpy (Gcal/hr)	-0.04	-0.023	-0.014
Mass flow (kg/hr)			
H_2O	5.591	5.429	0.162
MEA	trace	trace	trace
N_2	0.055	trace	0.055
CO_2	1.251	trace	1.251
H_2	0.003	trace	0.003
CH_3OH	9.261	1.852	7.409
CO	<0.001	trace	<0.001
Mole flow (kmol/hr)			
H_2O	0.31	0.301	0.009
MEA	trace	trace	trace
N_2	0.002	trace	0.002
CO_2	0.028	trace	0.028
H_2	0.001	trace	0.001
CH_3OH	0.289	0.058	0.231
CO	trace	trace	trace

4.5.1 Final product

The final product of this simulation is a purified methanol stream. The data for this stream is shown in Table 42.

Table 42: Stream data for the crude methanol product stream

	CRUDEMET (kg/hr)	**Composition (wt%)**
Total Mass flow	8.881	
CH_3OH	7.409	83.4
H_2O	0.162	1.82
CO_2	1.251	14.1
N_2	0.055	0.62
H_2	0.003	0.03
CO	<0.001	<0.01
MEA	trace	trace

5 Discussion

This section discusses the results that are presented in the previous section. The results of the absorption step, stripping step and conversion step are discussed individually. Afterwards, some general discussion points regrading the overall scope of this thesis are presented.

5.1 Absorption

This section discusses the absorption results, discussing amongst others the high absorption numbers and the matching of the results to plant data.

5.1.1 High absorption numbers

The simulation show relative high absorption numbers, up to 99.5%. In literature, high absorption numbers are also mentioned, however, not all literature mention removal of such high numbers. For example, Desideri and Paulucci (1999) mention a CO_2 removal of 90.4% for their natural gas fired power plant, which is significantly lower compared to the removal obtained in this simulation. In order to obtain realistic results, simulation data is often matched to real-life plant data. In Aspen Plus, there are several ways of match the absorption results to plant data, by for example using different flow models. In this thesis, it was shown that different flow models yield slightly different results, ranging from a CO_2 absorption from 98.6% to 99.5%. In literature, there is no consent on which flow model matches the absorption process the closest, and different articles mention the use of different flow models to match results to plant data. For example the Aspen Technology Inc. guide uses a VPlug flow model for their simulation, while Plaza et al. use a countercurrent flow for their simulation [4, 69]. Often, the flow model that closest matches plant data is chosen.

5.1.2 Matching to plant data

In this thesis, the absorption process is simulated in Aspen Plus, using data and parameters provided by literature. Afterwards, the results are compared to results given in literature. To further improve the validity of the results, it would be optimal to match them to plant data.

5.2 Stripping

This section discusses the stripper results.

5.2.1 Optimizing the condenser block

In the condenser block, the CO_2 is separated from the remaining water and MEA that are still present in the top stream leaving the stripper. At the top, a CO_2 rich stream leaves the condenser and at the bottom a stream with high amounts of water and smaller amounts of MEA leave as waste stream. Around 4.7% of the CO_2 entering the condenser block, ends up in the waste stream with the MEA and H_2O. The waste stream further contains relative large amounts of water and MEA. In order to further optimize this block and the entire process, it would be interesting to recycle this stream back to the absorber. Thereby decreasing the amount of water and MEA needed in the make-up stream.

5.3 Conversion

This section discusses the conversion results, including the temperature of the reactor and the H_2 recycle stream.

5.3.1 Temperature of the reactor

The reactor is in this thesis simulated with a temperature inlet of 67 °C. The conversion reaction of CO_2 to H_2 is generally done around temperatures of 200 °C. In the simulation, the reactor is modelled as an adiabatic reactor with no intercooling, therefore the temperature rise in the reactor is due to the exothermic reactions taking place. This leads in the simulation to an increase in temperature in the reactor to 200 °C. Therefore an inlet temperature of 67 °C yielded the highest methanol conversion. In reality, the temperature of the reactor should be controlled and kept at a constant temperature of 200 °C.

Using an inlet temperature of 206 °C leads in the Aspen Plus simulation to a rapid increase of the temperature inside the reactor. The conversion of CO_2 into methanol only takes place at the beginning of the reactor, where the temperature is still relatively low. The temperature profile and the molar composition profile of methanol are shown in Figure 40.

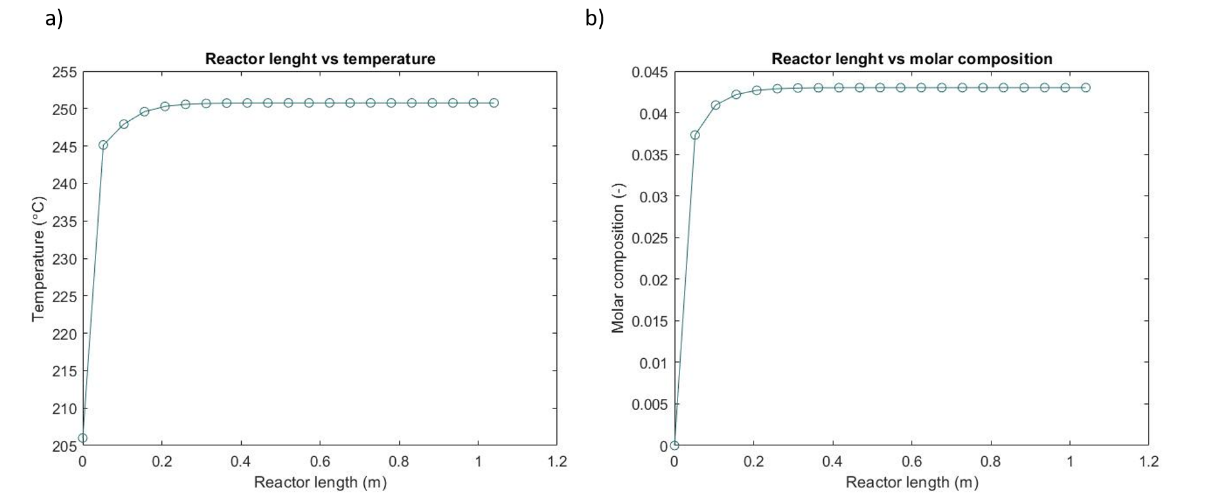


Figure 40: a) Temperature profile along the length of the reactor at an inlet stream temperature of 206 °C. b) Molar composition of methanol profile along the length of the reactor at an inlet temperature of 206 °C.

5.3.2 Recycle stream

The purger before the H_2 recycle stream splits the recycle stream into a 3% purge stream and 70% recycle stream. The purge stream is relatively large and more H_2 and CO_2 could be recycled to the reactor optimize the process. However, large recycle streams complicate the convergence the mass balances in the Aspen Plus simulations. Therefore, it was chosen to simulate the recycle stream with a larger purge stream in order to facilitate convergence.

5.4 General discussion

The next section discusses some general points regarding the overall process and the complete thesis.

5.4.1 Treatment of the flue gas

Before the absorption of CO_2 from a flue gas into any kind of solvent, the flue gas should be treated. Acidic gases such as NO_2 and SO_2 should be removed. When this is not done, they can form heat-stable salt when reacting with MEA. In order to remove SO_2 from a flue gas stream, a Flue Gas Desulfurization (FGD) unit should be installed before the absorber [94].In order to remove nitrogenoxides from the flue gas stream, Selective Catalytic Reduction (SCR), Selective Noncatalytic Reduction or NO_x burners can be used [94]. In this thesis, it is assumed that acidic gases are already removed from the flue gas. However, it is important to take this into account when looking at the whole process and when evaluating the energy requirement of the process.

5.4.2 Degradation of the MEA solvent

Degradation of the solvent is one of the main concerns when using MEA as absorption solvent. There are two degradation pathways of the MEA solvent: carbamate polymerization and oxidative degradation.

One major concern with MEA is the degradation of the solvent at high temperatures by carbamate polymerization. Amines can form polymers at higher temperatures and in the presence of CO_2. The carbamate polymerization reaction is initialized by the formation of an oxazolidone, a five-ring formed by internal reaction of an alcohol and a carbamate. The amine then reacts with the oxazolidone and produces a substituted ethylenediamine. This reaction is insignificant for temperatures under 100 °C, therefore only relevant for the stripper part of the simulation. Degradation reactions are favoured by high CO_2 loading, so the rich end of the stripper is more prone to degradation. Furthermore, degradation also depends on the amine concentration, solvents with a lower amine concentration therefore experience lower degradation rates as well [46].

Another concern is degradation of MEA due to oxidative degradation, which can be a problem when oxygen is present in the flue gas. Oxidative degradation can occur at all temperatures and also without the presence of CO_2. It results in the production of various aldehydes, or organic compounds such as acetate, formate, glycolate, acetate, oxalate amines, ammonia, and nitrosoamines. One of the problems is the environmental impact when these products are released into the environment, for example nitrosoamines are known to be carginogenic. Another issues it the formation of heat stable salts due to oxidative degradation, leading to a loss of solvent which has to be compensated by a higher make-up stream. Overall, this leads to increased costs in the process. Furthermore, the degradation reaction can also increase the corrosion in the column and the column internals, which sould be takin into accunt as well. In industry, inhibitors are often added to the process in order to prevent the oxidate degradation of MEA [46].

5.4.3 Environmental impact of MEA

It is important to consider the environmental impact of MEA when this process is used to produce methanol in a more sustainable manner. Luis (2015) describes the usage of MEA for CO_2 capture on a global scale [54]. For the production of MEA, there are direct and indirect CO_2 emissions. In order for the capture of CO_2 by MEA to be a feasible sustainable option, the CO_2 emissions related to the production of MEA have to be considered as well.

Furthermore, post combustion capture of CO_2 using amines leads to amine losses from the absorber column. This can potential lead to amine degradation in the environment, which can be toxic as well. The main concern is degradation to the products nitrosamines and nitramines [54].

5.4.4 Hydrogen production

The hydrogen that is used in this simulation is a stream with pure hydrogen at a temperature of 25 °C and a pressure of 62 bar. It is essential that this hydrogen it produced in a sustainable manner. The most promising pathway to do this is via the electrolysis of water to form H_2 and O_2, which is discussed more extensively in Section 2.3.6. This has not been simulated in this thesis, since it is out of the scope of this thesis. However, it is an important step to evaluate when producing chemicals from renewable sources. The production of H_2 is also an energy intensive step and should therefore also be taking into account when calculating the overall energy needed for the production of methanol. In order for the process to make sense, the energy needed for the production of H_2 should come from a renewable source with limited CO_2 emissions, such as solar energy or wind energy.

5.4.5 Energy source

In order to fulfill the overarching goal of this thesis, developing chemicals in a more sustainable manner without depending on fossil fuels, it is important to also consider the energy source of this process. The energy source has not been discussed in this research, but renewable energy sources should be used for the process. This sources include solar and wind energy. There are still several challenges for using renewable energy sources in industries, such as the varying energy supply. These challenges have to be further researched in order to make this process sustainable and efficient.

6 Conclusion

The objective of this thesis was to develop a simulation for the capture of CO_2 and the conversion of CO_2 into methanol using H_2 from a renewable source. This process is simulated in the simulation environment of Aspen Plus V8.8. The process is divided into three units: absorber, stripper and reactor.

6.1 Answering the sub-questions

First, the sub-questions of this thesis are answered.

> *Which techniques are available for the separation of CO_2 from a flue gas stream?*

There are several techniques available for the separation of CO_2 from a flue gas stream, these include physical and chemical absorption, adsorption, cryogenics, membranes and microbial systems. The composition of the flue gas used in the simulations in this thesis has a relative low partial pressure, therefore chemical absorption is considered as most promising separation technique. There are several solvents available for the chemical absorption of CO_2 from a flue gas stream, including amines, ammonia and alkaline solutions. Amines are still considered the most feasible solution for absorption of CO_2 from a coal-fired or natural gas fired power plant. Therefore, it is decided to use a chemical absorption process with MEA as solvent for the simulation of CO_2 absorption from a flue gas stream.

> *What are the optimal operating conditions (pressure, temperature and solvent wt%) for the separation of CO_2 from a flue gas stream using an aqueous MEA solution?*

From the sensitivity analysis, it was found that the maximum amount of CO_2 absorbed from a flue gas stream was at operating conditions of 46 - 48 °C and and MEA concentrations of 30 wt%. For the further simulation of the process it was decided to use operating conditions of 40 °C, since the amount of CO_2 absorbed only increased by very small amounts when the temperature if further increased. However, increasing the temperature, does also increase energy requirement in the process further on. Therefore an trade-off between energy requirement and amount of CO_2 capture has to be made and thereby 40 °C is chosen as optimum temperature for the rest of the simulation. Furthermore, it was chosen to use 30 wt% MEA as optimum solvent concentration. This yielded the highest amount of CO_2 absorption. Different flow models were also reviewed, choosing a VPlug model for further simulations.

For the stripping block, it was seen that increasing the temperature in the stripping blocks yield significantly higher stripping results. A temperature of 130 °C was chosen for the further simulation, since this yielded the highest CO_2 conversion.

> *What are the possible conversion techniques for the conversion of CO_2 into CH_3OH?*

Three types of reactors for the conversion of CO_2 into CH_3OH are reviewed in this thesis: (1) adiabatic reactor, (2) water-cooled reactor, (3) gas cooled reactor. It is decided to use an adiabatic reactor for the simulation of the process in Aspen Plus. An adiabatic reactor is chosen on the basis of reactors costs and composition of inlet stream. Since CO_2 rich inlet streams have a decreased demand for robust cooling-systems, adiabatic reactors can be used for the simulation.

> *What are the optimal operating conditions (hydrogen input, pressure and temperature) for the conversion of CO_2 into CH_3OH*

The conversion process has been simulated for a hydrogen input between 0.5 kmol/hr and 3 kmol/hr. From this graph, it could be seen that a maximum of CH_3OH is produced with an inflow of 2.5 kmol/hr. In this simulation it is chosen to use an reactor inlet temperature of 68 °C, since this yielded the highest methanol conversion and selectivity. Using an inlet temperature of 68 °C shows a temperature profile inside the reactor between 68 °C and 210 °C. In a sensitivity analysis, the pressure is increased from 60 bar to 70 bar inside the reactor. With increasing pressure, the methanol conversion also increases. It is chosen to use a pressure of 62 bar for the rest of the simulation.

6.2 Answering the main question

In this section, the main question of this thesis is answered. The main question is formulated as followed:

> *What is the optimal process design and operating conditions for the production of CH_3OH from CO_2 from a flue gas stream using an aqueous MEA solution?*

A flue gas with a CO_2 content of 13 wt% enters a 12-stage rate-based absorber at the bottom stage. An aqueous MEA solution enters the absorber at stage 3. The solvent contains 30 wt% MEA, the rest is H_2O. The CO_2 from the flue gas stream is absorbed into the solvent and undergoes a reversible reaction with MEA. The operating conditions of the absorber are 40 °C and 1 atm. This results in 99.5% of CO_2 absorption.

The bottom stream leaving the absorber is led to a stripper. Before entering the stripper, the pressure of the stream is increased to 1.6 bar and the temperature to 130 °C. The stripper is simulated as a column similar to the absorber, with 12-stages and rate-based calculations. In the stripper, the CO_2 is recovered from the solvent. The stripper operates at 130 °C and 1.6 bar. The reboiler duty of the stripper is set to 29.9 kW, corresponding to an energy requirement of 4 GJ/tonneCO_2. In the stripper, 78.3% of the $MEACOO^-$ in the stream entering the stripper is stripped and converted into CO_2. In relation to the flue gas stream, 77.9% of the CO_2 entering the process, leaves the stripper at the top stream. The top stream leaving the stripper contains a gas with high CO_2 content. The remaining water in this stream is separated from the gas using a condenser block, operating at 25 °C. The condenser is simulated in Aspen Plus using a Flash block. The top stream leaving the condenser is the CO_2 rich stream, while the bottom stream leaving the condenser contains mainly H_2O and smaller amounts of MEA. The condenser is able to separate 95.3% of the CO_2 entering the condenser block, having less than 5% CO_2 loss in this block. The resulting CO_2 rich stream contains 90.6% CO_2, 7.4% N_2, 2.0% H_2O and trace amounts of MEA.

Overall, the amount of CO_2 leaving the condenser block is 0.589 kmol/hr, the amount of CO_2 entering the process in the flue gas stream equals 0.793%. A total of 74.3% of the CO_2 is recovered in the process of separating CO_2 gas from a flue gas stream.

The CO_2 rich stream leaving the condenser is further compressed to 62 bar and mixed with H_2 in a mole-ratio of CO_2:H_2 of 1:4.2. This mixed stream is cooled to 68 °C before entering an adiabatic reactor, with a length of 1.04 m and a diameter of 0.104m. In the reactor, the CO_2 and H_2 are converted into CH_3OH. The optimum operating conditions for the conversion of CO_2 and H_2 into CH_3OH are at temperatures around 200 °C and a pressure between 60 and 70 bar. In this simulation it is chosen to use an reactor inlet temperature of 68 °C, since this yielded the highest methanol conversion and selectivity. Since the reactor is simulated as adiabatic reactor, the temperature in the reactor increases as a result of reaction energies. It can be seen that the temperature inside the reactor increases up to around 210 °C when an inlet temperature of 68 °C is used. The reactor converts 37.9% of the input CO_2 into methanol. The selectivity for methanol is 99.9%.

Each unit has been evaluated individually before integrating them in the complete process. The process is completed by adding recycle streams of MEA and H_2. The bottoms stream leaving the stripper is recycled back to the absorber. An make-up stream with MEA and H_2O is included to make-up for the MEA and water losses in the process. The unreacted H_2 and CO_2 leaving the reactor are first separated from the methanol using a flash separation block, operating at 50 °C and 62 bar. The final product stream leaving the flash separation block is a crude methanol stream with remaining water in it. The product stream contains 83.4wt% methanol, 1.82wt% H_2O, 14.1wt% CO_2 and smaller amounts of N_2, H_2, CO and MEA.. Furthermore, there are trace amounts of MEA and CO present in the product stream. The product stream could be further upgraded towards a higher quality methanol stream by removing the water from the methanol with a distillation column, which was outside the scope of this thesis.

6.3 Recommendations

The following section discusses the recommendations for future research, including the matching to plant data, evaluation of different solvents, increasing the conversion yield, improving the reactor temperature and .

6.3.1 Matching absorber and stripper to plant data

To further improve the Aspen Plus simulation of the absorber and stripper block, the data should be matched to plant data. Real-life plant data should be used to increase the validity of the results of the simulations.

6.3.2 Evaluation of different solvents

There are several solvents possible for the chemical absorption of CO_2. MEA is one of the most widely studied solvent in literature. However, there are also other solvents available for the capture of CO_2. Common solvents used for this include potassium carbomate and chilled ammonia [46]. Furthermore, ionic liquids can also be an interesting option for the capture of CO_2. Ionic liquids are able to both physically or chemically absorb CO_2. Currently the main limitations of ionic liquids include the low CO_2 uptake capacity, limited to below 0.5 moles per mole ionic liquid. Furthermore, ionic liquids are relatively expensive compared to MEA, making it currently less applicable for large-scale applications [88]. Another interesting group of solvents to evaluate are deep eutectic solvents. Compared to ionic liquids, deep eutectic solvents are simpler to synthesize, have a lower material cost and are biodegradable in nature. Deep eutectic solvents consist of a hydrogen bond acceptor, such as organic halide salts, and hydrogen bond donors, such as amines, amides, and alcohols.

6.3.3 Increasing the conversion yield

From the CO_2 entering the process in the flue gas stream, 36.4% is converted into methanol and ends up in the crude methanol stream. After further purification, this number 29.2%. To make this process interesting, the overall efficiency of the process should be increased. In order to achieve higher conversion yields, it is interesting to evaluate different types of reactors, especially the inter-cooling of the reactor is an important aspect which has not been evaluated in this thesis. Better control over the temperature has a great influence on the thermodynamic equilibrium that is reached inside the catalyst bed. This can be used to further improve the efficiency of the overall process.

Furthermore, methanol is also losses in the purification step, which should be avoided as much as possible. In order to do this, the efficiency of the purification step, the distillation column, should be further improved by using a more rigorous distillation column.

6.3.4 Temperature of the reactor

Further research should be performed on how the temperature inside the reactor can be best simulated. In this thesis, it is decided to use an inlet temperature of 68°C since this gave the highest conversion rates and gave a reasonable temperature profile inside the reactor. However, in literature, inlet temperatures of around 200 °C are often mentioned. Therefore, it would be interesting to do more research about how the temperature profile in the reactor can best be simulated in order to match literature. Eventually, if possible, the temperature of the reactor should be simulated in such a way that it matches plant data.

6.3.5 H_2 Recycle stream

To optimize the H_2 recycle stream, a smaller purge fraction could be used. This case, more H_2 and CO_2 can be recycled back to the reactor and therefore optimizing the process and increasing the overall methanol yield. To simulate this in Aspen Plus, more robust convergence settings should be investigated to overcome convergence issues with larger recycle streams.

6.3.6 Work-up of methanol

The final product of this thesis is a methanol solution with 83.4wt% methanol, 1.82wt% H_2O, 14.1wt% CO_2 and smaller amounts of N_2, H_2, CO and MEA. Further research include the working up of this crude methanol stream to a product with higher methanol purity. The methanol should be separated from the remaining CO_2, which can be recycled back to the absorber. Furthermore, the remaining H_2O, N_2, and H_3 should be removed.

Part II

Communication Design for Innovation

1 Introduction

In the Chemical Engineering part of this research, a simulation for the conversion of CO_2 into methanol has been developed. This falls within the context of the e-Refinery institute, which focuses on researching and developing electrochemical conversion technologies for the sustainable production of chemicals and fuel. The e-Refinery institute is an interdisciplinary research group, involving multiple research domains and researchers with a range of different backgrounds.

This part of the research focuses on the collaboration aspect of the e-Refinery institute. A shared vision is the key concept as means to improve the collaboration. The outcome of this part of the research is a communication tool to aid the e-Refinery institute in collaboration.

This section gives some background information on interdisciplinary research groups, shared vision in interdisciplinary research groups and adaptivity. Afterwards the context of complex problems and uncertainty is introduced. Later, the scope of the thesis is explained. The section finalizes with the structure of the report.

1.1 Interdisciplinary research groups

Working in interdisciplinary research groups often requires more attention compared to collaborations with colleagues from own areas of expertise, who often share the same vocabulary and have a shared understanding of concepts [29]. In interdisciplinary research groups, each party often have different, or contrasting, worldviews due to difference in underlying paradigms. Bridging this while recognising the underlying differences forms the basis for strong interdisciplinary research. Finding common ground and the development of a shared vision aids in forming this bridge [43]. A shared vision as the basis for interdisciplinary collaboration is widely recognized in literature [81, 96, 43, 68, 61].

1.1.1 Shared vision in interdisciplinary research

A shared vision within interdisciplinary research institute has multiple benefits, ranging from motivation to external visibility, from internal communication to the evaluation of impact [96]. It can also aid in generating awareness and raising support for partnerships, which in turn improves the efficiency and minimizes competing agendas [15]. Different literature on collaboration acknowledges the creation and development of a shared vision as a critical component for the success of the collaboration [77].

A shared vision is in this research defined as the overlap between goals and ambitions, values, future perspective, external visibility and concerns. A shared vision in research institutes is not a once defined static element of the collaboration, it is dynamic and changes over time. A shared vision should therefore be adaptive in nature. A more extensive explanation of the concept shared vision can be found in Section 4.2.3.

1.1.2 Adaptivity in interdisciplinary research

Adaptivity can be defined as the state of having the capacity of being adaptive or the capacity to adapt [102]. For adaptive researchers, this means that researchers have the capacity to adapt to new situations and act according to this. Adaptability or adaptive capacity is defined by Engle et al (2011) as the ability of a system to prepare and deal with stress and change and adjust and respond to the effects caused thereby [27]. Increasing the adaptive capacity of a system, improves the system's ability to manage and deal with a range of issues, while maintaining flexibility to alter research approaches when necessary [27].

The goal of this research is to develop a tool to aid the development of a shared vision in research institutes. Since a shared vision is a dynamic and changes over time, therefore, a tool that aids in the development of a shared vision should also be adaptable to this change. For an adaptive tool, it means that the tool itself can be adaptive to the situation. So the tool has different functionalities, or can be used in a different manner dependent on the situation or need at that moment.

1.2 Scope of this thesis

The aim of this thesis is twofold:

1. Deepen the knowledge on how a shared vision can aid in interdisciplinary research institutes.
2. Develop a tool for the members of the e-Refinery institute to deal with uncertainty when developing the optimal solution for the capture and conversion of CO_2.

The two-folded goal of the thesis leads to the main research question defined as:

> *"How can members of the e-Refinery institute be enabled to develop a shared vision to deal with uncertainty in the project?"*

The sub-questions are defined as followed:

1. How can a problem direction be defined for research projects, taking into account the uncertainty that is inherently integrated in them?
2. How can a shared vision be developed in an interdisciplinary research institute?
   (a) How can the concept 'shared vision' be defined as an adaptive concept?
   (b) What are the drivers and barriers for developing of a shared vision within an interdisciplinary research institute?
3. How can a tool be designed to aid the e-Refinery members in the development of an adaptive shared vision?

1.3 Structure of the report

This research starts with a methodology section, presenting and elaborating on the methods used in this research. Afterwards, this part of the report is structured in three parts: (1) discovery phase, (2) deepening phase, (3) design phase. The first phase, the discovery phase, consists of a preliminary research, including interviews. This phase wraps up with a problem direction, which is the starting point for the next phase. The second phase, the deepening phase, consists of a more in-depth review of the problem direction. This phase includes a systematic literature review, as well as a second round of interviews. This phase concludes with the essence of the problem, which is again the starting point for the next phase. The last phase, the design phase, consist of the designing of a tool, based on criteria that are drawn from the problem essence formulated in the deepening phase. Afterwards, the results are discussed in the discussion. Finally, the report wraps up with a conclusion.

2 Methodology

This section gives an overview of the methods used to address the research questions. First, an overview of the overall structure used for this research is presented, based on a triple diamond research model. Second, this overall structure is further explained in detail, explaining the different research methods used in the research. The methods is divided into three phases, based on the overall method: the discovery phase, the deepening phase and the developing phase. For each phase, a goal has been formulated.

2.1 Overall Structure

A triple diamond model is used as the structure for this research. The triple diamond model can be seen in Figure 41. This method is based on the double diamond model by the Design Council, but has an additional diamond before the first diamond [14]. This additional diamond allows for an introduction to the case before starting the double diamond research model. The method is based on a process of first exploring (divergent thinking) and than taking a focus (convergent thinking).

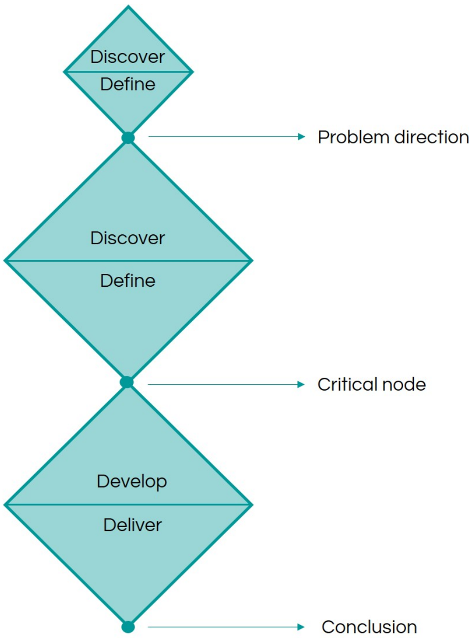


Figure 41: Triple diamond model used for this research

In the first diamond, the *discovery diamond*, the case is discovered in a broad sense. The e-Refinery institute is further explored and the first diamond eventually leads to chosen problem direction. In the second diamond, the *deepening diamond*, the problem is further discovered by looking at with a more in-depth view. After discovering the problem direction further, the critical node is specified. In the third diamond, the *developing diamond*, the end-product is developed. This is done by first exploring the possible possible directions and later converging towards the deliverable.

During all those phases, the design principles are taking into account [14]:

- **People first** the starting point will be the people with their strengths, aspirations and needs.
- **Visual and inclusive communication** a shared understanding of the problem for all the people involved.
- **Collaborate and co-create** working together and using work from others as inspiration
- **Iterate** constant iteration to spot errors early

The process is shown in more detailed steps in Figure 42. As can be seen, the starting point is the initial problem definition (1). After a first round of preliminary interviews and the formulation of the results (2), the problem statement is redefined and further specified (3). Afterwards, a second round of interviews is held and those results are formulated as well (4). Together with a literature study and the results of the second round of interviews, an analysis leads to a redefined problem statement in which the essence of the problem becomes clear (5). This is the critical node as seen in Figure 41. This is the starting point for the first definition of the solution (6), after which a tool or advice is developed (7). This tool is tested inn practise (8), which allows for feedback and leads, after further design and adjustments, to the final tool or advice (9).

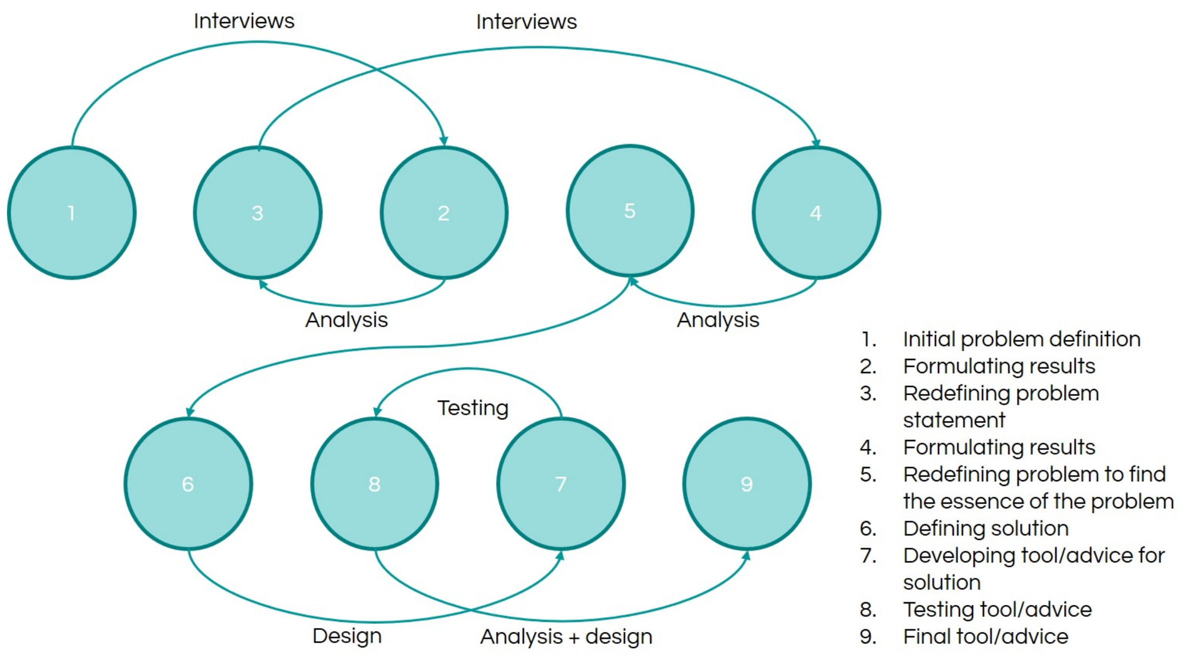


Figure 42: Iterative process used in this thesis project

2.2 Discovery phase

The discovery phase is the first diamond and consists of interviews. The research question related to this phase of the research is states as followed:

> *How can a problem direction be defined for the e-Refinery institute, taking into account the uncertainty that is inherently integrated in research projects?*

2.2.1 Goal of the interviews

The preliminary interviews are explorative in nature. This means that the goal of the interviews is to get to know the case better, without diving deep into theoretical aspect of collaboration. The focus of this round of interviews is to gain more insights in the structure of the project group, their current way of working and decision making processes. Furthermore, it is important to get a clearer overview of how different roles are defined and divided amongst the different individuals working in this institute.

In this round of preliminary interviews, the focus is on gaining more insight in how the e-Refinery institute is functioning. The focus is less on the details of the research that is performed, but more on the general overview of what types of research is currently performed. Another aspect of this round of interviews is to check if current knowledge regarding the institute is correct.

Furthermore, this round of interviews is used to gain more insight in the multiple stakeholders involved in the project and how they relate to each other. The following key focus points are drawn for the preliminary interviews:

- Get an overview of the different types of research that is currently performed in the e-refinery project group
- Gain more insight in the different roles that are currently employed in the group and who are the key individuals in the institute.
  - Who are responsible for which part of the research?
  - Who are responsible for decision making and in which areas do they make decisions?
- Which problem direction for further research can be identified?

2.2.2 Interview structure

Semi-structured interviews were held with 3 members of the e-Refinery institute. The interviewees are also all connected to the TU Delft. The interviewees all have different roles within the institute, including a board member, an assistant professor and a full professor. The website of the TU Delft dedicated to the e-Refinery institute is used to find the participants for the interviews.

The interviews are semi-structured. The interview protocol is shown in Appendix E.

2.2.3 Data processing

All interviews were conducted and recorded via Zoom. The interviews were fully transcribed and analysed in ATLAS TI. The transcripts were made anonymous and names of others were blanked out. All interviews were conducted and processed in English. The transcripts of the interviews can be found in Appendix F.

2.2.4 Problem direction

The discovery phase concludes with a problem direction. This problem direction is the starting point for the next phase, the deepening phase.

2.3 Deepening phase

The deepening phase consists of a systematic literature review and interviews. This section elaborates on the methods used in the deepening phase of this research.

2.3.1 Systematic literature review

A systematic literature review is performed to structure the literature and forms the basis of the theoretical framework.

The literature review is performed around the problem direction that originates from the preliminary interviews. The research question that relates to this part of the research is stated as followed:

> *What are the drivers and barriers for developing a shared mission and vision within a virtual research institute?*

Criteria SCOPUS is used as database. Articles between the year 2010 and 2020 were included in the results and the language is set to 'English'. The keywords that are used for the systematic literature review are listen in Table 43. It is specified that the keywords of list 1 should be within three words of list 2 (using PRE/3). List 1 and 2 are combined with list 3, resulting in 72 articles.

Including all articles between 2010 - 2020 results in 57 articles. These articles are screened based on their title and abstract, which resulted in 8 articles. An overview of the search queries can be found in Appendix G

During this first search, one relevant article mentioning 'social capital' as keyword. This was the reason to conduct a second literature review, using list 1 and 2 (using PRE/3) in combination with the keywords of list 4 from Table 43 to also include articles focusing more on social capital, social learning, collaborative learning and collaboration in combination with developing a shared mission or vision. This search resulted in 156 articles. Including all articles between 2010 - 2020 limits it to 119 result. Screening those articles based on title and abstract resulted in 11 articles.

In order to also include articles that focus more on barriers and drivers for developing a shared mission and vision, it is decided to also include these therms in a third search query. This is done by again using list 1 and list two (using PRE/3) in combination with list 5 from Table 43. This resulted in 144 articles. Only articles in the field of Social Sciences were included, resulting in 24 articles. These articles were screened on title and abstract, resulting in 6 articles.

Table 43: Synonyms of the search terms that are used in the systematic literature review

List 1	**List 2**	**List 3**	**List 4**	**List 5**
Develop	Shared mission	Research institute	Social capital	Driver*
Development	Shared vision	Scientific institute	Social learning	Barrier*
Creating	Shared goal*	Academic institute	Collaborative learning	Factor*
	Shared objective*	Academic research	Collaboration	Condition*
	Shared target*	Interdisciplinary research		Variable*
	Common mission	Interdisciplinary institute		Determinant*
	Common vision	Research organisation		
	Common goal*	Scientific organisation		
	Common objective*	Researchers		
	Common target*	Research collaboration		

Analysis of the articles The articles were read and analyzed in ATLAS TI. The articles were first open coded and afterwards axial coded. The further analysis of the articles is explained in Section 4.1.

2.3.2 Interviews

Goal of the interviews The goal of this round of interviews is two-folded: (1) deepen the knowledge on what a shared vision means in the context of research institutes and how this concept depends on the phase of the research project, and (2) verify and identify drivers and barriers for the development of a shared vision.

Interview structure Semi-structured interviews were held with 9 individuals that are part of the e-Refinery institute. The interviewees are also all connected to the TU Delft. Interviewees with different roles within the institutes are interviewed, this includes full professors, assistant professor and PhD students.

The interview consist of four different parts:

1. **Introduction** First the interviewees are ask to introduce themselves and to elaborate more on their role within the institute
2. **Statements** In the second part of the interview, the interviewees are asked to fill in a short online survey. This survey consists of 15 statements regarding the drivers and barriers of the development of a shared vision within the context of research institutes. The interviewees are asked to rate all statements on whether they agree or disagree with the statement in relation to the e-Refinery institute, and whether they find the particular statement important in research institutes or not.
3. **Definition** After the survey, the interviewees are asked about their definition of a 'shared vision' and they are asked to rate the importance of the five different aspects that literature mentioned regarding a shared vision: shared goals and ambitions, shared values, shared perception of the future, external visibility and shared concerns.
4. **Drivers and barriers** In the also part of the interviews, the interviewees are questioned about the drivers and barriers for the development of a shared vision within the e-Refinery project. In this part, the statements are also used in order to steer the conversation and to ask more in-depth questions regarding the answers they gave in the statements.

The complete interview protocol and the survey are shown in Appendix H.

Data processing All interviews were conducted and recorded via Zoom. The interviews were fully transcribed and analysed in ATLAS TI. The transcripts were made anonymous and names of others were blanked out. Interview 1, 4 and 7 were conducted in Dutch, for the processing of the results they were translated to English.

2.3.3 Essence of the problem

The deepening phase concludes with the essence of the problem. This essence is distilled from the problem direction, which is further explored in the deepening phase, and with the systematic literature review and the interviews further narrowed down to a problem essence. This forms the basis for the last phase, the design phase.

2.4 Design phase

In the design phase, the final tool or advice is developed. This phase consists of multiple steps. First the criteria for the design of the tool are specified. Afterwards, a literature investigation is performed to gain a broader perspective of methods used to tackle the design criteria.

2.4.1 Goal of this phase

The design goal of this research is formulated as followed:

> *The goal is to design a tool that aids e-Refinery members in the development of an adaptive shared vision.*

The criteria for the development of the tool are obtained in the deepening phase. The design criteria follow from the essence of the problem and are further elaborated and molded in the form of design criteria as a first step of the design phase.

2.4.2 Literature investigation

A literature investigation is performed for the five design criteria that were drawn in the previous phase. For this literature investigation, the five design criteria were used as search terms in combination with the search terms related to multidisciplinary research institutes. The search terms for the literature investigation include 'developing shared language', 'developing shared goals', 'stimulating interaction', 'collective goal development', 'sharing of concerns'. These search terms were used in combination with the terms "multidisciplinary collaboration' and interdisciplinary collaboration'.

The articles that were found were selected on whether they related to multi- or interdisciplinary research institutes and whether they provided enough practical insight for the development of a tool regarding the five criteria that were drafted.

Furthermore, using a snowballing method, additional articles were found as a result from the articles that were found using the search terms. Those articles often mentioned other articles which mention different methods and techniques for the one of the five criteria. Those articles were obtained from the references and again selected on whether they related to multi- or interdisciplinary research institutes and whether they provided enough practical insight for the development of a tool.

2.4.3 Brainstorming sessions

A brainstorming session is conducted with an expert in the field of education. A total of two sessions were held regarding the five design criteria. The brainstorming sessions were used to provide more practical insights in how the five criteria could be integrated in a tool. The brainstorming sessions were conducted for all five criteria via the set of the eight house rules:

- The problem or target of the session is explained and discussed till there is consent and mutual understanding of the target
- A time limit of 20 minutes is set for each criteria
- No judgement or negative comments were given in the time frame of the 20 minute brainstorming session
- All ideas are encouraged, how weird or unrealistic they might seem, as long as they stay on topic
- Aim for quantity, the brainstorming session aimed for high quantity of ideas, the selection for quality of ideas comes later
- Building on ideas, during the session it is encouraged to associate with other ideas and build upon them.
- Visualization: it is encouraged to visualise the brainstorming process

Even though five criteria were treated in separate brainstorming session of 20 minutes per criteria, it is decided to use one large overview of all five criteria. This decision is made because the five criteria are not stand-alone criteria, but are all connected to one-other. The result of one criteria, could be inspiration or input for the next criteria. Therefore, it is also decided to spend time on an additional session on the overview, focusing on connecting different output ideas together.

2.4.4 Morphological chart to concept formation

The morphological chart is designed by combining the results from the literature investigation and the brainstorm sessions. Three tool concepts are formulated by combining functions in the morphological chart together and designing tool concepts based on the combination of different functions. This has been an iterative process, going back and forward between the morphological chart and the tool concepts.

Each concept is subjected to a feedback-session with a recently graduated Science Communication student. This feedback-session aims at improving and further developing the draft concepts. This session was also a process of going back and forward between the morphological chart and the tool concepts. For each concept, the following steps have taking in the feedback-session:

- Explanation and elaboration of the tool concept.
- Evaluation of the tool based on the five design criteria, using the following questions:
  - Does the tool help the participants to formulate and make time for shared concerns?
  - Does the tool allow the participants to gain insight in which goals are shared?
  - Does the tool stimulate in the collective development of goals?
  - Does the tool aid in the development of a shared language?
  - Does the tool stimulate interaction between the members of the institute?
- Based on the answers above, the tool is improved and further developed. Going back to the morphological chart and integrating the missing features into the tool.

The final tool is chosen after evaluating each concept. All concepts are scored based on their design criteria, with scores ranging from $--$ to $++$. Furthermore, the context in which the e-Refinery institute takes places is also taken into account, making sure the tool fits within the institute. Taking both the scores and the context into account, a tool is chosen for further development.

2.4.5 Final tool reviewing

After choosing one of the tool concepts, that tool is further developed and designed. To improve the concept, four feedback sessions are held. The first session is held with a recently graduated Communication Design for Innovation student. This session has as main goal to improve the tool concept. The second session is held with a PhD student that is currently doing research that falls within the activities of the e-Refinery institute. This session focuses more on whether the tool fits the institute, which functionalities would be more or less interesting for the PhD students involved in the institute, and how the tool can fulfill the needs of the researchers. In a third session, the focus points retrieved from the second session are discussed with a fellow student from the Communication Design for Innovation master track. Together, it is discussed how these focus points can be integrated in the tool and the tool is adjusted accordingly. A fourth session is held with a Communication Design for Innovation graduate. This session focused on visualizing the current structure between members of the e-Refinery institute and visualizing the connection between collective and individual goals and concerns. This session is used to improve the structure of the tool, the visualizations aided in this.

Afterwards, the tool is tested with two PhD students from the e-Refinery institute. This is done by letting the PhD students fill in two pages of the tool: the sub-goal page and the concerns page. The PhD students are provided with instructions for filling in the two pages, as well as an example of how the pages can be filled in. This example retrieved from the chemical engineering part of this thesis, using a sub-goal of this part, as well as concerns related to this sub-goal. Afterwards, the PhD students are asked several questions regarding the tool. The format for the testing of the tool can be found in Appendix I

3 Discovery phase - preliminary research

In order to get more insights in the nature of uncertainties in the e-Refinery project group, a preliminary research is done in the discovery phase of this research. The methods for this preliminary research are explained in Section 2.2.

3.1 Preliminary interviews results

Three researchers from the e-Refinery institute were interviewed during the preliminary interviews. All three researchers are both part of the e-Refinery institute as well as a employees at the Technical University of Delft.

3.1.1 The e-Refinery institute as virtual institute

For the preliminary interviews, three members of the e-Refinery institute have been interviewed. All three interviewees are also connected to the Technical University of Delft. The interviewees fulfill roles as appointed assistant professor, associate professor and professor. The interviewees work for different faculties of the Technical University of Delft: Electrical Engineering, Mathematics & Computer Science (EEMCS), Technology, Policy and Management (TPM), and Mechanical, Maritime and Materials Engineering (3mE). The institute is supported by five faculties of the Technical University of Delft in total, also Aerospace Engineering and Applied Sciences are participating in the institute.

The e-Refinery institute has a board of 12 people, consisting of a director, scientific director, managing director and 9 experts. Everyone in the board is from the Technical University of Delft as well. [63] One of the interviewees is also a member of the board. Furthermore, over 40 Principal Investigators and over 50 Post-Doc and PhD Researchers are part of the e-Refinery institute.

During the preliminary interviews, the institute was described as "a virtual institute", in relation to how the research is funded. Described more clearly: "It's not like an institute who is going to fund your research, they [e-Refinery] don't have money for that. (...) We fund the research via normal research goals, so NWO [Nederlandse Organistatie voor Wetenschappelijk Onderzoek - Dutch Organization for Scientific Research], Horizon 2020, European money, or even companies, and then, in this consortium, which is larger than the university, then we integrate." This means that the e-Refinery institute is not an institute that imposes for example rules or research directions upon it's members, but works the other way around. Researchers performing research that is somehow related to the overall goal and direction of the institute, can become part of the institute. This is supported in the interviews as well, in which is said: "we don't have any employees, everyone is there voluntary" and "we don't do this full-time either".

During the interviews, the different roles within the e-Refinery institute were also discussed.

3.1.2 Goals of the e-Refinery institute

When asking the three interviewees to describe the goals of e-Refinery institute, their answers are shown in Table 44

As can be seen from Table 44, the goals are defined differently by different people within the e-Refinery institute. The e-Refinery institute itself defines the goals on their website as only the development of the technology, as can be seen in Figure 43. Furthermore, in given interviews, it is also said that e-Refinery is more than just the development of a certain technology: "It also includes educating the future workforce, and close collaboration with industry. It's TU Delft's mission to contribute to a modernising industry" as told by Paulien Herder.

Table 44: Goals defined by different people in the e-Refinery institute

Interview	Quote
1	"The final goal is to reach large scale application"
2	"- So are you aware of them [the goals]? - no not by heart"
3	"Trying to increase technology development by making information flow between different aspects of technology development really fast" "The ultimate goal is more like the direction of where we are going and why we are doing it and a lot of what we do is how we create the tool that would allow that to happen"

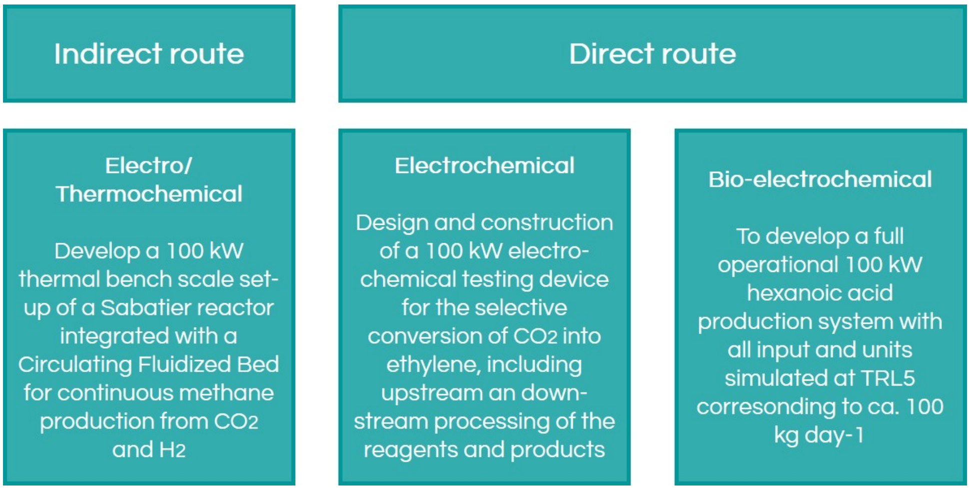


Figure 43: Goals e-Refinery institute as defined by e-Refinery itself (figure retrieved and edited from Delft University of Technology, n.d. [65])

Interviewee 3 also explained more about the process of defining the research goals. As part of the board, this interviewee was more involved with the overall research goals compared to the other interviewees and explained more about how the goals were defined. Multiple strategy sessions were bold with the board of the e-Refinery institute as well as other people involved. In these meetings, small groups worked together in sessions of 3-4 hours and questions like "What are we doing? What are our targets? What makes us different? What are our limitations? What are our lines? Do we miss something? What are the technologies we work on" are asked. In these sessions, members from different facets of the institute are consulted and developing the overall research lines and goals "took a lot of polder"; meaning that it took a lot of discussing and making compromises before reaching the goals as they are now. Decision had to be taken which were only supported by some and not by others. To get to the research goals as they are now, took over a year. This is also due to the fact that the board doesn't work full-time for the e-Refinery institute.

Uncertainty in the goals The interviewees were also asked what happens if their personal research goals were not reached fully, and how this would impact the overall research goal of the institute. The answers to this question are shown in Table 45.

An interesting observation is that interviewee 1 at first did not see 'efficient' or 'cost efficient' as a considerable problem of not reaching certain research goals. This interviewee focused mostly on the technological aspect of the research and less on other aspects, such as economical feasibility and whether or not the technology could be implemented or not. Interviewee 2 acknowledged

Table 45: Answers from the interviewees to the question *In what way would not reaching your personal research goals affect the overall research goal?*

Interview	**Quote**
1	"It's not going to be most efficient, or most cost efficient, but it's fine" "It would affect the, let's say, economical feasibility of such projects, right? (...) So in terms of 'will it work' it has very little impact, but in terms of economic feasibility of the total project, yes it would definitely have an impact." "The goal is defined in such a way that there is no uncertainty, but the way that you reach that goal can be fastely different from what I think it will be now and it probably will be different from what I think it will be now. I wouldn't say there is uncertainty in the goal, but the final solution is very unclear. "
2	"Probably in some sense, for instance you would say, not reaching means probably no that we fail, but that we reached something different than we expected."
3	"You cannot take the goals as draft into stone and regardless (...) for me it's obvious that goals are always moving goals" "We are open to failure, and if we are going to fail, let's fail really fast so a new option can come"

that there were multiple pathways, and that reaching a certain research goal is not a failure, but more a different direction that was taken, or different outcomes than expected. Interviewee 3 did not answer the question directly, but instead explained again that the overall research goals of the e-Refinery institute or not set in stone goals, but more a direction of where to go. So in that sense, it is not really possible to not reach certain goals, since the focus is on a learning trajectory, in stead of on the end-point.

3.1.3 Perceived challenges and uncertainty

In the preliminary interviews, the perceived challenges are also asked to the interviewees. These perceived challenges are summarized in Table 46.

Table 46: Quotes from the interviewees on challenges within the e-Refinery institute

Interview	Quote
1	[On research performed by others in the institute] "They are really doing new stuff and usually that is on, let's say, an extremely small scale. So that's a challenge." "The final goal is to reach large scale application and I think that some faculties with there research are not at that level yet"
2	"We are removing all these matureness and we are putting new things, which are very difficult to control." "We need to make society more aware of the importance of the scientific challenges we really have to tackle"
3	"A part of the problem is the Paris agreement and the sustainable development, we need to reach there." "Now with corona, are you losing the community?"

As can be seen from Table 46, challenges on multiple aspects of the research are experiences. Not only technological challenges (as given by interviewee 2) are perceived but also challenges related to external factors and policies (as mentioned by interviewee 3) as well as challenges related to research performed by others (mentioned by interviewee 1). Furthermore, interviewee 3 also mentioned the COVID-19 pandemic and voiced doubts about whether and how this would have an impact on the institute and the feeling of having a community.

Uncertainty All interviewees agreed that uncertainty is a part of research and is unavoidable. However, the way uncertainty within the overall research goal is perceived differs among the researcher. As interviewee 1 states that there is "no uncertainty in the goal itself", interviewee 3 defines the overall goal more as a direction instead of a set in stone point that should be reached. This is both a very different way of looking at the overall research goal.

The parts in which the interviewees perceive uncertainty are listed in Table 47. Both interviewee 2 and 3 mention that they work with different scenarios. Interviewee 2 is glad with this approach and mentions: "it really is better than just working with the best and worse case, so maybe you have a worst case but now we are talking about different paths and different kinds of worst cases."

Table 47: Quotes from the interviewees on uncertainty within the e-Refinery institute and how they deal with it

Interview	Quote
1	"The final solution is very unclear"
2	"Most uncertain is what happens politically everywhere" "We have different scenarios, three, four, paths. We defined some case studies around
3	"We do a lot of by-work that deals with this uncertainty, like scaling of things that are not there, or systems that are not there. So deal with the part that uncertainty is in the system, and it's large. " "We look at uncertainty in the larger: 'what are the scenarios, what are this conditions, what are the parameters in terms of rangers, but also, how much do you know about the technology and how much are you guessing' "

3.1.4 Communication and cooperation

Table 48 lists quotes from the interviews related to the cooperation between different members of the e-Refinery institute.

Table 48: Quotes from the interviewees on communication and cooperation within the e-Refinery institute

Interview	Quote
1	"From my perspective, I see the most, let's say, a couple of colleagues from 3ME and a couple of colleagues from chemical engineering and the reason that i collaborate the closest with them is because I need to know how these cells behave and what kind of electrical energy they prefer before I can set the requirements for the components or devices that I'm trying to make. So a lot of the times I'm in calls with them or collaborating with them or negotiating with them on what they need." "For me, the interaction with the companies that participate in the e-Refinery is very little, but I am collaborating with some parties, companies, let's say, other research institutions, on these topics. But they are not necessarily par of e-Refinery, it's just people I know that i think we can work together with."
2	"I'm a bit more familiar with some researchers, professors, phd's, postdoc's who are more or less closer to what I do."
3	-

As can be told from interview 1 and 2, those members were more inclined to work more closely together with researchers that do research close related to their own field. Or otherwise with parties that were perceived as being directly beneficial or necessary for own research. Interviewee 2 also mentions that with the e-Refinery institute, working together with third parties was more common: "With this project, we know more people, also manufactures from electrolyzers and suppliers and converters, but also people working for environment, policy making, people that are more connected to the society. (...) That was new for me, that was really out of my comfort zone (...) In the beginning it was really complex". Later was explained that in order to work successfully together with these parties, it was important to improve communication and presentation skills.

Meetings Table 49 list some quotes of the interviewees on the meetings they have within the e-Refinery institute.

Table 49: Quotes of the interviewees on the meetings

Interview	Quote
1	"Sometimes it's multiple times in one week, sometimes it's not at all, but I think on average once a week I talk to one of my colleagues within e-Refinery "
2	"At least once a month"
3	"It is not the number of meetings of meetings that count, it is the possibility for me to send emails, as well with the real question and get answers."

Interviewee 1 described three different types of meetings that are being held as part of the e-Refiner institute:

1. "Acquiring funding for research, so those are usually not that in-depth but more focused towards what approach are we going to take."
2. "What are we going to research and how can we collaborate?"
3. "Me and my colleagues just have questions for each other, that goes really in-depth and it goes into he technical details"

By Interviewee 3, it is added that for the whole institute, there are e-Refinery launches every month: "[those] are designed for internal and external people. So once a month, someone from the group would present results, or someone from outside would present results to us, so that we know what they are doing". Furthermore, it is also stated that for projects within the e-Refinery institute, communication within the projects is handled internally and thus the way meetings are organised and executed are dependent on the project itself.

How cooperation between different parties is perceived Furthermore, they way in which is collaborated currently is described mainly as positive. interviewee 1 described it as "collaboration of equals" and mentioned that "within the university I think it's actually working very well". Interviewee 2 agreed with this and described the collaboration as "it is going smooth" and mentions that members are "always open and positive trying to discuss". Interviewee 3 was also largely positive about the cooperation, but also described a learning process: "We are learning, it is no friction, we are learning how to work together in a way that we are not used to work together. I think we are doing a lot of trial by doing, so sometimes you notice we are meeting too frequently, and sometimes we went the other way, let's meet more frequently. And sometimes the meetings are too general, and sometimes the meetings are too specific, it goes back and forward.

3.2 Problem Direction

From the preliminary research, two observations are highlighted that lead to the problem direction:

1. There is a difference in interpretation of the research goals of the e-Refinery institute amongst individuals involved in the project.
2. There is a difference amongst individuals within the e-Refinery institute about cooperation between different parties within the project.

First, the two observations are elaborated further in Section 3.2.1 and 3.2.2. Afterwards, the observations are linked to an overall problem direction. The problem direction is explained more deeply in Section 3.2.3.

3.2.1 Research goals

The way the overall research goal is defined by all three interviewees differs quite a bit, as well as the way the goal is presented on the website of the Technical University of Delft. The goal is on the one had defined as reaching a certain technology, while on the other hand the goal is defined as a direction to work towards. While interviewee 1 perceived the goal more as the development of this technology, interviewee 3 perceived the goal as a way of defining the learning process. While the website of the TU Delft shows the goal as the development of the technology, the director the institute mentions that the goal is more than just the technology, it also includes education as well as collaboration of multiple parties.

3.2.2 Cooperation Between the Parties

From Section 3.1.4 it could be seen that researchers were more inclined to work with members there were more closely related to their own field of research. Working together with researchers performing research not directly related to their own field, was not as intuitive. However, it is also stressed that in this e-Refinery project, there is a focus on bringing together multiple parties and cooperation with this parties is a large part of the project. In one of the interviews, some concerts regarding the COVID-19 pandemic are also expressed, and how this would impact the cooperation between the multiple parties in the institute.

3.2.3 Problem Direction

The problem direction is the end point of the first diamond and is the starting point for the second diamond of the triple diamond research method that is used for this thesis. Figure 44 shows the triple diamond research method and indicates the problem direction in this research method. The problem direction is distilled from the preliminary interviews that were held in the first phase of this research.

The two observations made in the preliminary interviews are translated into an overall problem direction. The two observations consist of a more practical question (e.g. with whom do research have to cooperate in order to successfully participate and do research in the e-Refinery project?) and a more underlying question (e.g. what is the vision of e-Refinery institute and the overall goal to work towards?). The overall problem statement should contain both of these aspects and take a more overarching look at the issue.

It is important to note that both observations should not be seen as two separate issues, but they both overlap and are entangled in each other. A lack of consent on what the exact goal or vision of the institute is, might also lead to a difference in approach towards the goal. If the goal is formulated more as a technological challenge, cooperation and communication between researchers would be a more prominent aspect of the institute. While if the goal is formulated with a stronger focus on social embedding of a certain technology, stakeholders such as politicians and citizens play a more dominant role in the institute. Therefore, it is important to develop a stronger shared vision within the institute, in order to better understand how communication and cooperation should be shaped in order to facilitate in reaching the goals of the institute.

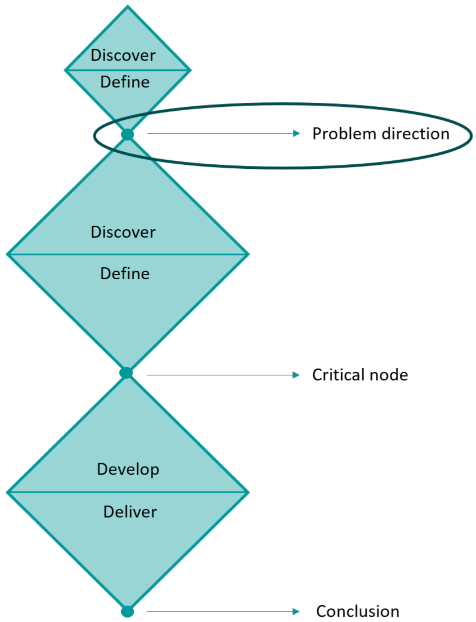


Figure 44: The triple diamond is used as the basis for this research. This step gives the problem direction, the end point of the first diamond and the starting point for the second diamond.

The problem direction is therefore stated as followed: *There is a difference in insight amongst individuals within the e-Refinery institute about the vision, goals and means of the e-Refinery institute.* This contains both the underlying issue of a difference in shared vision between the individuals in the e-Refinery institute on what the overall goal of the institute is, as well as the difference in which means should be deployed in order to reach there.

4 Deepening phase - Theoretical framework

The problem direction described in Section ?? forms the basis for the systematic literature review. The research question that relates to this problem direction and forms the basis for this part of the research is stated as followed:

> *What are the drivers and barriers for developing a shared mission and vision within a virtual research institute?*

A systematic literature review is performed to find the drivers and barriers for the development of a shard vision in research institutes. The method for the this systematic literature review is elaborated upon in Section 2.3.

4.1 Analysis of the articles

An overview of the systematic literature review is shown in figure 45. The systematic literature review yielded a total of 24 articles, which have been read and analysed.

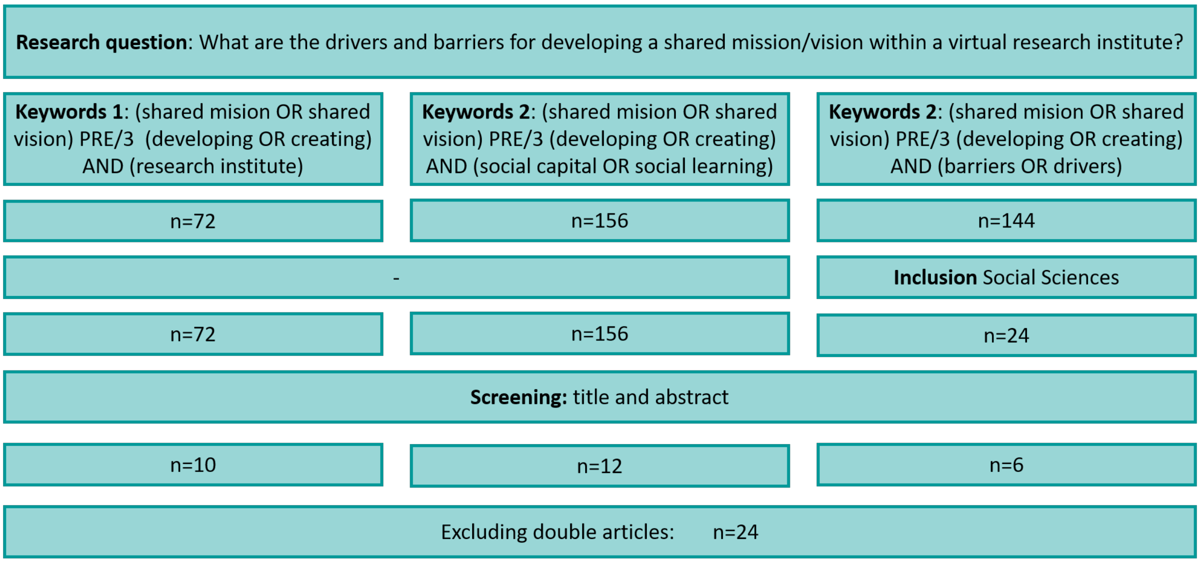


Figure 45: Overview of the systematic literature review

The open codes that were used in the analysis of the articles are shown in Table ??.

Table 50: Overview of the codes used for the systematic literature review

Code	Occurrence	Explanation & example
Action planning	5	Relating to action planning names as driver in an article. *Example: "Action planning helps collaborative partnerships determine who will do what and when, and is thus key to successfully achieving goals and objectives [15]"*

Advantages	9	Advantages of a certain concept, idea, driver or barrier. *Example: "Through shared vision, relationships between professionals improve, learning is facilitated, and long-term commitment is stimulated [34]"*
Barriers	27	Concepts with a negative influence on another concept (also used for factors or variables with a negative influence on a concept) *Example: "Due to lack of trust in certain organisations some key stakeholder groups were less willing to take part or share their motives [30]"*
Case details	35	Details of the cases used in the articles. This codes were later used to make Table 51
Collaboration	66	Codes regarding collaboration, including different forms of collaboration
Collaboration for impact	6	Collaboration with the focus on making impact or succeeding in something
Common language	10	Related to a common language or a shared language or vocabulary *Example: "Shared language embodies the degree to which network members use the same language, i.e., the means by which people discuss and exchange information [50]"*
Definition	42	Definition of a concept, barrier or driver
Documentation	5	Codes relating to the documentation process in a project *Example: "Documentation refers to creating feedback systems for evaluating outcomes throughout the project [15]"*
Drivers	87	Used to code concepts with a positive influence on another concept (also used for facilitators, factors or variables with a positive influence on a concept)
Financial resources	5	Related to financial resources as driver or barrier. *Example: "Securing financial and human resources is foundational for the work of collaborative partnerships [15]"*
Goals	15	Goals, ambitions or objectives as a driver or barrier. *Example: "Shared goals are an important relational resource and also a necessary condition to facilitate meaningful communication between parties in an exchange relationship [12]"*
Interdisciplinary	28	Related to interdisciplinary and multidisciplinary research or collaboration

Leadership	7	Leadership as a driver or barrier. *Example: "The strong leadership of the site coordinators was an especially critical resource for creating collaborative relationships [61]"*
Mission/vision	68	Related to the shared mission or vision
Resilience	8	Segments of articles related to resilience of research, researchers or collaborations *Example: "Community resilience can be threatened by action at other scales (e.g. at the scale of national policy), but it could also be supported and enhanced there [68]"*
Social capital	9	Segments of the articles related to social capital *Example: "most management scholar generally agree that social capital represents the resources an individual or social entity gain through its network relationships [50]"*
Trust	17	Trust as a driver or barrier *Example: "Trust is a significant concept in corporate governance research since it has a positive effect on the relationship between two or more parties and is regarded as a vital component for long-term cooperation, as well as for directing and controlling inter-organizational exchange relationships [20]"*
Understanding other's perspective	7	Mutual understanding between individuals, or an understand for other's perspective or worldview *Example: "Understanding the other collaborator' perspective was a key ingredient to creating a more shared vision [77]"*

Figure 46 shows the code tree that is used for the analysis of the articles. The first column shows the two main concepts: collaboration and shared vision. The second column shows the second iteration of codes: drivers and barriers. Those codes are in a third iteration split up between the individuals factors that influence collaboration or the development of a shared vision. Those codes include: social capital (entailing amongst others human and financial resources), mutual understanding, trust, resilience, action planning, time, common language, commitment, communication, documentation, leadership and goals. So the third code iteration uses more content related codes, while the first and second iteration focus on the two main concepts (collaboration and shared vision) and the identification of drivers and barriers.

Furthermore, three other codes were used besides the codes given in the code tree. These codes include 'advantages', 'case details' and 'definition'. The code 'case details' is used to get an overview of the case characteristics of each article, later used in Table 51. The code 'definition' was used to code definitions that were given by articles and 'advantages' was used to get an overview of advantages of a certain concept, idea, factor or driver. ATLAS TI has a functionality that allows to combine certain codes. So for example combining 'definition AND collaboration' gives an overview of all the definitions of collaboration mentioned by all the articles.

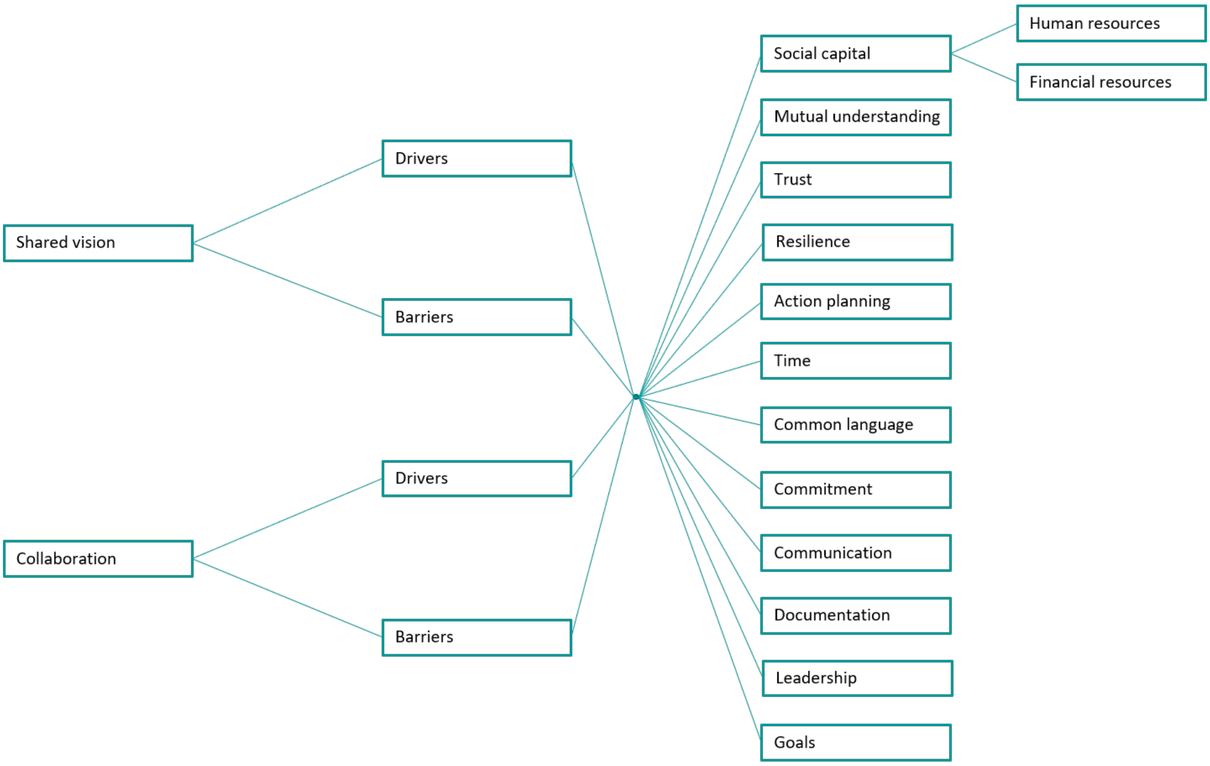


Figure 46: Code tree for the systematic literature review

4.2 Theoretical model

This section elaborates on the theoretical framework that is used in this thesis

4.2.1 Overview of the articles

The articles used to draw the theoretical model are:

- Brömmelstroet and Bertolini (2008) - Developing land use and transport PSS: meaningfull information through a dialogue between modelers and planners [7]
- Chen et al (2014) - how to facilitate inter-organizational knowledge sharing: The impact of trust [11]
- Daiser and Wirtz (2019) - Strategic corporate governance factors for municipally owned companies: an empirical analysis from a municipal perspective [20]
- Esler et al (2015) - Interdisciplinary and multi-institutional higher learning: reflecting on a south African case study investigating complex and dynamic environmental challenges [29]
- Gutiérrez Gutiérrez et al (2008) - Six sigma: from a goal-theoretic perspective to shared-vison development [34]
- Jean et al (2018) - Serious games as a catalyst for boundary crossing, collaboration and knowledge co-creation in a watershed governance context [40]

- King et al (2007) - Seeking common ground: how natural and social scientists might jointly create an overlapping worldview for sustainable livelihoods: A South African perspective [43]
- Lefebvre et al (2016) - Social capital and knowledge sharing performance of learning networks [50]
- Morgan et al (2015) - Observation of inter-professional collaborative practice in primary care teams: An integrative literature review [58]
- Porras et al (2018) - Unravelling stakeholders perceptions to enable adaptive water governance in dryland systems [70]
- Robertson (2006) - Development of Shared Vision: Lessons from a science education community collaborative [77]
- Schöttle and Tillmann (2018) - Explaining the benefits of team-goals to support collaboration [82]

Furthermore, the rest of the articles from the systematic literature review were read, but not used in the theoretical framework. Those articles include:

- Anito et al (2020) - Praxis for accelerated improvement in research (PAIR) [2]
- Bargen (1996) - Community visioning and leadership [5]
- Besterfield-Sacre et al (2014) - Changing engineering education: views of U.S. faculty, chairs, and deans.
- Lim et al (2019) - Embedding and sustaining motivational interviewing in clinical environments: a concurerent iterative mixed methods study [52]
- Prior et al (2013) - Resourcing the future: using foresight in resource governance
- Saville et al (2012) - Creating learning communities in the classroom [80].

The articles by Anito et al (2020), Besterfield-Sacre et al (2014) and Saville et al (2012) were excluded after reading since those articles focus solely on education and not on collaboration, making the articles irrelevant for the purpose of this literature review. While for example the articles by Esler et al (2015) and Robertson (2006) also take place in an educational context, those articles have a main focus on the collaboration aspect and not on the educational aspect, making them relevant for this systematic literature study.

The articles by Lim et al (2019) and Prior et al (2013) are both excluded from the literature review since both articles focus mainly on the technological and case-specific details and less on the collaboration part.

The article of Bargan (1996) was excluded from the literature review since the article focusses on building

4.2.2 Defining the concepts

Collaboration is described by Schöttle (2014) as a relationships between organizations, based on trust and transparency, with the intention to create a common project organization, based on a shared vision, a commonly defined structure and a collective project culture [81]. Robertson (2007) characterize collaboration by a mutually beneficial relationships between organizations in order to achieve results [77]. Chen et al (2014) describe collaboration as interactive and as task-oriented [11].

Goals are defined by Locke and Latham (2006) as *"future desired outcomes"* and by Widmeyer and Ducharme (1997) as *"guides for action"* [53, 98]. Johnson and Johnson (2009) formulated two ways to increase commitment of team members towards group goals: (1) making goals specific, trackable and measurable, achievable, challenging and relevant enough for the members of the group, or (2) goals were formulated together with the team [41].

In the article of Parkhill et al (2015) workplace communities are defined by Lave and Wenger (1991) as a group of individuals that participate in a system in which a shared understanding exists about their activities and the meaning thereof regarding their life and their community [68].

In the article of Parkhill et al (2015) community resilience is defined by Wickes et al (1999) as the process in which a (working) community shows the ability to deal with stress or change and to positively respond to it [68, 97]. Resilience is achieved when a community or a group of people are able to adapt to social-ecological changes [41]. Resilience relates to the attitude of the community regarding stress or change and the process of dealing with it, while adaptivity corresponds to the level in which a group is able to responds to this change or stress. Community resilience can both be endangered as well as enhanced by change on larger scales (for example national policies). On the one hand, national policies can create opportunities which can in turn empower and strengthen workplace communities. On the other hand, communities are not always able to adapt to a certain policy fast enough, acting as a barrier towards community resilience [68]. Chen et al (2014) define trust in terms of a positive psychological state in which one believes in the other's integrity and benevolence by holding to promises and working towards common results [11]. Daiser and Wirtz (2019) describe trust as having a positive effect on relationships and call it a vital component in order to successfully collaborate.

Social capital is defined by King et al as the intrinsic capacity of a group of collaborators and their social relationships that can provide means for the group [43]. Lefebvre et al (2016) define the concept of social capital as the resources a group of collaborators have through their social network. They divide social capital in three dimensions [50]:

1. **Structural dimension** the structural dimension refers to the social interaction that is part of social capital. Social interaction is the process of establishing relationships and making contacts. It is assumed that through this relationships and contacts, information and resources can be gathered.

2. **Relational dimension** the relational dimension of social capital is linked to trust. Trust between parties increases the willingness to collaborate and to share knowledge.

3. **Cognitive dimension** the cognitive dimension of social capital relates to a shared vision and a shared language. Through a shared vision, it is easier for the collaborators to align their focus and direction, which allows for enhanced knowledge sharing and better direction of resources. A shared language increases knowledge sharing and gives better access to information.

In Figure 47 the three dimensions of the social capital are shown. All dimensions of the social capital are said to influence the performance of the network. Also the dimensions mutually influence each other [50]. This is shown in the figure with arrows.

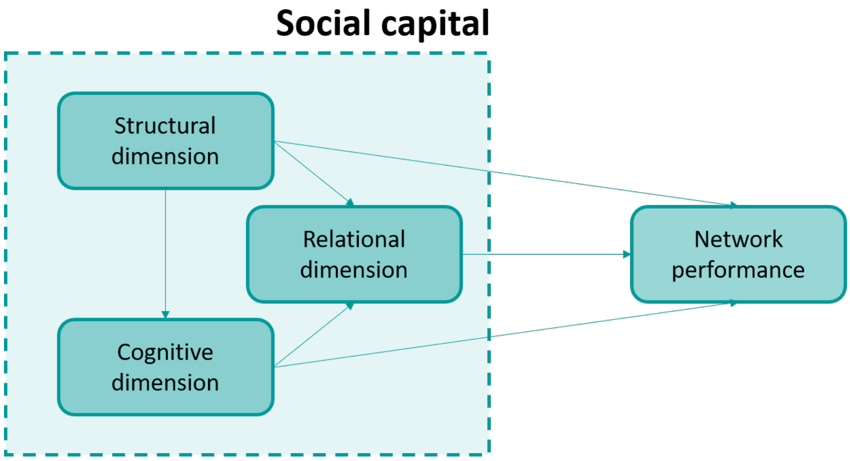


Figure 47: Social capital as three dimensions: structural dimension, relational dimension and cognitive dimension; influencing the performance of the collaborative network (adapted from Lefebvre et al [50])

4.2.3 Shared vision as time-dependent concept

Having a shared vision between multiple collaborative parties is defined by Daiser and Wirtz (2019) as having common goals and ambitions [20]. Lefebvre et al (2016) extend this definition by including common concerns and a shared perception of the future state [50]. Parkhill et al (2015) add to this definition having an agreement on the common good, as well as an alignment in worldviews, culture and lives, and shared values [68]. Shared values are defined by Chen et al (2014) as *"the extend to which partners have beliefs in common about what behaviors, goals, and policies are important or unimportant, appropriate or inappropriate, and right or wrong* [11]. Gutièrez-Gutièrrez et al (2008) focus their definition of a shared vision more on the future perspective of the collaboration, defining a shared vision as a shared future image amongst the members of the group and having individual commitment towards this image [34]. Weber et al (2015) note that a shared vision does not necessarily have to be consensus oriented, it can also be an alignment of existing different interests or ideas [96].

A shared vision is described by the articles with different important aspects. For the sake of this research, a shared vision is visualized as the overlap between goals and ambitions, values, future perspective, external visibility and concerns. Figure 48 shows this concept.

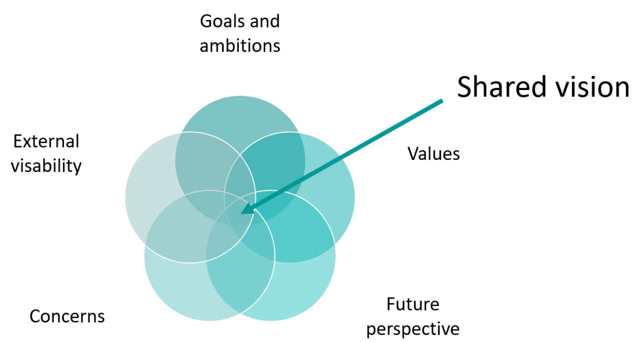
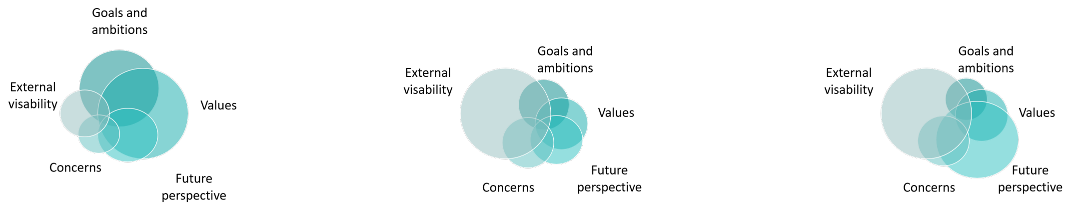


Figure 48: Shared vision as the overlap between goals and ambitions, values, future perspective, external visibility and concerns.

However, it is also noted in the articles that during different phases of the collaboration, a shared vision can be beneficial for different purposes. In the initial stage of a collaboration, a shared vision can aid in bringing people together. In this stage, shared values and a shared sense of the goals and ambitions are more important compared to external visibility. While later on in the collaboration, when (financial) resources have to be established, external visibility becomes more important. In the end phase, goals and ambitions might not be the main focus of a shared vision, but external visibility and future perspective might be more important. Figure 49 gives an idea on how a shared vision might change over time. Figure 49 (a) shows how a shared vision might look like at the initial phase of a collaboration, in which individuals share an initial idea of what the collaboration will look like based on shared values and shared goals and ambitions. Figure 49 (b) shows a later phase in which resources have to be secured, a phase in which external visibility might be more prominent. Figure 49 (c) shows the end phase of a project



(a) (b) (c)

Figure 49: Shared vision illustrated as a concept that is dependent on time. Figure (a) represents the initial phase of a collaboration in which individuals come together, figure (b) shows the start up phase in which (financial) resources have to be secured, and figure (c) shows the end stage of a project in which goals and ambitions are already met and the collaboration is about to finish

4.2.4 Drivers and barriers for (interdisciplinary) collaboration

Crooks et al (2018) uses seven factors for successful collaboration in a multidisciplinary and multi-organizational project described by Roussos and Fawcett (2000) to research effective collaborative partnership leading to community and system change. These seven factors include:

1. **Clear mission and vision** This refers to the purpose for the work. Having a clear and shared purpose amongst the individuals involved in the project is beneficial for creating awareness and support amongst partners. It also improves efficiency of the collaborative initiative and limits ambivalent personal goals in a project [78]. Crooks et al (2018) mention three drivers for the development of a shared mission and vision amongst the partners involved: (1) prior developed relationships from previous (larger, state) initiative, (2) resources available for an outcome of shared interest, and (3) a feeling of equal ownership amongst the parties involved, despite differences in organizational background and roles in the project [15].

2. **Action planning** Here defined as the planning of who will do what and and which time, which is essential for achieving goals and objectives [78]. Drivers for successful action planning are named by Crooks et al as: (1) strong relationships amongst partners in order to be flexible and efficient in response to challenges, (2) deep understanding of the capabilities of the individuals and the organizations involved in the process, (3) trust amongst each other that each member involved in the project is working towards the same shared mission and vision. [15]

3. **Leadership** Leadership is done by one or more individuals in the group and guides the group to achieve their objectives [78]. It can be either a key individual in the group that takes on this role, or leadership can be distributed between multiple team-members. Different sub-projects often have their own leaders as well, those are often members with a strategic position in the project, chosen based on their competences and role in the organisation [15].

4. **Documentation** Documentation is defined by Roussos and Fawcett (2000) as the feedback systems that are in place in order to evaluate the (intermediate) results of the project, a method for ongoing quality improvement, a way of identifying barriers and making them part of the formal conversations, as well as celebrating (intermediate) results. Drivers for effective documentation are identified by Crook et al (2018) as (1) a strong connection between the documentation and the accountability of individuals, (2) solid interpersonal

relations between the individuals in the project, (3) clarity about roles, and (4) formal documentation of roles.

5. **Technical support** Technical support is described as "the training and support needed to implement and sustain a collaborative partnership" (Roussos and Fouwcett, 2000, p.387) [78]. Two different ways of enabling this support are mentioned by Crooks et al 2018): (1) internal support, relating to the mutual learning between members of the group, and (2) external support, often accessible through already existing relations between members of the group and individuals or organizations outside the group [15].

6. **Dedicated resources** Resources can be both human resources or financial resources, and is often the foundation of a collaborative partnership since it can aid in making the collaboration both formal and legitimate. Having a clearly formulated and shared mission is describes as a driver in securing financial resources [15]

7. **Results orientated** Outcomes of the project should be relevant beyond the scope of the established partnership, they should also be relevant to the members on an individual level. This is a driver for steering more human and financial support towards the project [78].

Crooks et al (2018) furthermore identified three cross-cutting themes that were drivers for the successful collaboration [15]:

- **Flexibility** On all levels present in the collaboration: individual, organizational, system-wise and regarding the action planning. The flexibility in the project was a result of having a shared mission as a driving force behind the collaboration.

- **Transparency** in this case referring to transparency in both personal and organization strengths and weaknesses. Having a common mission made transparency between individuals around (financial) resources easier.

- **Prioritizing of relationships** relationships were prioritized and a sense of shared success exceeded personal successes.

4.2.5 Drivers and barriers for developing a shared vision

A shared vision can be the initiator of a partnership [68], however a collaboration can also be formed on basis of a shared concept, while a shared vision may come to place later on [7]. Having a vision that is shared between the collaborative partners, can be beneficial for multiple reasons. A shared vision can be beneficial in order to facilitate both social action and social resilience [68]. A clear vision can also aid in raising external awareness and increasing support for the collaboration [**?**]. Weber et al (2015) observed that a shared vision had a positive effect on motivation, external visibility, internal communication and goal setting [96]. Part of having a shared vision, is having shared values. They are mentioned by Parkhill et al (2015) and Silk et al (2010) as the fundamentals that a (workplace)community needed to build the collaboration upon [68, 83].

According to Robertson (2006) the following factors influence the process towards the development of a shared vision in a collaboration [77]:

1. **Time** Having sufficient time for collaborators to meet and to discuss is one of the key factors in the development of a shared vision and creating a successful collaboration initiative

2. **Communication** Communication is mentioned to be vital to create a mutual understanding. Besides, it is one of the most time consuming aspects in collaboration. Communication via email and telephone is more efficient, however, face-to-face communication takes more time but allowed for other's perspectives to be better heard.

3. **Understanding other's perspective** Having a better understanding of other's perspective and on the basis of the collaboration, leads to developing a more shared vision. It takes time and communication between members to create a mutual understanding of each other's perspective. In the article by Schöttle and Tillmann (2018) it is mentioned that the process of agreeing on goals lead to a more clear understanding of mutual expectations and a better understanding of the perspective of other members [82].

4. **Dedication, motivation an ownership** Having a sense of dedication and motivation towards the project, helps collaborators in feeling more connected to a collaborative initiative, which in turn is a driving factor for creating a shared vision. Furthermore, if collaborates can take ownership in (parts) of the collaboration, they feel more responsible towards the collaboration as well. Increased sense of responsibility also leads to a greater dedication and motivation towards the project.

5. **Collaborative environment** The collaborative environment and successfulness of a project is largely determined by the individuals in the project. Factors that might play a role in this are the eagerness of individuals to collaborate, the amount and flexibility to spend time on a project and how they perceive the usefulness of the spend time on the project.

Crooks et al (2018) name the three factors that influence the development of a shared vision [15]:

- Relationships between members prior the the collaboration, past relationship can either negatively or positively influence the development of a shared vision
- Amount of ownership felt by each member of the institute, having equal ownership regardless of the role in the collaboration is a driver for developing shared vision
- Availability of resources. Having resources available positively influences collaboration around a shared interest.

Daiser and Wirtz (2019) name trust and mutual understanding as drivers for creating a shared vision for a long-term collaboration [20]. Trust is also mentioned by Chen et al (2014) as a driving factor for knowledge sharing [11]. Fielke et al (2017) identified the lack of trust in their case study as a barrier to communication and a barrier to share individual motives [30]. According to Lefebvre et al (2016) social interaction (the structural dimension of social capital) increased trust between members and this in turn was is a driving factor for the development of a shared vision [50]. Furthermore are a shared vision, shared values and shared vocabulary all named to be drivers for the development of trust [50].

Brommelstroet and Bertolini (2018) names a shared vocabulary as a pre-requisite to the development of a shared vision.

Nelson et al (2018) list consensus building, open dialogues and mutual respect as three factors that positively affect the member's sense of commitment en belonging towards the collaboration [61]. One of the main constraints for this is time. There must be sufficient time for the members dedicated to familiarize themselves with the project, to build personal relationships, establish a shared vocabulary, and agree upon a common goal or outcome [61]. Weber et al (2015) elaborate that alignment of interests takes place in both informal and formal ways, and documented as well as oral [96].

Robertson (2007) name the following drivers and barriers for the development of a shared vision [77]:

- Different priorities of the members of the collaboration
- Amount of time that is available to meet and to collaborate.
- Time spend on communication
- Ability to understand perspectives of others'
- The degree of dedication, motivation and ownership the collaborators feel towards the project
- Collaborative environment, which is largely defined by the individuals working on the project.

Lefebvre et al (2016) further mention that a shared vision can also be a driver for the amount of knowledge sharing in and between organizations in a collaboration.

4.2.6 Overview

An overview of how the different concept relate to each other according to the systematic literature review is shown in Figure 50. The two most important concepts, shared vision and collaboration, are shown in bold. The concepts shared goals and shared values are shown as part of a shared vision and connected to a shared vision, since those two concepts are in integral part of having a shared vision, but can also be evaluated as concepts on their own. The arrows show positive relationships between multiple concepts. For example the arrow from trust to shared vision, indicates that trust has a positive influence on a shared vision, and is thus a driver for the development of a shared vision.

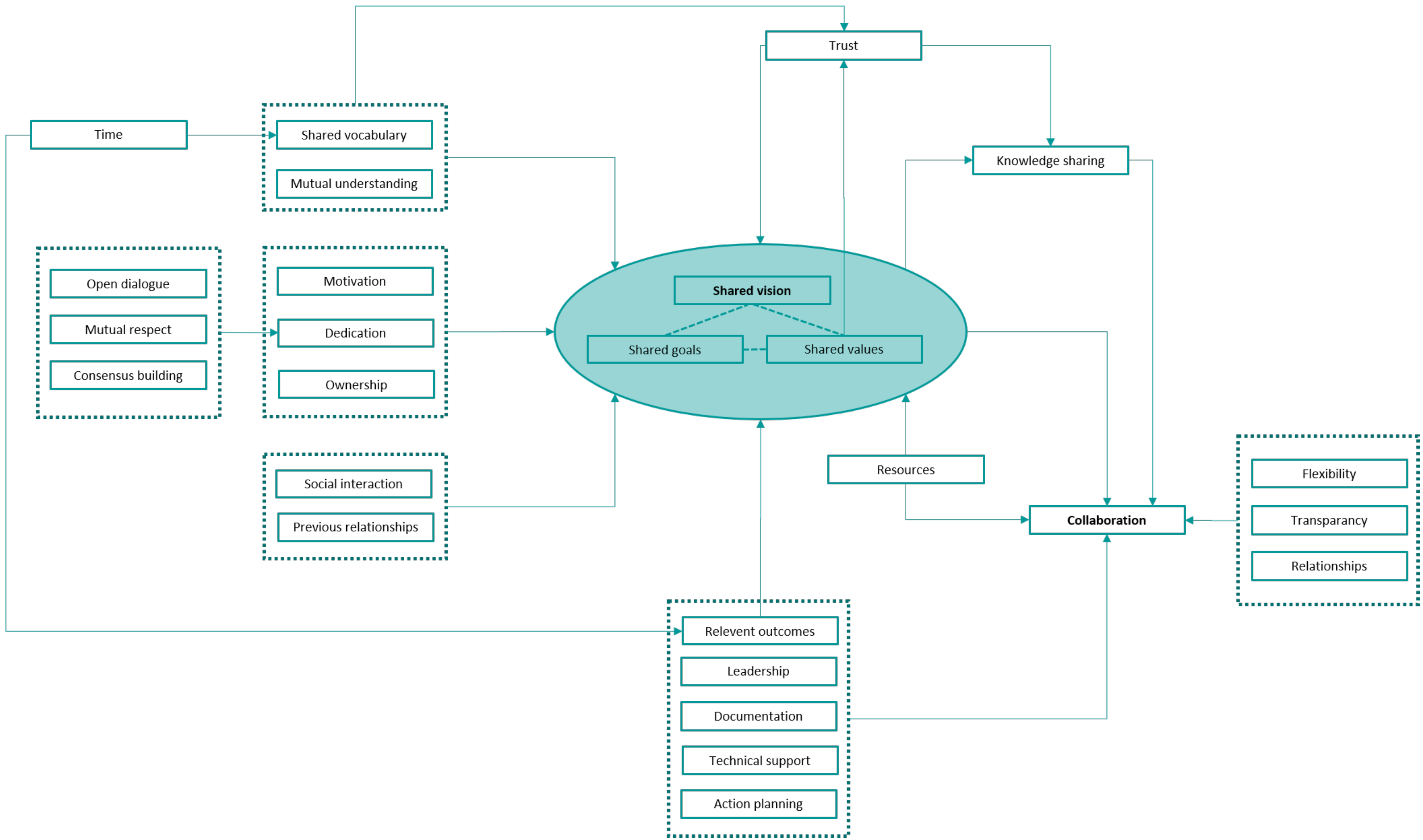


Figure 50: Overview of the interaction between the different concepts

4.2.7 Characteristics of different cases

Table 51 gives an overview of the cases used in the articles and some characteristics of those cases.

Table 51: Characteristics of the cases in the articles from the systematic literature review

Article	**Case / Research context**	**Characteristics of the context/case**
Anito et al (2020 [2]	Research production and publication in higher education instituteions in the Philippines	-
Brömmelstroet et al (2008) [7]	Development of land use and transport through mediated planning support	Cooperation between transport planners and land use planners. Transport planners have a stronger focus on quantitative information and problem solving, while land use planners focus more on qualitative information and on bringing together multiple goals.
Chen et al (2014) [11]	Industrial manufacturing parks in Taiwan	-
Crooks et al (2018) [15]	Sexual and domestic violence prevention in Alaska	Committee including organizations related to education and public health, both governmental as well as non-governmental. Complexity due to diversity in both population and geographical sense.
Daiser and Wirtz (2019) [20]	Municipality owned companies	-
Esler et al (2016) [29]	Interdisciplinary education in higher learning institutes	Social-ecological challenges characterized by large spatial scales, unpredictable changes and involvement of multiple stakeholders with different interests
Fielke et al (2017) [30]	Agricultural innovation	Involvement of multiple stakeholder groups with different interests. Both economical and environmental factors set constrains on innovation.
Gutiérrez-Guttiérrez (2008) [34]	Electronics industry	Six sigma methodology to improve organizational performance in the electronics industry

Jean et al (2018) [40]	Governance of watersheds	Involvement of multiple stakeholders (e.g. public, industry, small business owners, politicians, decision makers); Complex issues due to e.g. possibility of asymmetry in resources, political structure and governmental agencies;
King et al (2007) [43]	Two cases: 1) ecotourism in South Africa, and 2) Invasive alien species in South Africa	Complex due to interaction of environmental with socio-economical factors, influencing local communities
Lefebvre et al (2016) [50]	European learning networks	
Morgan et al (2015) [58]	Interdisciplinary collaboration in health care teams	Collaboration between different professions
Nelson et al (2014) [61]	Housing for mentally-ill homeless people in Canada	Complexity due to physical environment, lack of transparency, changing parameters, involvement of multiple stakeholder groups
Parkhill et al (2015) [68]	Energy transition projects in the UK	Local projects involving multiple stakeholders
Porras et al (2018) [70]	Water governance in Mexico	Multiple challenges in a complex socio-economical context with conflicting interest of multiple stakeholders.
Poulsen et al (2019) [71]	Integrated health care to support people on sick leave due to common mental disorders	Multidisciplinary collaboration
Robertson (2006) [77]	Improving science education by field trips	Collaboration between teachers and researchers with different perceived outcomes
Prior et al (2010) [72]	Resource management in Australia	Interaction across social, techno-, logical-, ecologial, governance and economic domains
Saville et al (2012) [80]	Educational learning communities	
Schöttle and Tillmann (2018) [82]	Lean construction	Team-goals setting and tracking as means to support collaboration in the lean construction industry
Weber et al (2015) [96]	Ad hoc disaster management	Real time collaboration, ad hoc collaboration, highly unpredictable, involvement of both global and local network partners

5 Deepening phase - interview

This section shows the results of the second round of interviews. The section starts with an overview of the definition of a shared vision given by the interviewees. Secondly, a shared vision, defined as the vent-diagram of five different pointers (goals and ambitions, values, future perspective, concerns and external visibility) is discussed in more detail. This is followed by an overall analysis of the presence of a shared vision within e-Refinery. Afterwards, the drivers and barriers for the development of a shared vision are discussed. The section finalizes with a critical node regarding the drivers and barriers of a shared vision.

5.1 Shared vision definition

Table 52 gives an overview of the definition of the concept 'shared vision' given by the interviewees. As can be seen, a shared vision is mostly described in terms of having a shared goal. The way to reach that goal, the road towards the goal, is also mentioned by some interviewees.

Table 52: Definition of a shared vision given by the interviewees

Interview	Quote
1	I would define it as having a common goal Yes yes and also the means. In the case of e-Refinery, the way towards the goal is also very important
2	We have a sort of end goal and we aren't necessarily working to get to that goal in the same manner.
4	It's a good question, but also a hard one. I think there needs to be consent about the functionality of the things you'll develop. Consent about functionality. And that functionality can be developed in different ways, or can be contributed to with different sub-disciplines. I think you also need consent about the scientific renewal it brings, otherwise it's not publishable. It needs to have a scientific value.
6	In my opinion a shared vision is a common goal, that people agree with and would like to strive for
7	For me a shared vision exists of having an end goal and knowing the steps you have to take to get to that end goal.
8	I would believe a shared vision means where we want to end up, how we would image the future to look like. So that for me would be vision, to have the same goals.

5.2 Shared vision within e-Refinery

This section first gives an overview of the answers given to the open question regarding whether e-Refinery has a shared vision. The subsections following go into more detail about the five aspects of a shared vision: shared goals and ambitions, shared values, future perspective of the institute, shared concerns, and external visibility.

5.2.1 Open question

Table 53 gives quotes from the interviewees regarding whether they see a clear shared vision within the e-Refinery institute or not. As can be seen from the quotes, the opinions on whether this shared vision exists in e-Refinery, is rather diverse. Some interviewees believed this shared vision to be very present, while others believe there is room for improvement or the vision is not as much shared between all members. One explanation for the difference in opinion about this, might be that some parts of a shared vision are more present, while other aspects are less present.

Table 53: Shared vision within e-Refinery

Interview	Quote
1	The shared vision is there, definitely
3	My impression is that right now most members have a different understanding of this vision actually, that is my impression
5	There are some people who work on different topics and also topics including the interest of e-Refinery. So the answer is yes and no. So on some level yes, but not fully
6	Not really, I think that could be improved.
7	Oh yes for sure we have [a shared vision], I think that is the beautiful thing of this institute, there is a clear line of where we want to go. That makes it easier to set up collaboration as well, so I'm absolutely positive about that.
8	I would say that is very present

5.2.2 Shared goals and ambitions

Table 54 gives an overview of the quotes regarding the existence of shared goals and ambitions in the e-Refinery institute. Having a shared goal is one of the first components mentioned in having a shared vision by the interviewees. There is consent on what this shared goals and ambitions are, but there is less consent on ho the reach those goals. However, even though most agree on the goal and the ambitions, there is still some division in whether this goal is a set and fixed goal, or more a moving goal.

Table 54: Shared goals within the e-Refinery institute

Interview	Quote
2	I think the overall goal is something, sort of, reminded to us everything we go to a big meeting you know, like the societal implication of it. So I do think there is an overall goal, but within that people are quite disperse. We have a sort of end goal and we aren't necessarily working to get to that goal in the same manner, we have quite a lot of different ways of getting there. We disagree quite a lot on how to get there, because we all have the same idea of the end goal, that is what unifies us, and we all care about different aspects of it. Then there are some people on sort of higher, I don't want to say management level, but let's say implementation level that do care about fitting those people together.
3	One could also facilitate interactions and driving more fundamental and applied research using this e-Refinery institute, but the goal wouldn't be just one direction, right? And I think e-Refinery is functioning more on this mechanisms now, but a shared vision becomes a bit weaker, because everyone has their own goals.
3	Here is this kind of goal also and at the same time it is also not really a fixed goal
4	I think it is important to have shared ambitions
7	That there is a shared goal that is shared between the members, I definitely agree with. And I think it is important that it is there.
8	I think that is very much the same
9	If there is a defined goal, that is always nice for everybody to stay on track
9	I would say it is of the utmost importance because if there is no overall goal, there is no need to continue the research.

5.2.3 Shared values

Table 55 gives an overview of the statements of the interviewees regarding the shared values within e-Refinery. The interviewees agreed on that the societal and environmental values behind the e-Refinery institute, such as reducing CO_2 emission and striving for a greener future, are shared between the members of the institute. This value is for some an extra motivation to join the institute and to work towards the shared goals. Even though these values are said to be an extra motivation, they are not on their own the big unifying factor in the institute.

Another mentioned value is more related to the way science is practised, relating to how people in scientific projects can cooperate with each other. Even though this value is mentioned and said to be present in e-Refinery, it is agreed that this is not often made explicit.

Table 55: Shared values within the e-Refinery institute

Interview	Quote
1	- So an example of a shared value could be 'striving for a greener future' or 'decreasing CO_2 emissions', or values related to doing research. - I agree with them and I think these are important. It is essentially also the societal context and part of the motivation behind this
2	I think that is something we all agree on, but, I think, I don't know (...) I think a lot of us are a little bit less emotional about it, we sort of know that this is something that needs to be done and let's go ahead and do it.
3	If there is a shared value everyone can appreciate and can agree on, that is a good thing. But at the same time, I don't know if this is at all possible.
4	I'm hesitating a bit, because there are different values. There are societal values, like reducing CO_2 emission and I think everyone in the group shares that, but at a scientific level those values can differ a bit. I can understand that a pure chemist is very happy if he can research for example chemical reactions on a surface within the e-Refinery group, while an engineer might want to do something that is eventually being implemented. So there is a certain diversity.
5	Of course, there are modelling people and experimental people and they should be well connected together. I think e-Refinery is kind of bridging this gap between different fields
6	Of course [e-Refinery shared vales]. There are modelling people and experimental people and they should be well connected together and I think e-Refinery is kind of bridging this gap between fields. Of course we want to change the world, right. We want to make things sustainable, we want to advance science. This are some of the shared values.
7	Those are important. We all work on different aspects of course, so these kind of things come up when you for example come up with a new idea and you get appreciated for that, or the feeling that nobody runs off with your ideas. So in that sense shared values are important to reach the goal. And I believe they are there, and even though they are not often told explicitly, I believe it's going well
8	It is maybe a little bit implicit in the goal, but I think it is important if you have the same vision to also have the same values
9	We work for the same topic so the vision is that one, reducing CO_2 in the environment and creating an electrolyzer in 2050, so there is a global shared vision amongst the group definitely

5.2.4 Future perspective of the institute

In the interviews, some agreed that the future perspective of the institute is more agreed on, while others said it to be less agreed on. The difference in views over whether there exists a clear shared perception over the future of the institute can be explained in terms of how specific that future perspective is defined and described by the interviewees. A more general future perspective (e.g. transition towards an electro-chemical based future) is very agreed upon between the members in the institute, while the more detailed and specific future is less agreed upon (e.g. the difference in whether to strive for a small scale or large scale).

Table 56: Future perspective of the e-Refinery institute

Interview	Quote
1	Yes I agree with that, I would say it is less important compared to the first one [shared values], because a perception is something that can also work against you. If we would focus too much on one route for example, when we don't really know how yet... Well that is not scientific, you also need to let yourself be guided by the facts and be open for possibilities
2	- Do you share the same idea of what the future of the project should look like? - Yeah! Yeah yeah yeah We definitely have a vision for the future were we see this is going to carry on.
3	Yes I think that that is probably more agreed on. Everybody understands the importance of the transition.
4	I think this is important, but it will result in a vigorous debate. And maybe that is a good thing, because eventually you have to decide a main road in which you're going to work and make priorities.
6	For some people this is more clear and for others it is less clear. Also for me, as a scientists or as a researcher, you work at your own piece of the puzzle and depending on which piece you're working on, you may see a bigger picture or you may see a smaller picture
7	The first one [shared perception of the future] there may be a difference. While one might thing, if we can show it, at small scale in the lab, and we write an article about it, it is done. While another might also thing we need to bring it towards industry, that's our job. So there might be a difference absolutely.

5.2.5 Shared concerns

The quotes regarding shared concerns are shown in Table 57. Most interviewees agreed that the level of shared concerns is not that high yet in the e-Refinery institute. The most mentioned reason for this is that everyone is focused on their own research and own field, and having also concerns related to that. Most interviewees agreed that there is room for individual concerns within the larger institute, however a certain level of shared concerns can be necessary to eventually reach the shared overall goal and to decide which things to bring attention to and to locate resources well.

Table 57: Shared concerns within the e-Refinery institute

Interview	Quote
1	I think the concerns aren't there yet I think this is really important so the right things get attention and resources are spend well, so it is definitely important if you want to really reach your goal.
2	I think we have the three main problems, the sort of vent-diagram that we started with. One was CO_2 capture and storage, one was carbon neutral fuels, and one was chemical feedstock. Within, usually when someone within e-Refinery talks about something, we talk about one of those three.
3	If we have a shared vision, we need to have shared concerns also to achieve this shared goals and ambitions I think everybody has many different types of concerns They are really busy or really focusing on their topics and their concerns are really different from other concerns, so I think shared concerns are probably not that high level yet.
4	There is a certain extend of concerns, or things people are concerned about. But those can still be quite diverse.
6	Not everyone has the same kind of concerns, but depending on the kind of people and research, everybody has a different opinion on this. But I do think we do agree on many of the shared issues we have and we see that we need to tackle them.
7	Partly yes, but I think this can be improved. I don't think that everyone is equally inclined to share their concerns in the group. There could be more attention for this
8	There might be a difference in concerns, but I feel like e-Refinery is at least trying to bridge that

5.2.6 External visibility

The concept 'external visibility' is understood by the interviewees as a concept that entails the image that is held by e-Refinery and is used to portrait itself towards the outside world, the way e-Refinery interacts with the outside world in terms of collaboration and knowledge sharing, and the level of visibility of the e-Refinery institute. From the interviews, it is seen that the image e-Refinery wants to present to the outside world is already quite agreed upon and also clearly shared within the institute. However, this image is not yet often brought the the outside world in terms of visibility. So put it simple: the 'what' is established, but the 'if', 'how' and 'when' is still up for discussion. There is a clear idea of what to represent to the outside world, but not yet a vision on if this is something to be done, how this should be done, and when to do it.

Table 58: External visibility of the e-Refinery institute

Interview	Quote
1	I think it is very important [having a shared image of what e-Refinery is]
2	I think a lot of the leaders, a lot of the stuff they created, we do have quite a clear image of the overall goal. So whenever I'm talking to someone outside e-Refinery I can go sort of back to that stuff they have already done and had presentations about and use that. (...) We definitely have a good image decided from the start about what we want to represent ourselves as.
3	I think it is important, the core team of e-Refinery, they need to know exactly how to sell it to the outside world. I have been observing how things have been going on, and I've seen that it is quite a heterogeneous mixture.
4	I don't think everyone is equally capable of doing this [communicating towards the outside world], but that grows with the years. There are some older people involved, that already took a few steps in their scientific career and are a bit more trained in this compared to the younger generation. But there are surprisingly good talents amongst the younger people as well. But there are also some researchers really, I don't want to say trapped, but fascinated by their own subject so they dive in too deep instead of keep an overview.
5	- Do you think e-Refinery has a coherent image of how they want to portrait themselves towards the outside world? - Yes this is what they are doing, but as far as I'm seeing up until now, maybe they have done that in the past, but I wasn't there yet, but they don't do it systematically
7	I think there are... I think most of the people are focused on collaboration but there are some gradations. One would think to keep it more a Delft-thing, while other's are more open for collaborations
8	I actually believe for something like being visible or being... or someone knows about e-Refinery, put it out there in the world, that is also something that we can work on a little bit more. (...) You heard people talk about it, but there was no website or so. I think it's also very important to identify yourself a little bit more with the collaborators.
9	There is now this discussion about creating a website. I think soon we develop this type of way of communication and I think this is even better because then everybody can juts google e-Refinery and get some information about it.

5.2.7 Overall analysis - Shared vision within e-Refinery

Overall, it can be said that within the e-Refinery institute, the overall vision is especially present in the goals and ambitions of the institute. The shared values are currently less present in e-Refinery. There are some shared values, but those are not very explicitly mentioned or agreed upon by the members. The future perspective of the institute is on the one hand quite clear in terms of a general and overall idea of what the future should look like for the institute. On the other hand, there are still discussions going on about the details of this future perspective. A similar situation can be described for the external visibility. The image of the e-Refinery group is agreed upon and set, however, there is not yet much activity going to actually make the group visible. The shared concerns are currently the least present in the e-Refinery institute.

The shared vision of e-Refinery is visualized in Figure 51. In the vent diagram, the goals and ambitions are shown as a larger circle and the values, future perspective and external visibility are shown as slightly smaller. The concerns are visualized as the smallest circle.

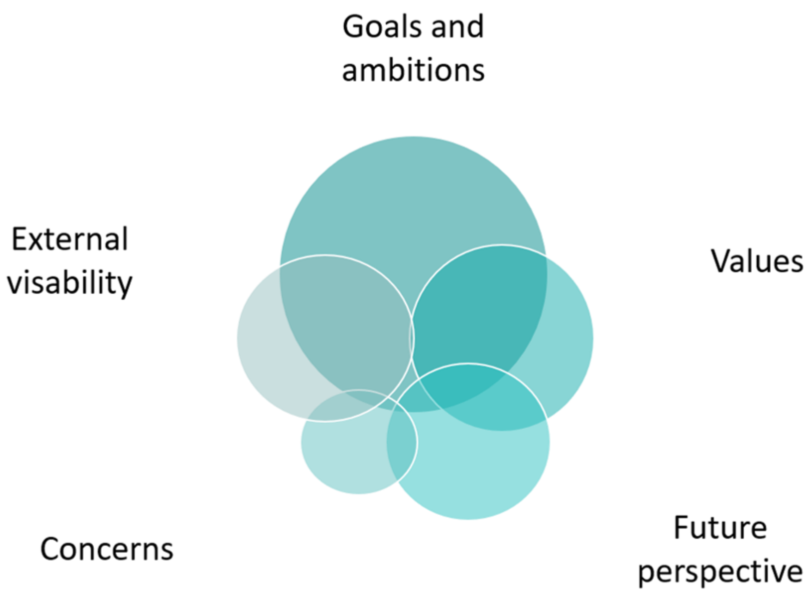


Figure 51: Shared vision visualized for the e-Refinery institute

The e-Refinery institute is now already a few years old and the institute is changing and expanding a lot over time. A shared vision is also always a dynamic process and certain aspects of a shared vision are more or less important over the time of the project. This is also described by interviewee 1, focusing on the shared concerns aspect of a shared vision: *"In the beginning you have to make sure that everyone is standing for the same. The context, the goal, it has to be clear. Once you're making progress, you hopefully, in the ideal situation, the restrictions and the concerns to reach that goal slowly become more clear. That's something you can hope and expect. And from a pure rational point of view, you need to pay more attention to those".*

A shared vision as a concept changing over time is also acknowledged by interviewee 4, emphasizing the shift from a more internal focus to a more external focus: *"During the starting phase, a lot of energy was invested in getting to know each other, working together, so internally focused. How do we get this club going. But after a year of 3 to 4, the external world is starting to ask: so what is coming from this? And then the selling of research results, and the* *translation thereof into pilot applications is becoming more important. But you have to make sure the internal frame, the structure, is working".*

5.3 Drivers and Barriers

The next section discusses the drivers and barriers for the development of a shared vision.

5.3.1 Survey results

In the interviews, the interviewees were asked to fill out a survey. This survey has been filled out by the interviewees in an interactive manner to simultaneously get the though process and train of thought behind the answers that were given. The survey consists of 15 statements relating to the drivers and barriers found in literature. All statements were asked to rate on a 5-point Likert scale from 0 to 5, the first scale ranging from "strongly disagree" to "strongly agree" and the second scale from "not important" to "very important". The results of the survey are shown in Figure 52, in graph (a) both the presence and importance average ratings for each statement number are shown while graph (b) shows the difference in rating between both scales.

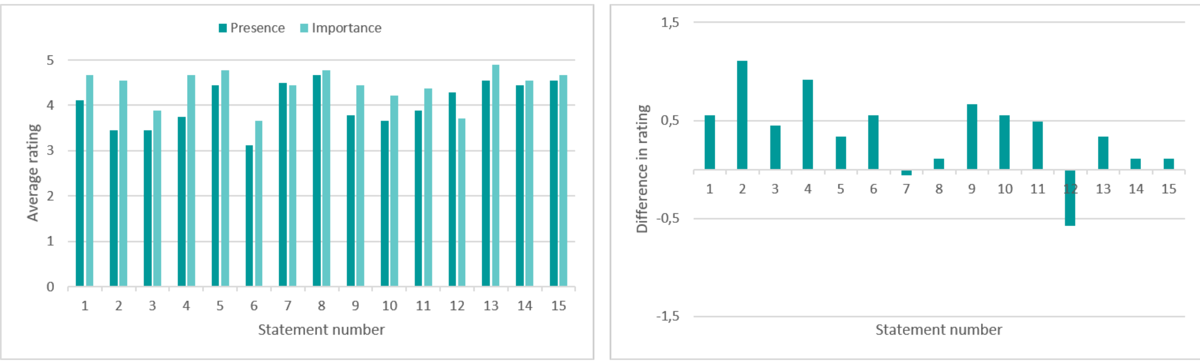


Figure 52: Results of the survey, in graph (a) showing the average rating of the statements on the presence scale and the importance scale and (b) the differences between both ratings, calculated as difference = importance - presence

Table 59 shows the statements, their average ratings and the difference in rating between the important and presence scale.

Table 59: Results from the survey held amongst the interviewees. In the second column the presence, the average rating on the disagree/agree scale, and in the third column the importance, the average rating on the unimportant/important scale, the fourth column gives the difference in rating

Statement	Presence	Importance	Difference
1. The members of the e-Refinery institute share the same overall goal	4.11	4.67	0.56
2. The members of the e-Refinery institute developed goals collectively	3.44	4.56	1.11
3. It is clear what is expected from each member in the institute	3.44	3.89	0.45

4. There are enough financial and human resources to successfully participate in the institute	3.75	4.67	0.92
5. The members of the e-Refinery institute share knowledge and views with each other	4.44	4.78	0.34
6. The members of the e-Refinery institute care about the same issues	3.11	3.67	0.56
7. I feel like I have ownership over the part I do for the e-Refinery institute	4.5	4.44	-0.06
8. I am motivated to be part of the e-Refinery institute and to work towards their goals	4.67	4.78	0.11
9. In general, there is sufficient interaction with other members from the institute	3.78	4.44	0.67
10. It feels like the members of the institute use similar language	3.67	4.22	0.56
11. It feels like the members of the e-Refinery institute communicate on the same wavelength	3.89	4.38	0.49
12. Previous relationships with others positively influenced the say we shaped this project	4.28	3.71	-0.57
13. I trust the other members of the institute	4.56	4.89	0.33
14. I feel like the work I do is respected and appreciated within the institute	4.44	4.56	0.11
15. In general I experience the collaboration as positive	4.56	4.67	0.11

5.3.2 Shared goal

The quotes regarding a shared goal are given in Table 54. All interviewees agreed that a shared goal is one of the main components of having a shared vision and therefore also important for the collaboration. This is also confirmed in the survey, in which a shared goal is rated with a score of 4.67 out of 5 o the important scale. On the presence scale, a shared goal is rated with a 4.11 out of 5. This number is a bit lower since some agreed on a shared overall goal, but noticed still some differences in how members of the institute are working towards that goal. Furthermore, the overall goal of e-Refinery is not a fixed goal, as said by interviewee 3, which was also mentioned in the preliminary interviews by interviewee 3: *"The ultimate goal is more like the direction of where we are going and why we are doing it"* (see Table 44).

5.3.3 Collective development of goals

The quotes regarding the collective development of goals is given in Table 60. From the survey it was clear that collectively developing goals is important of the e-Refinery members, since it is rated with a 4.56 out of 5 points. However, the presence of developing goals is rated with a

3.44 out of 5, so there is quite a difference between the perceived importance and the perceived presence of this aspect.

The process of developing goal is not done completely collectively according to the interviewees. The goals and the vision is developed by the researchers and the board that took initiative in the institute and set it up. Researchers and PhD students that joint the institute later, were less involved in the development of this overall goal and vision. They found overlap in what e-Refinery is doing and what they are doing (or wanting to do) and contribute in that way.

Table 60: Collective development of goals within the e-Refinery institute

Interview	Quote
2	What you define as what is valuable is up for discussion (...) We do talk quite a lot about what is important, so I do agree that it is collectively done.
3	The concept behind was already defined and I'm following now the evolution
4	I feel like there is an overall vision of where we want to go and everyone is looking from their own expertise: how can I contribute to this overall goal. But that is different from sitting together and deciding what you're going to do and basing research on that.
6	There are these workshops and so which have been organized, but it is a continuous process and it should happen more
7	[developed goals collectively] hmm not so strong, it is important though, but it has been something growing.
8	That is tough to answer for me as a PhD, but you get a certain degree of freedom
9	So for this it depends, because there are people doing photocatalysis, that are doing something different from the people that are modeling or doing fundamental electrochemistry. So it depends on, let's say, there are some boundaries in between and if those boundaries are a bit weaker then you can still have developed goals collectively, otherwise finding a link between a group in electrochemistry or somebody doing photocatalysis.

5.3.4 Mutual expectations

From the survey it can be seen that the e-Refinery members don't hold very many expectations of the other members of the institute, since it is rated with a 3.44 out of 5 on the presence scale. The members do not think it is that important, rating the expectations a 3.89 out of 5. From the interviews it became clear that there are some general expectations the members hold for each other, *"just do research"* and *"contribute towards the institute as best as they can"*, but besides that there is also a level of independence for the members to shape this in their own way.

Table 61: Mutual expectations within the e-Refinery institute

Interview	Quote
2	I think it's less clear what is expected from everyone. That is partly because there is a level of independence
4	Yes I think it's pretty clear, I think each member is contributing towards the institute as best as they can, but within the framework of their own research lines
7	Yes I think this is quite clear, although it is also a bit organic and people can say what interests them and work with that
9	It is expected to just do research, but there is no clear rule

5.3.5 Financial and human resources

In the survey the members rated the presence of enough financial and human resources with an average of 3.75 out of 5 while the importance is rated with a 4.67 out of 5. In the interviews it was mentioned that the limited budget can be a barrier in what e-Refinery can achieve eventually. The quotes regarding the financial and human resources in the e-Refinery institute are given in Table 62.

The interviewees agreed that the members currently involved in the e-Refinery are all professional and excellently qualified for the research they do. So when talking about human resources, the members are very content with the members currently involved. Nevertheless, it is also said that there is still room for more members taking on different roles that are currently not yet deployed. Most of the members involved in the e-Refinery institute are there voluntarily and do not work on e-Refinery full time. Especially a person full-time dedicated to the e-Refinery institute and taking on auxiliary tasks is seen as a great addition to the institute.

In the interviews, financial resources in the form of funding is mentioned as a driving factor for the development of a shared vision. Funding from industry and governmental funding drives universities into a certain research direction. As said by interviewee 5: *"I think funding facilitated the shared vision here. If there are more activities towards the attraction of funding, so people will be more connected to the e-refinery and be more connected to the same goal"* - Furthermore, interviewee 8 acknowledges the role of politics in driving companies to invest in certain research or not: *"The politics drove companies to invest money in certain parts of research. And it is then also important for universities to sort of guide the vision and make it possible to actually work on it, right"*

Table 62: Financial and human resources within the e-Refinery institute

Interview	Quote
1	When we talk about scaling-up, we also talk about manpower and human resources, and then we run into a limited budget. I think we're slowly started to feel the limited budget, maybe also partly due to the crisis
2	There is a lot of financial incentive for going into this direction, and that financial incentive exists because other people have said, you know this is very important for the world and the government should give us money and big companies should give us money. A lot of people who work for e-Refinery didn't make those deals you know, they got hired afterwards, they are not really on the forefront making big moral decisions.
4	I cannot judge about the financial resources, but regarding the human resources I think Delft is excellently qualified with the people they have on that subject
5	This could certainly be improved. - Both human and financial resources? - Both I think funding facilitated the shared vision here. If there are more activities towards the attraction of funding, so people will be more connected to e-Refinery and more connected to the same goal So I think having a person dedicated to e-Refinery, arranging meetings, also doing the job of approval, program manager, ring industries. Kind of trying to help to put people together and putting ideas together. I think that kind of person is missing.
6	- Which human resources would you really like to add at e-Refinery? - Dedicated people that do this maybe full-time and not part-time
7	I'm neutral about this. It is rather important, but at the same time, it's not all at once. It's a big goal and if you wanted to do that instantly you need millions, and that's not the amount we can find in one go.
8	I have no clue what to place here [regarding financial resources] I believe we have different people working on the project, which is actually quite nice because everyone knows something

5.3.6 Knowledge sharing

In the survey the statement on knowledge sharing is rated with a 4.44 out of 5 on the presence scale and a 4.78 out of 5 on the important scale. One of the main ideas behind e-Refinery is knowledge sharing and the sharing of ideas. This is also a driving factor for researchers and industry to participate in the institute. The quotes from the interviews regarding knowledge sharing are shown in Table 63.

The interviewees were all content with the level of knowledge sharing and the way this is formally organized within the e-Refinery institute, such as meetings, presentations and symposiums. The only one concern mentioned by members is the level of sharing knowledge and ideas in informal places. The interviewees mentioned that before the COVID-19 pandemic there were also sufficient informal interactions at for example the coffee corners and the social drinks, but since the pandemic this had decreased drastically: *"so before maybe there were a little bit too many [informal meeting moments], but now there are basically zero"* - interviewee 9. Also interviewee 2 mentioned missing the informal meeting moments and the value it has for their research: *you collaborate with people when you have a beer with them afterwards and you see people and you talk about stuff and hear 'yeah I work on this idea' and then you decide to talk about that more.* During the interviews it was noticed that this type of informal contact moments were especially important for the PhD students involved in the e-Refinery institute. Those moments were places to find others involved and to start collaborations. With the current COVID-19 pandemic and the shift to more online contact and meetings, it becomes harder for the PhD students involved to find collaborations. This is also acknowledged by interviewee 8: *We lately had a discussion because for PhD's it gets a bit tricky because for me when I started it was very easy to learn what every-body was doing and to find collaborations. You talked to people and you know. Now everything is online.*

Table 63: Knowledge sharing between the members of the e-Refinery institute

Interview	Quote
4	I'm a little bit in doubt what to answer, but let me walk you through my though process. The people go to the lectures, they listen and they come up with good questions. So there is certainly exchange, but I cannot oversee to which extend people communicate, shared knowledge, share frustrations and exchange information with each other behind the scenes
5	This is an ongoing activity, there are some biweekly meetings that each members is presenting the most updated results and sharing the new findings with other members.
7	There are frequently gatherings, presentations and discussions at which this is done. There are also internal symposiums and such things, and there are several interrelations where people informally discuss and internally share information
8	We do have lectures once a month, but before we had more like, really interactions within the TU Delft. We had meetings ad lunch presentations from industry, that was quite nice.
9	We have this meetings so there is always the change to share ideas. Unfortunately these are like once a year and last time we were showing our research in like 15 minutes or something.

5.3.7 Caring about same issues

In the survey, the statement regarding caring about the same issues is rated by the interviewees with a score of 3.11 out of 5 on the presence scale and with a 3.67 out of 5 on the importance scale. Table 64 shows the quotes of the interviewees regarding caring about the same issues.

The most mentioned reason for the difference in rating is the existence of different interests within the e-Refinery institute. The members involved in the e-Refinery institute have multiple interests, such as for example also profiling themselves scientifically, which can at times be more personally more important compared to the e-Refinery interests.

Table 64: Caring about the same issues

Interview	Quote
2	It's hard for me to guess what other people care about, I assume they care
3	I cannot really answer this
4	I always have the feeling that a lot of people, especially who are in the initial phase or the first 50% of their career, feel the necessity to profile themselves scientifically in their own field. Of course the societal profiling also plays a part in that, and makes that they want to cooperate with e-Refinery. But to which they are committed to help someone from another department with their research by shifting their own research line, I don't know.
6	I think so as well, of course not everybody has the same kind of concerns, but depending on the kind of people and research, everyone has a different opinion on this. But I think we do agree on many of the shared issues we have
7	In general we care about the same issues, and I think that is rather important. However, some look at the problem a bit more focused on the application, while others are more scientifically interested. But that's not such a big deal when you're working towards the same goal.
9	We are dealing with issues like global warming and environmental change of course. About research issues specifically what you find hard exactly about experiments, maybe not, but the same issues in the sense of global warming and environmental issues: yes of course

5.3.8 Ownership over the project

In the survey, the statement about ownership over the part the interviewees do for the e-Refinery institute is rated with an average of 4.5 out of 5 for the presence and an average of 4.44 out of 5 for the importance. Since these numbers are very close together, it can be seen that there are no real issues in this aspect.

Table 65 shows the quotes regarding ownership from the interviewees. Having ownership over the part they do for e-Refinery was also mentioned by some interviewees as a driving factor for being motivated to work for e-Refinery and ownership was also mentioned to be a prerequisite for participating.

Table 65: Perceived level of ownership amongst the members of the e-Refinery institute

Interview	Quote
2	I definitely feel I have ownership over what I do.
3	I cannot really answer that, they don't own anything about what I do and I don't own anything about what they do, so we share the knowledge at the moment
4	For me personally I can do exactly what I want
7	I for sure have ownership and for me it is important. There are some people that find this less important, especially when they are a bit earlier in their career it might be easier to have a bit less ownership
9	I have the ownership and that is shared with the e-Refinery community and with Shell because they are part of the funding.

5.3.9 Motivation and commitment

From the interviews it was clear that all interviewees were motivated to work towards the goals of the e-Refinery institute. In the survey this factor was rated with a 4.67 out of a total of 5 points, so the motivation is clearly present in the e-Refinery institute. The quotes regarding motivation for the project are shown in Table 66.

There is also an interplay between the development of a shared vision and the motivation of the members. A shared vision, or shared values, motivate others to join the institute and to work towards the e-Refinery goals. This is confirmed by interviewee 5: *"- These shared values of making the world more sustainable, do you think that is a motivation for other's to join? - Yes definitely "*. While interviewee 1 acknowledged that motivation is also coming from the way e-Refinery organizes people around a goal: *"- We have people with a lot of skills and when you want to execute a project, you put it together a project with people with different skills. - Does that influence the development of a shared vision as well? Because it's not ordered from higher up but from your own initiative? - Yes I think it's a good thing, because the motivation is there (...) We organize people around a goal."*

Table 66: Motivation of the members of the e-Refinery institute

Interview	Quote
1	- We have people with a lot of skills and when you want to execute a project, you put it together a project with people with different skills. - Does that influence the development of a shared vision as well? Because it's not ordered from higher up but from your own initiative? - Yes I think it's a good thing, because the motivation is there (...) We organize people around a goal.
2	Generally for me personally it is the fact that e-Refinery is essential working towards an ethically good thing, there is a morally positive outcome at the end. It wasn't really the deciding factor for me, but it was a bonus. I can feel good about what I do.
4	Yes I'm motivated, it is one of the reasons why I'm still connected to the TU Delft.
6	- These shared values of making the world more sustainable, do you think that is a motivation for other's to join? - Yes definitely
7	For sure I agree, and it's important as well
9	yes I'm motivated

5.3.10 Interaction with other members

In the survey, the level of interaction was rated with a 3.78 out of 5 on the presence scale, while the important scale got an average rating of 4.22. Table **??** gives an overview of the quotes regarding the interaction between the members in the institute. Overall, the interviewees were quite content with the amount and the set-up of the interactions planned by the e-Refinery institute. However, there is still room for improvement, especially in the area of interactions that lead to real collaboration and stimulates working together on projects. Especially the interviewed PhD students declared a need for more interactions. This goes also hand-in-hand with the lack of informal interactions, previously discussed in Section 5.3.6.

Interviewee 6 also mentioned the interaction as a driver for the development of a shared vision: *"The time to brainstorm and to say: look this is what we're doing and this is what others are doing, and this is what the future is probably going to be and so forth and so forth. So yeah workshops and discussion, that is what helps. "*

Table 67: Interaction between the members of the e-Refinery institute

Interview	Quote
2	Yes I meet with a few people, mostly because my part has a lot of overlap with other people I would say there is sufficient [interaction] but there is definitely room for more Whenever we have proper e-Refinery meetings, which haven't been as frequent as we would have liked, but whenever we do, there is always sort of getting everyone up to speed on the current state. A lot of these meetings are something we missed in the last year, we don't really collaborate with people when they give a presentation

3	Yes the interaction, that is good.
4	The interaction is well organized with colloquiums, we have it twice a year, or at least one general meeting at which people share their work in an informal way and they can present and discuss, so that's a strong point.
5	The interaction is only limited to presentation, so people are coming from industries to academia to share ideas and to share results but still what is missing is really the initiatives for doing projects. I think it happens once in a while, but in not a very systematic way and not everybody is involved
6	- Were there any factors that really helped in getting a shared vision? - Yes I think we had a couple of workshops, and I think that really helped. (...) The time to brainstorm and to say: look this is what we're doing and this is what others are doing. And this is how the future is probably going to be and so forth and so forth. So yeah workshops and discussions, that is what helps.
7	There are regularly meetings, presentations and discussions at which that [sharing knowledge and views] is done.
8	We have lectures once a month, but before we also had more like, really interactions within TU Delft. We had meetings lunches, presentations from industry. That was nice. We lately had a discussion because for PhD's it gets a bit tricky because for me when I started it was very easy to learn what everybody was doing and to find collaborations. You talked to people and you know. Now everything is online and they started working on a website so PhD's can see who is working on what I think it is mostly also due to corona, so before that was for me a short period. So now the interaction is also lacking sometimes. I think it would be important to do that at least a little bit more
9	Sometimes they are really really far away from each others, the topics, and maybe if we have this type of talks at the theater [a symposium were everyone presented their work] it was even a little bit easier to communicate because after the talk you could interact with someone and have a better and more clear vision Of course this pandemic is not helping in this interactions because we are forced to follow the rules of social distancing

5.3.11 Shared vocabulary

In the survey, the statement regarding a shared vocabulary is rated with a 3.67 out of 5 for the presence, while the importance is rated with a 4.22 out of 5. Table 68 show the quotes from the interviewees regarding a shared vocabulary. Most interviewees agreed that there is room for improvement regarding the way people interact with each other and the scientific language that is used. Even though all e-Refinery members communicate on a scientific level, there is still some differences between the way researchers from different fields talk and the language they use.

Table 68: Shared vocabulary within the e-Refinery institute

Interview	Quote
2	There are quite a few different fields covered in the e-Refinery institute, and the things is, the stuff I do with the modelling, we use sort of different terms, like if someone comes up to me and comes with x-Ray spectroscopy, well I can't even say the word, let alone talk about it, and than you have the different groups in catalysis or something that are all be talking about these structures
3	I think quite good actually
4	We're dealing with three faculties, well four faculties, which are the technology, policy and management faculty, electrical engineering, mechanical engineering, and chemical engineering. What I notice is that the language that electrical engineers use, regarding energy security and such, is a very abstract engineering language. They talk more in the the frequency domain then in the time domain, and I feel like the applied chemists and chemical engineers don't always pick that up, and vice versa the same. When chemical engineers start talking enthusiastically about their science, the mechanical engineers mentally drop out. This is a bit of a universal problem within the TU Delft.
6	So e-Refinery is also a multidisciplinary project and what happens is that every discipline has it's own kind of language and priorities and so on, but that really improves over time.
7	There are some people on the more fundamental side, the small scale of the electro-chemical side, who use different terminology then the people from the engineering side
8	This is a bit tough right, because e-Refinery is so big that like of course people working on electrolysis use a little bit different terms then battery people
9	It is harder to please everybody because they may have different background in knowledge and maybe different scientific background. You have to find the right balance in being clear but not being like low level.

5.3.12 Communicating on the same wavelength

In the survey, the statement regarding communicating on the same wavelength is rated with a 3.89 out of 5 for the presence, while the importance is rated with a 4.38 out of 5. Table 69 show the statements regarding communicating on the same wavelength. Overall the interviewees saw no big differences in how different members communicate with each other. There are some members more theoretically focused, while others are more focused on application. Furthermore are some more scientifically driver, while others more driven by societal issues. However, these gradations in which people talk and work within e-Refinery are not perceived to be a problem for the institute.

Table 69: Communicating on the same wavelength

Interview	Quote
2	We are all in this same level of theoretical or applied (...) I think overall we're on the same wavelength
3	yes certainly, in a manner, yes.
4	I don't think they do. It is difficult enough though. (...) I think everyone tries their hardest but it is quite difficult.
7	You could look at it very scientifically, focused on content, or more applied, focusing on solving the climate issues. I think for most members those two are connected. They think it is scientifically interesting, but also feel the importance to solve a societal issue. I don't think there is a member focused on only one of the two, but there might be some gradations
9	If you say wavelength as in goal and purpose, yes. It is CO_2 reduction we are doing.

5.3.13 Previous relationships

In the survey the positive influence of previous relationship was rated with a 4.28 out of 5 on the present scale and with a 3.71 out of 5 on the important scale. The interviewees that already knew members before joining the institute, all agreed that this had a positive influence on their decision to join. Furthermore, already established relationships helped in the initial phase of the institute to shape the institute and to develop the shared vision. From the survey can be seen that even though this factor has been acknowledged to have a positive influence, it is not perceived as a very important factor in collaborations.

Table 70 shows the quotes related to the previous relationships.

Table 70: Previous relationships between members of the e-Refinery institute

Interview	Quote
1	I worked closely together with [name] and I sat down for a day, maybe one and a halve day and we sat down with roughly 20 people from Delft and from other universities and we talked about the three subjects we perceive to be very important (...) and this eventually resulted in one, or two years later, the e-Refinery project
4	Good and personal work relationships help a lot
6	It made the decision to join e-Refinery quite easy
7	You already know you can count on the people and this establishes a relationship of trust within the collaboration
8	I already had a lot of discussions with other PI's that were not from my department or faculty who work on something related but a little bit different and that really helped in shaping the research questions and getting the knowledge and those were good discussions.

9	One of my colleagues was part of the project so I already knew her so I could talk with someone already there (...) I could understand a little bit how it goes, how many talks do we have, hos everything is going

5.3.14 Trust

In the survey the statement regarding trust has been rated with an average rating of 4.56 out of 5 on the presence scale and a 4.89 out of 5 on the importance scale. All members agree that trust is important in projects where research is done. Overall the interviewees trusted the other members of the institute. Furthermore, in a discussion with interviewee 7, it was mentioned that trust is one of the implicit shared values within e-Refinery and within universities in general. This is not often made explicit, but it might be a good idea to once in a while also talk about this subject more explicitly, especially with junior researchers. The quotes regarding trust are shown in Table 71

Table 71: Trust between the member of the e-Refinery institute

Interview	**Quote**
2	I like to think that I can trust them, I've been given no reason to distrust them. I think very least through the nature of sort of controlling the separate project, so there is a level of industry involved as well and everyone is very careful with information as well so no one is going to publish unfinished work and steal anything from you.
3	I trust the other members? Ha-ha what a question, yes good yes.
4	I really trust the people and their competencies that work with e-Refinery and yes it is very important as well
7	I think especially towards the junior members, the PhD's involved, some might thing 'this is my research and I'm afraid to share or loose my smart ideas, others might take them', you could make it more explicit what a good way is of working together and how we do that in a fair manner.
9	Yes of course otherwise it would be harder to keep working.

5.3.15 Respect and appreciation for work

From the survey it was clear that the interviewees were content about the respect and appreciation they got for their work. The average rating was 4.44 out of 5 for the presence and was rated a 4.56 out of 5 for the importance. The quotes regarding respect and appreciation for the work are shown in Figure 72

Table 72: Respect and appreciation for work within the e-Refinery institute

Interview	Quote
2	it is definitely respected if you're giving it the correct respect it deserves and nothing more. I know that the stuff I have done isn't the best thing in the world and when you told me it was, I wouldn't believe you. When people sort of value your work it is very honest.
3	Good question, I don't know. I think so.
4	I'm a bit of a side player, but the times I did some things it definitely was appreciated.
7	Yes absolutely yes
9	Yes of course, it always is.

5.3.16 Collaborative environment

All interviewees were very positive about the e-Refinery institute and about working in this institute. Interviewee 2 mentioned: *"I enjoy the collaboration, I enjoy it a lot"*. Interviewee 7 also expressed positive feelings regarding the institute: *"Yes, I'm positive about the collaboration"*. This is in agreement with the results from the survey, where the presence of a positive collaboration was rated with a 4.56 out of 5 and the importance a 4.67 out of 5.

5.3.17 Drivers and barriers - other

Table 73 gives an overview of all other drivers for the development of a shared vision mentioned by the interviewees.

Table 73: Drivers for the development of a shared vision

Interview	Quote
1	A community has been created, we have lunch lectures at different levels. The contact between people is good, they talk amongst each other, so people really try to create this community. Also, they try to keep each other updated on progress and problems of which individual PI's [principal investigators] are responsible.
1	Communication is key, that's where it starts and that has been set up very well
1	Shell also gave a push, but they weren't the only one. [When setting up this institute] they looked around and saw multiple interested partners, which facilitated realising this initiative.
2	The shared vision is helped by people in the institute who make sure that everyone stays relevant to this final goal we're all thinking of.
4	Those factors are in the communication by the people that lead this institute. From the beginning they invested in getting everybody on board by communicating clearly about the program, asking good feedback, meeting sufficiently often. You need to create a new community and that asks for robust communicative investments.

7	I think especially intern there is quite some attention for the togetherness. And on the other side also external, there is a lot of attention for the climate issues and the energy transition
8	For me this is really nice because we have a lot of PhD's who are involved in e-Refinery and even though the you work on a lot of different projects, but because you meet under this -Refinery umbrella you feel like a team.
8	I think that everyone [PI's, PhD's and people from industry] was really concerned about where we are going and wanting to contribute and that is basically what everyone had in common and got them talking.
8	I believe it is also partly politics, so I think politics drove companies to invest money in certain parts of research, and it is also important for industries to sort of guide the vision and make it possible to actually work on it.
8	Someone needs to pay for it, so I think that paved the way I would say. And also the input from industry and also politics shaped the vision, I would say.
9	The most important thing is having the floor to chat with each other. Maybe even formally, but it is a way to get in touch and develop new skills and knowledge, this is what I think is most important.

Table 74 gives an overview of all other barriers for the development of a shared vision mentioned by the interviewees.

Table 74: Barriers for the development of a shared vision

Interview	**Quote**
1	People are very concerned about their own field and you notice that. For them, their field is very clear and they know a lot about it, but problems in other scientific fields, which are also there, it is very hard to measure that regarding their own. The tendency is to preponderate the things you know more about
1	I hope this will still come, that there will be more collaboration between researcher not only because there is a certain overlap of a certain subject, because that is obvious, but especially the insight that they are not able to solve all problems alone.
1	Especially the creative part, where people are around a whiteboard or a piece of paper and work together [is now lacking with COVID-19]
3	It is a big team, and people from different fields have different types of vision
3	It comes from the difficulty of having a shared vision. Everyone is expert in their own field, it is fine, but it is also not an easy thing to combine, combine to tackle one big case that is this idea.

4	In the ideal situation you would want to have a physical space were people regularly have contact with each other. The fact that this community is divided over, well, let say 3, 4, 5 different buildings, who also all speak their own language, scientifically, that makes it more difficult
6	So of course there are interactions planned and meetings and so on, but nevertheless I think, even though meeting online is quite good, but certainly when it comes to sort of having a shared vision and talking and so on, it is best to have it face-to-face in a room where you can brainstorm with your colleagues and so on
6	For some of the main people in e-Refinery it is a primary thing, but for me, and for most of us, it is not what I do on a day to day basis
8	During the lunch lectures we always met new people each month and even though we now have it on Zoom, it is not at all the same. So you have to work a little bit harder to know who is doing what and to form collaborations.
9	We work in quite different fields, so the topic is the same but there are several branches. So maybe people are in different departments and maybe because of the distance it is sometimes harder to find each other especially during corona times.

5.4 Critical node

The critical node is the end point of the second diamond and is the starting point for the third diamond of the triple diamond research method that is used for this thesis. Figure 53 shows the triple diamond research method and indicates the critical node in this research method. The critical node is distilled from the systematic literature review and the results of the interviews and the survey that were held in the second diamond phase of this research.

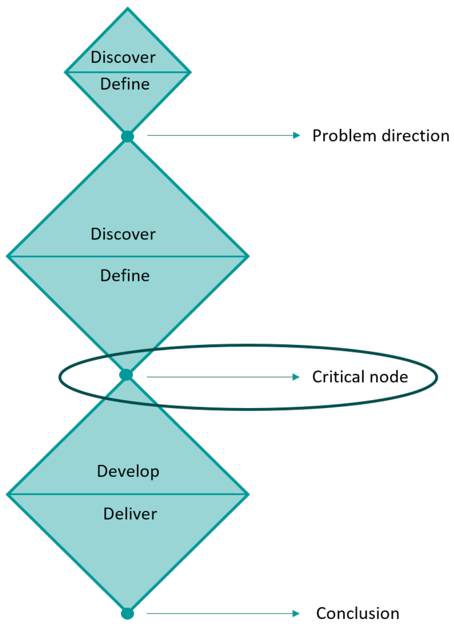


Figure 53: The triple diamond is used as the basis for this research. This step gives the critical node, the end point of the second diamond and the starting point for the third diamond.

To come to the critical node, the starting point is the survey that is held during the interviews. From the survey, a top six factors that scored the highest are taken into account, see also Figure 52. This six factors include the following: (1) the collective development of goals, (2) social capital (including financial and human resources), (3) interaction between members, (4) shared vocabulary, (5) shared concerns, and (6) shared overall goal.

It is decided to not further include social capital into the next steps of this research since this is not a factor that can by influenced by communication means. The resulting five factors are clustered into two pointers that form the critical node for the last phase of this research. In order to cluster the five factors, it is decided to use the concept of 'content' versus 'process' of interaction, in which content deals with the 'what' and process deals with the 'how' [45]:

1. Content-based interaction: including the content based side of the interaction between the members, so this pointer includes the shared concerns, shared issues and shared goal.

2. Process-based interaction: including how the communication and interaction takes place between the members. This pointer includes the amount of interaction between the members, the development of a shared vocabulary and the collective development of goals.

6 Design Phase

This chapter describes the design phase of this research, in which a communication tool is designed. The design goal of related to this chapter is formulated as followed:

> *The goal is to design an tool that aids e-Refinery members in the development of an adaptive shared vision.*

This goal is very broad and is further specified by making design criteria, which are presented in the first section. The design criteria are discussed and further evaluated during an interview with a PhD student related to the e-Refinery institute. In the following section, a combination of a literature investigation and brainstorming sessions lead to the development of a morphological chart. Based on this chart, three tool concepts are proposed, of which one is chosen for further development. The chosen concept is further developed and fine-tuned by holding multiple feedback sessions. Theories that are relevant in the development of the tool are presented. The chapter wraps up with a presentation of the final tool.

6.1 Design Criteria

The design criteria are divided into two categories: content-based design criteria and process-based design criteria. The content-based design criteria focus on the content of the communication, while the process-based criteria focus on how the interaction takes place.

The content-based design criteria are the following:

1. Development of shared goals: the overall goal of e-Refinery is already developed and communicated widely across the members. However, based on the shared issues and shared concerns, sub-goals could be developed collectively.

2. Sharing of concerns and care for similar issues: the tool should give the participants more insights in the concerns and issues that other's have within the e-refinery institute. This should give the participants more insight in which concerns are shared amongst the members of the groups and which concerns are more individual concerns. This should give more insight in which concerns should be prioritized and which should not.

The process-based design criteria are the following:

1. Shared vocabulary: The tool should aid in the development of a more shared vocabulary between the members of the institute. The tool should make the members more aware of the language they use and the language that is universally understood amongst the members, and the language that is more field-specific.

2. Interaction between members: The tool should stimulate more interaction between the members of the institute. Especially interaction between members that is not that straightforwards should be stimulated, so interaction that is not directly focused at working together because there is a need to work together, but also working together because it might be beneficial. Another aspect is the informal interaction, since from the interviews it became clear that especially this form of interaction can be increased.

3. Collective development of goals: The tool should aid in helping the members to develop goals more collectively.

6.1.1 Relation to the e-Refinery institute

In order to get more insight in the five above mentioned criteria and how they relate to the e-Refinery institute, an additional session was planned with a PhD student involved in the e-Refinery institute. This section shows the outcome of this session, including quotes in italics.

Within the institute, a difference can be made between individual goals and collective goals. There is an overall goal for the institute, defined in the initial phase of the institute, when the e-Refinery institute also consisted of much less people. This overall goal is a big part of what defines the institute and the vision of the institute, so in that sense there is not much flexibility or adaptability in this overall goal, which also does not pose a problem at this moment. However, how to reach this overall goal, the road to get there and the sub-goals that need to be defined, are much more uncertain, constantly in development and allow therefore as well for more adaptability and molding. Therefore, the collective development of shared goals should mainly take place in the development of these, more individual, sub-goals that are part in the road towards reaching the overall vision of e-Refinery. In this group, especially the PhD students are an interesting group, since they are the group that does most of the research work. Most of them work on such an in-depth level and on such a specific part within the institute, the link towards their research and the overall vision of the institute might not always be that visible or straightforward. Especially for other's involved in the institute, this link might not always be that clear. This is also suggested by the PhD student: *The e-refinery project is quite wide and so there can sometimes be, between one project and another one, great differences. In terms of PhD projects as well. So that [connections between projects and e-Refinery] is not always [clear], it can be somehow related, but it depends on the subject itself. I'm more of an experimentalist, but if you deal with somebody doing modelling for instant, then the connection is a bit harder to find. It can always be linked to a project, but it can be somehow difficult.* Therefore, this is one aspect that should be paid attention to when talking about the goals. The link between individual research goals and the overall vision of the institute should be clear for each member, not only regarding own research but regarding the research of other's as well.

Another part of the shared vision is the shared concerns. This relates to concerns related to the overall goal of the institute that are shared between multiple members of the institute. Not all concerns are shared with multiple members, there can also exist concerns related to own research or related to other aspects of collaboration. It is important to get insight in these concerns, and how these concerns to own research goals and collective goals. For the PhD students involved in the e-Refinery institute, it becomes clear that the main concerns exist in two areas: (1) regarding the PhD track and process itself and (2) regarding the content of the research. Concerns regarding the PhD track and the process itself, are often shared amongst other PhD students, but less often with supervisors or others. Concerns related to the research itself are discussed between PhD students amongst each other as well as with other colleagues, however it is not structurally integrated in e-Refinery's meetings. Relating to concerns regarding the research, the following is mentioned: *Well the problems in research life are always kind of personal. Because you have to reach your goals, your research and the outcome, and what is good about your research. The rest is a bit underneath. Because what you show for the e-refinery, because you have little time, you show the tip of the iceberg, you show what is good, but the rest underneath, your worries and that kind of stuff, you can share with colleagues, your friends and family, but not during the e-Refinery community meetings.*

The development of a shared vocabulary can related to use of certain words, definition and jargon, but underneath there is also a layer of a shared understanding of how research is performed. This layer underneath relates more to a general understanding about methods used in different types of research, and to a broad understanding of the topic itself. This is also mentioned in the interview: *No it is not only jargon but sometimes the topic of the research itself. Because you're* *just not familiar* An example is given of a misunderstanding in a presentation: *Something that happens usually is, they have model and an equation, and you may wonder, who is this guy that developed this kind of equation? What is the basis of that? What are the terms? Even the letters, what is that Greek letter? Sometimes that is something that is hard to understand because I have no background in that topic.*

When asked what types of interaction are lacking or would be valuable, it was mentioned: *brainstorming sessions, dealing with problems, discussions, share ideas. Especially maybe with some other post doc's or other researchers, some people maybe a little bit more experienced..* Other research to have this sessions with are mostly found through connections and through networking. To summarize it, the interactions that are needed should be focused on the content, content-wise they should go in-depth on the subject, and they should be interactive sessions (versus presentation-like meetings).

Regarding the collective development of goals, it is mentioned that within the process of defining PhD tracks and making goals for PhD research, there exists a tension between the TU Delft and e-Refinery. Research performed by PhD students within the e-Refinery institute, is performed at the TU delft and therefore also bound to regulations, procedures and policies of the TU Delft. Furthermore, for PhD students involved in the e-Refinery institute, there is also a tension between the individual aspect and the collective aspect, since a PhD project is quite an individual process. *We as PhD'ers we also have to think about this TU delft procedures and as PhD'ers we have to think also, unfortunately, about ourselves. Therefore neglecting sometimes a little bit this aspect of collectiveness. But this is just how it goes, we have this contract which we have to sign with our supervisor. We have to decide our pathway within this four years. And this also requires individually in stead of collectiveness.*

6.1.2 Link with uncertainty

The design criteria can be seen as rooted in the complexity of the project and therefore increasing the uncertainty in the project. In the general introduction, five areas of uncertainty as mentioned by Ward and Chapman (2001) have been listed. These five areas of uncertainty include: (1) estimate of project parameters, (2) basis of estimates of project parameters, (3) design and logistics, (4) objectives and priorities, (5) relationship between project parties.

The development of shared goals is closely related to uncertainty in objectives and priorities. The structure of goals and the link between individual goals and collective goals is quite complex within the e-Refinery institute, giving rise to the level of uncertainty in the objectives and priorities as well.

Concerns within the e-Refinery project can be seen as a result of uncertainty in the institute. From the previously described session with a PhD student involved in the e-Refinery institute, it was seen that concerns mainly manifest itself in two areas: (1) regarding the PhD track and process itself and (2) regarding the content of the research. Where the first type of concern is mainly rooted in uncertainty in the relationship between project partners and uncertainty regarding the peripheral matters of the project. The second type of concern, concerns regarding the content of the research, can be a result of uncertainty in either of the five areas distinguished by Ward and Chapman.

The need for content-based interaction can be seen as rooted in uncertainty with regard to design and logistics, and objectives and priorities. Uncertainty in the area of design and logistics relates to uncertainty in the project deliverables and process of producing things. Uncertainty in objectives and priorities is related to this, but focuses more on the clarity about project objectives and relative priorities and trade-offs. The need for more content-based interaction, such as brainstorming sessions, and sessions to tackle issues in the project, indicates that researchers experience uncertainty with regard to the content of their project and seek for a way to deal with this, resulting in the demand for more interaction.

It can be seen that the design criteria of collective development of goals is rooted in uncertainty in the relationship between partners. The tension between the TU delft and the e-Refinery institute, as well as the tension between the collective part of the e-Refinery institute and the individual part of a PhD, form a barrier in the collective development of goals. Uncertainty in the relationship between these partners is the underlying cause of the tension that can be seen.

The design criteria of the development of a shared vocabulary can be seen a method or tool of increasing the adaptivity of the e-Refinery institute. Highly adaptive organizations tend to have to a greater extend a shared vocabulary and to a less extend agreed policies [56].

6.1.3 Conclusion

The results of the interview in Section 6.1.1 are used to further sharpen the design criteria.

- Development of shared goals: the tool should be able to show the link between individual goals and the overall e-Refinery goals.
- Sharing of concerns and care for similar issues: the tool should give more insight in which (content related) concerns are present for the individual researchers and which of these concerns are shared between researchers
- Shared vocabulary: the tool should at the minimum help in the development of a shared vocabulary, on the level of terms, jargon and equations. At best, the tool also aids in the development of a shared understanding of research approach, but this is more complex and might not be feasible for the tool. However, the tool could raise awareness in the existence of research approaches and methods.
- Interaction between members: the tool should stimulate the members to have more interactive content-based session or lower the bar for establishing connections based on shared goals or shared concerns.
- Collective development of goals: since there are quite some factors in the collective development of goals, it is quite difficult to intervene in this process. Therefore the tool should give more insights in the process of developing goals.

6.2 Literature investigation and brainstorm session

The design criteria are put in a morphological chart where solutions are found for the design criteria. These solutions are based on literature and on intuition. A literature investigation, using a snowballing method, for the two content-based criteria and for the three process-based criteria has been performed. A brainstorming session has been held with an expert in the field of education in order to fill in the intuition part of the morphological chart. This section first gives an overview of the literature investigation, afterwards an overview of the brainstorming session is performed. This section finalizes with the morphological chart.

6.2.1 Sharing of concerns and care for similar issues

To gain more insight in how issues are often dealt with, the issue attention cycle by Downs (1972) can be used. This cycle consists of five phases [24]:

- **Pre-problem phase** The initial phase of a problem, but the problem is not yet widely known among the total group of people.

- **Discovery/enthusiasm** The problem starts getting more attention and becoming more wide-spread amongst the group of people. In this phase, more attention is paid to the problem as well. In this phase, enthusiasm to solve the problem is rising and there is often still quite some optimism to solve the problem.
- **Realization of costs** In this phase, the costs needed to solve the problem slowly start to become more clear. This includes not only financial costs, but also the time, effort and knowledge of the people involved.
- **Decline of interest** Once costs of solving the problem have become more clear, interest is slowly declining over time. This is either to people realizing how difficult it is to solve the problem, or simply because they loose interest in the problem, or due to other, newer, problems appearing that ask for attention. Often it is a combination of the above mentioned factors.
- **Post-problem** The final stage is when most attention for the problem has disappeared. In this last phase, often only a small group of people still focus on the problem and deal with it. Another possibility is that in this phase the problem has mostly been solved or is solved too such extend that it is no longer a priority to pay attention to.

The issue attention cycle best describes issues that are in the pre-problem phase only shared by a small portion of the total group or problems that are shared amongst this small group, but not necessarily amongst the total group. In the discovery/enthusiasm phase however, the whole group starts paying attention to the problem and it is shared amongst the total group and becomes a group-problem.

The issue attention cycle is shown in Figure 54. Especially the enthusiasm gap is important to pay attention to. Once the level of attention decreases in the third phase, the 'cost realization phase'. In order to successfully solve the problem, it is important to pay more attention to it especially in this phase.

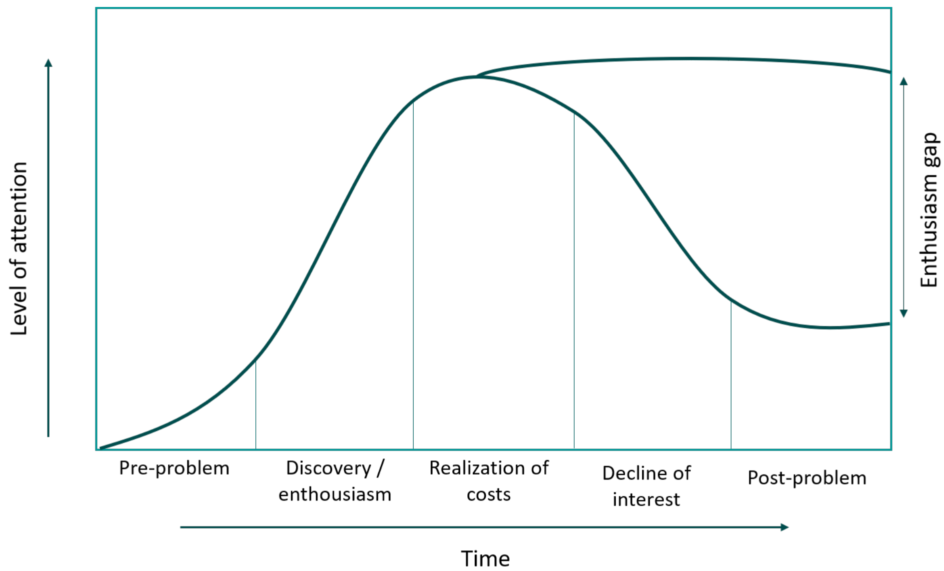


Figure 54: Issue Attention Cycle (adapted from Haase (2017) [35]

6.2.2 (Collective) development of shared goals

In literature there are already some techniques discussed and available for collective goal setting. These techniques include:

- Delphi groups [17]
- Leadership-based approach by Bennett et al (2018) [6]
- ASPIRe model by Haslam et al (2003) [36]

the Delphi group method can be seen as a form of expert brainstorm session. In this method, a selected group of expert respondents (the Delphi group) goes through a series of questionnaires, surveys, etc. and a facilitator leads this process and oversees the responses. The members of the Delphi group are selected on their expertise or knowledge. The process consists of the following rounds [17]:

- Selection of the members (Delphi group)
- Questionnaires, surveys, etc. are send to the Delphi group. The group does not meet, but they keep separate to avoid the negative affects that face-to-face discussions may have
- The Delphi group members are asked to assess and explain a problem and predict the future state of an issue.
- The facilitator is responsible for controlling the interactions. The facilitator selects the relevant information and filters out the irrelevant content.
- After processing, the results are send back to the members of the Delphi group
- The members make a new decision, based on the new information they gathered by the rest of the group. This process is repeated until consensus is reached

The ASPIRe model takes the personal (the attributes that makes us unique) and social identities (who are we as scientists) of the members of an interdisciplinary research team as the basis to start from. These personal and social identities are recognized to contribute positively to the organization and provide opportunities for the success of the organization. Personal and social differences are an important feature for the organization. The ASPIRe model, originally created by Haslam et al (2003) consists of four phases and a fifth phase is included by Cvitanovic et al (2020) [36, 18]. The extended ASPIRe model is shown in Figure 55.

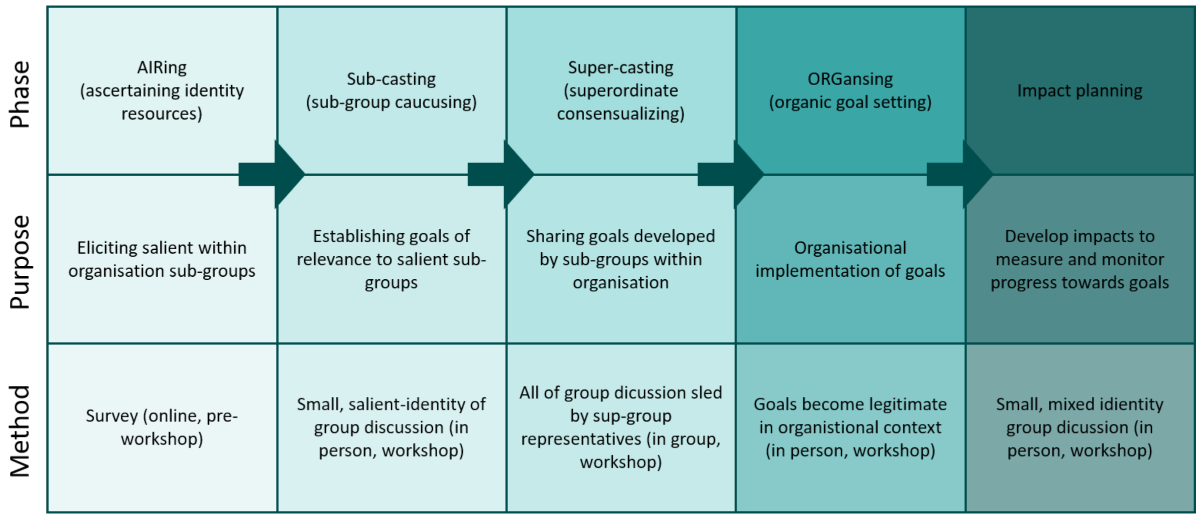


Figure 55: Extended ASPIRe model (adapted from Cvitanovic et al (2020) [18])

The phases in the ASPIRe model consists of the following phases [36, 18]:

- **AIRing phase**: the goal of this phase is to identify the relevant identities that each individual member of the organization has and to distinguish those from the identities that are not perceived to be self-relevant. The outcome of this phase consists of an increased knowledge of the social identities that are part of the organization and are relevant to the work-related activities performed within the organization. The task at the end of this phase is to form sub-groups within the organization that minimizes the perceived differences between members in the sub-groups and maximizes the differences between the subgroups [36]. The methods suggested by Cvitanovic et al (2020) to walk through this phase are online surveys or online pre-workshops [18].

- **Sub-casting phase**: in the second phase, the sub-groups of the first phase gather for discussion and debate. The goal of this phase is threefold. Firstly, the subgroup identifies and agrees shared goals. Secondly, they identify barriers that keeps them from achieving these goals. Thirdly, the contribution to the development of a shared subgroup-identify that is relevant to the goals should become clear. In this stage, the focus is on building a collective strategy, but also the differences between subgroups is made explicit and is recognized. One of the concerns in this phase, is that the groups start polarizing from each other; that there is emerge 'out-group' feeling towards members that are not part of the subgroup. This is one concern that should be paid attention too.

- **Super-casting phase**: The next step involves bringing all the subgroups together (or a representative of each group) to engage in further discussion and debate. This phase consists again of three purposes similar to the previous step. Firstly, the members should agree upon shared goals. Secondly, the barriers to achieve the goals should be made explicit. Thirdly, it should be made explicit how these activities aid in the development of a shared organizational identity. This organizational identity should be organic, able to change over time, and should allow and incorporate differences in subgroup identities.

- **ORGansing phase**: In this phase, strategic decisions have to be made in relation to the direction of where the organization is going. leaderships becomes more important in this phase and decision-makers should base their decision on the outcome of the previous phases, leading to organic goal setting. Even though leaders and decision-makers have a more prominent role in this phase, other members should continue to be (and feel) involved as well.

- **Impact planning phase**: The final phase, the impact planning phase, is added to the framework by Cvitanovic et al (2020) and involves reflecting on the goals. This includes monitoring the progress and the impact.

The leadership-based approach by Bennett et al (2018) [6] includes the following steps for the development of collective goals:

- **Step 1** writing down a vision statement for the collaborative initiative

- **Step 2** ensuring each member is able to reproduce this vision statement, each member should have the ability to see the bigger picture

- **Step 3** all members are encouraged to write down their own (research) goals and the connection of their own goals to the vision statement or the bigger picture

- **Step 4** discuss of each member the accomplishments and challenges, also discuss how this relates to the overall vision statement of the institute.

- **Step 5** each member is encouraged to take ownership over their own contribution to the overall bigger picture

- **Step 6** Besides ownership, each member is also encouraged to accept responsibility and accountability over their accomplishments and failures, without blaming others.

As can be seen, the model does not only involve the development of collective goals, but it also gives room to discuss challenges of each member, so also the shared concerns is an integrated aspect of this leadership-based approach.

6.2.3 Shared vocabulary

Monteiro and Keating (2009) discuss three aspects in which misunderstandings can take place when there is not a shared language within an interdisciplinary research team [19]. These aspects include:

- **Different understandings of validity of knowledge** Often different forms of evaluating data are use amongst different fields, which can be a source of misunderstanding in multidisciplinary teams.
- **Partial understanding** Accepting that there is partial understanding, is essential in managing uncertainty and in working with experts from different fields.
- **Interpretive discipline-crossing** When working with experts from a different field, it is possible to overestimate or underestimate the expertise of others, which can lead to misunderstandings.

In order to reach a more shared vocabulary, the model of remediation, compensation and dispensation can be used to gain more insight in the process of developing a vocabulary. This is a model often used for dyslexic children, children having a hard time developing their language skills, but gives also great insights in developing a more shared vocabulary on other levels of interaction. The model, shown in Figure 56, consists of three ways to cope with a difficulty in developing language [85]:

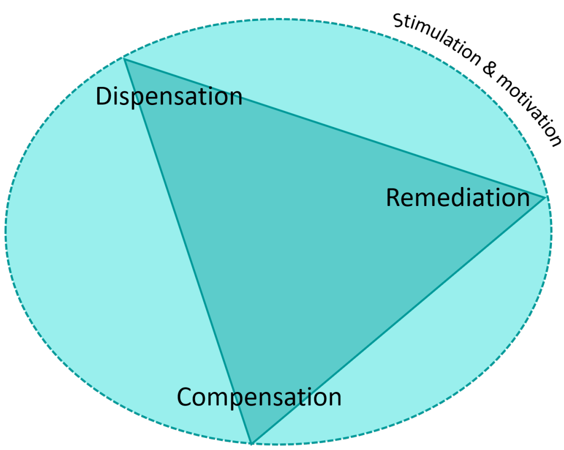


Figure 56: Interaction between the three strategies to cope with the development of a language: (1) remediation, (2) compensation and (3) dispensation, with stimulation and motivation visualized as the boundary conditions for applying the coping strategies (adapted from Smeets (2011) [85])

1. Remediation: relating to the process of improving the vocabulary.
2. Compensation: relating to the process of taking measures to make the vocabulary easier.
3. Dispensation: relating to the process of omitting parts of the vocabulary

The three ways shown in the figure are not to be seen separately from each other, as separate options to increase language skills, but are often used in interaction with each other. So not only remediation, developing new skills and improving current knowledge, but also compensation, taking measures to simplify language or terms, as well as dispensation, omitting certain terms or words that are maybe irrelevant or unnecessary to learn. Around these three ways, there is a circle with 'stimulation & motivation', there should always be an inner drive from the members to actually work on the development of a shared language and a stimulation to do so (which could be a function of the tool).

6.2.4 Interaction between members

E-refinery is presenting themselves as a knowledge sharing institute. They do not only collaborate in order to achieve common goals, they also focus on learning from each other by sharing knowledge. The model by Morley and Cashell (2017), see Figure 57 shows the overlap between collaborative behaviour and learning behaviour [59]. E-Refinery is operating mostly in the area of 'shared behaviour', incorporating elements of both collaborative behaviour and learning behaviour. So interaction that takes place in the e-Refinery institute, should also take place in both these areas. From the interviews, it became clear that interaction on the 'learning behaviour' side is taken care of sufficiently. Interaction focused on the collaborative side could be increased.

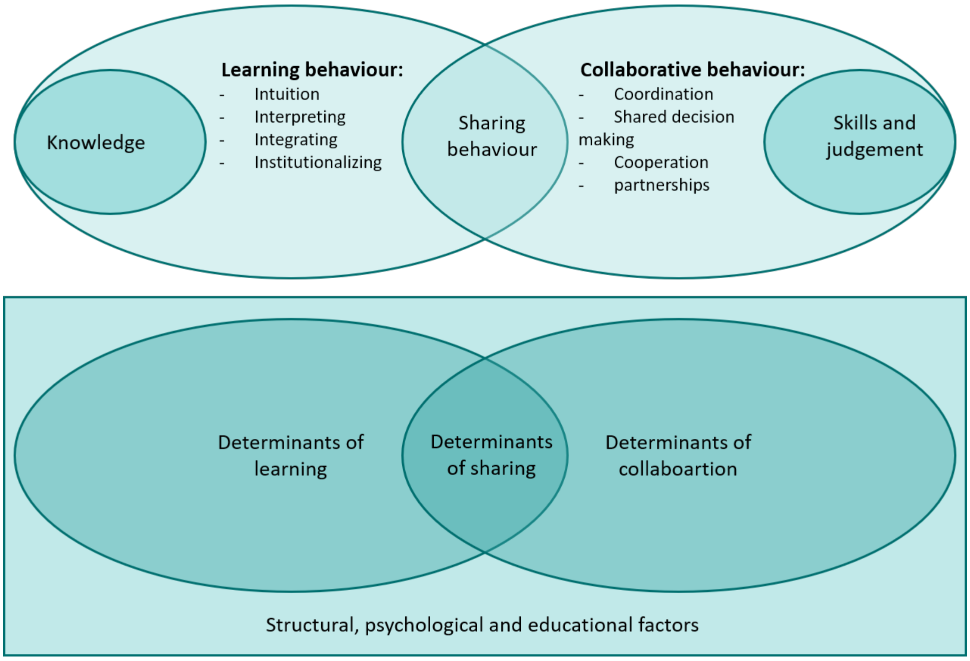


Figure 57: Overlap between learning behaviour and collaborative behaviour

6.2.5 Brainstorm-session

A brainstorming-session for the five design criteria of the tool has been held with an expert in the education field. This session was held in order to fill the intuition part of the morphological chart. An overview of the outcome of the brainstorm session is shown in Figure 58

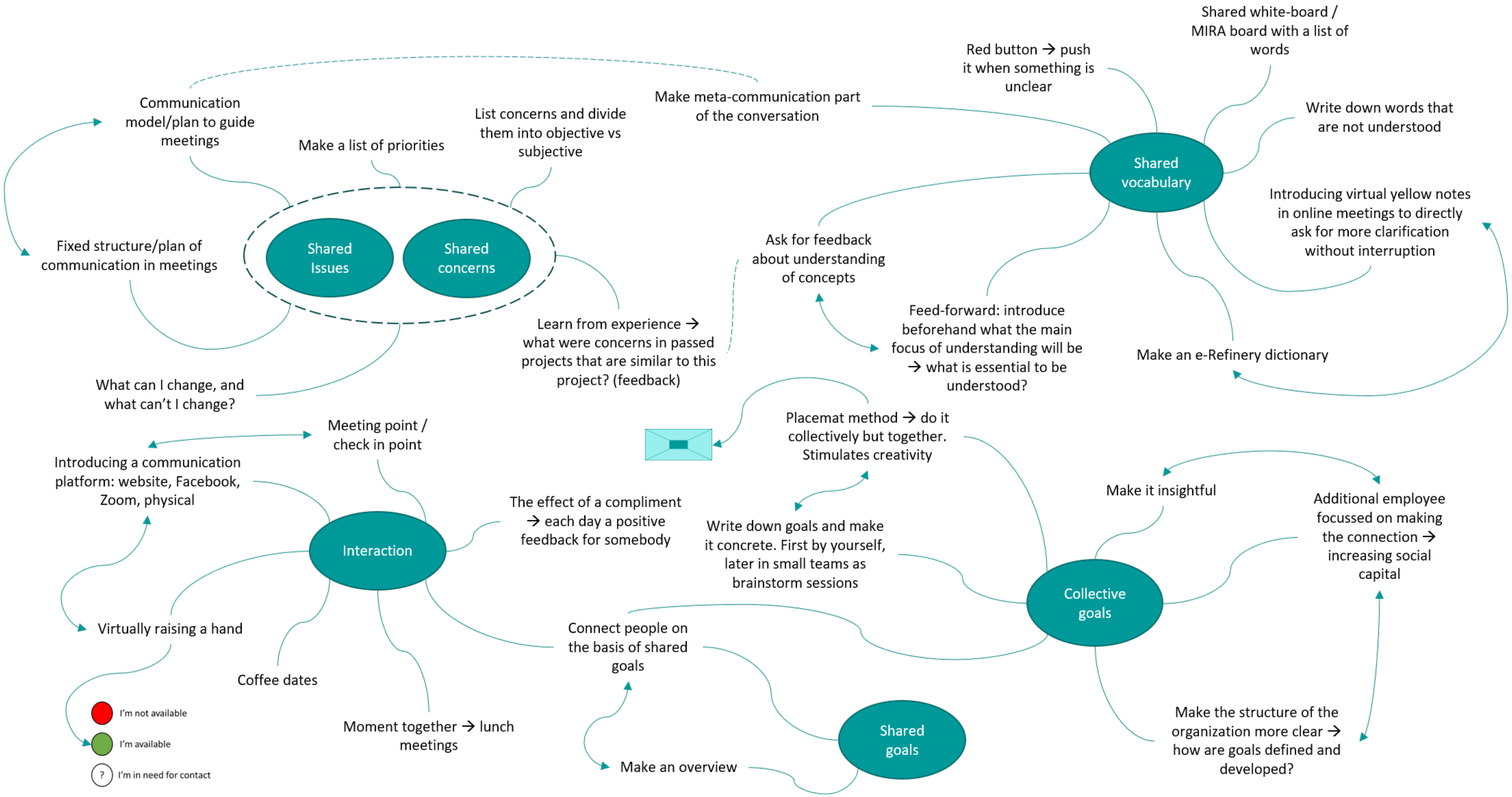


Figure 58: Brainstorm session for the five different functions of the tool

6.2.6 Morphological chart

Both the literature investigation and the brainstorm-session are put into a morphological chart, which forms the basis for the three tool concepts. The morphological chart is shown in Figure 59.

Design criteria	Theory	Theory	Theory	Intuition	Intuition	Intuition	Intuition	Intuition
Sharing of concerns	Issue attention cycle	Agenda-setting theory ⚡	-	Part of communication plan to guide meetings ☾	Objective vs subjective concerns	Learn from past projects	List concerns and connect them to goals ★	Prioritize concerns
Development of shared goals	ASPIRe method ☾	Delphi groups	Leadership-approach	Make an overview and find overlap	Connect people on basis of shared goals ★	Make the structure of the organization more clear ⚡		
Shared vocabulary	Monteiro and Keating's aspects of misunderstanding ★☾	Smeets' model of dispensation, remediation and compensation	-	interruption button: press when something is unclear ⚡	Develop a dictionary ★	Feedforward: what is the main focus of understanding? Feedback: what is clear and what isn't? ☾	Virtual yellow sticky notes to ask for clarification without interruption ★	
Interaction between members	Model of learning behaviour vs collaborative behaviour ☾	-	-	Introduce a virtual communication platform ★	Connect people on basis of goals	Virtually raising a hand (e.g. showing who is available, who isn't)	Plan physical meeting moments ⚡	
Collective development of goals	ASPIRe method ☾	Delphi groups	Leader-ship approach ★	First define goals individually, later together in teams	Placemat method	Give more insight in the structure of developing goals		

★ Concept 1 ☾ Concept 2 ⚡ Concept 3

Figure 59: Morphological Chart

6.3 Concept formation

In order to come to the final tool design, first three different concepts are suggested. These concepts are designed by combining the solutions presented in the morphological chart. Each concept should include at least one solution for each of the design criteria. The three concepts generated in this step are a virtual platform (concept 1, marked with a star in the morphological chart), communication road-map (concept 2, marked with a moon-sign in the morphological chart), and role-defined card game (concept 3, marked with a lightening bold in the morphological chart).

All three concepts are discussed with a graduated Science Communication student and with their feedback improved and further developed.

6.3.1 Concept 1 - A virtual platform

The first concept is a virtual communication platform. This concept can be integrated with the website that is currently being developed. The virtual platform can be integrated in this website an additional feature of the website that is only accessible for the e-Refinery members.

The virtual communication platform includes a Wikipedia-style dictionary for difficult words. There should be a functionality that allows the users to mark words they are not familiar with with a question-mark, other users can then click on this word and add a small description to it. This interactive process should help the members in learning each others' language and jargon.

The platform also allows for a more informal way of contact between the members of the institute. Especially the PhD-students could benefit from this, the virtual platform could aid as an accessible way of reaching out to other PhD-students.

Features	• Increasing contact between members of the institute • Facilitating informal contact • Wikipedia-like system for difficult terms
Users	• All members of the e-Refinery institute • Different features of the platform might be more or less applicable for different members
Strengths	• Virtual aspect of the tool makes it easy accessible for each member, no need to be physically present • Can be used both individually as well as collectively • Is accessible for all members and can be tailored to meet specific needs for all members • Easily adaptable • Can be integrated with the website that is currently under development
Weaknesses	• Needs clear direction on the 'how to use it' aspect • Might need a facilitator, a person dedicated to keep track of what happens on the virtual platform to bring it into the weekly meetings • Takes initiative to bring the online aspect to the offline way of working

Figure 60: Overview of concept 1, the virtual platform

6.3.2 Concept 2 - Communication road-map

The second concept is a communication road-map. This communication road-map should aid in giving structure to meetings and help the members of the e-Refinery institute to actively think and discuss certain parts of the collaboration. The communication road-map could be based on the ASPIRe-model for the development of collective goals. The communication road-map should also include a step that explicitly discusses the concerns and issues that are currently experienced by the members.

The communication road-map also includes a feed-forward and feed-back mechanism for the development of a more shared language. In the road map, there is a moment to discuss the question 'what is the main focus of understanding for this meeting?' to outline which parts are essential to be understood by all the members. At the end of the meeting, a feed-back moment is included, focusing on the question: 'Is the essence understood? What was clear, and what wasn't?'.

Features	• Gives direction on how to guide meetings • Integrates the current attention points of collaboration in a structured way • Makes meetings more predictable, gives grip.
Users	• Primarily useful for the board and PI's of the e-Refinery institute
Strengths	• Can be used both online and offline • Easily adaptable, e.g. time-needed per step, new aspects can be integrated in the route of needed, or aspects can be omitted.
Weaknesses	• Might be less applicable for PhD students involved in the e-Refinery institute • Needs a facilitator to use the road-map, needs expertise

Figure 61: Overview of concept 2, the communication road-map

6.3.3 Concept 3 - Role defined card game

The third concept is a role-defined card game. This card game includes cards in two different categories: process and content. The process cards are meant to let the members think and discuss the more process related side of the collaboration, so amongst others shared vocabulary, the interaction between the members and the collective development of goals. The content cards relate to the content of the collaboration, the shared goals and the sharing of concerns.

This role-defined card game can be used in meetings or other sessions were members work together. The card game consist of two phases. In the first phase each participants gets assigned one or more cards with 'who', 'how', 'when' and 'why' type of questions. They also get assigned a card regarding the process or content side of the collaboration. In the meeting, the members are responsible for bringing the statement or question to the attention. In the second phase, the cards are exchanged and each members now gets a different card. This members should give a short summary of what is said during this meetings regarding this card. The exchange of cards should also give an extra push to the participants see the importance of fully understanding everything that is said in the meetings, since in the end they have to be able to give a summary of a particular part of the meeting.

In order to help the members in comprehending each other and in being more aware of the language they use, a red-button that makes a sounds is included in this role-defined card game. This button can be pressed when the content becomes unclear, or when jargon that is not understood by everybody is used. This directly leads to an intervention and allows the members to discuss misunderstandings and as such develop a more shared language and shared understanding of concepts over time.

Features	• First phase: each members gets a card assigned with a question or statement regarding the functions. This members is responsible for bringing this point to attention in the meeting • Second phase: in the second phase, cards are exchanged to another • An intervention button as direct feedback system for misunderstandings
Users	• Used during meetings or discussions, accessible for all members of the institute
Strengths	• Concrete and tangible • Every members has an equivalency in role • Can be used to inspire the members, become more creative, and help them in moments when they are stuck • Gives a push to meet physically
Weaknesses	• Participants need to be physically present • Not as adaptable • Not easily integrated in everyday work live, more applicable for specific situations

Figure 62: Overview of concept 3, the role defined card game

6.4 Concept choice

The three concepts are scored on each design criteria with scores ranging from $--$ to $++$. The scores are shown in Figure 63. Concept one scores a $++$ on the design criteria of sharing of concerns since this platform allows members to share concerns with each other, but also allows them to react and discuss concerns via the platform. Concept two scores a $+$ on this criteria, since the sharing of concerns is integrated as a step in the communication road-map, so it is an integrated part of the session. However, it does only include the members that use the road-map in that particular session. Compared to concept one to concept two, concept one allows sharing and interaction on concerns between more members compared to concept two, explaining the difference in rating. Concept three, the role-defined card game, includes card related to the sharing of concerns and is therefore also sufficiently present in the tool and therefore scoring a +. However, similar to concept two, this tool only allows the members that currently use the tool to share concerns while concept one allows for more widely sharing.

Concept one is scored with a + regarding the shared goals. The platform especially allows the members to visualize the structure of existing goals and the relationship between these goals. Concept two is scored with a + regarding the shared goals. The road-map is focused on collective development of goals, which will lead to more shared goals over time. However, this road-map does not visualize and clarify the structure of existing goals. Concept three is scored with a + regarding the shared goals. Shared goals is one of the main topics that comes back with cards in the card game.

For the development of a shared vocabulary scores a ++ for concept one. The first concept allows members to develop a shared language in an interactive manner. Elements of both remediation (improving vocabulary) and compensation (taking measures to make vocabulary easier), as described in Figure 56, are present in this concept. The development of a shared vocabulary is scored with a +/- for concept two. This concept includes the development of a shared vocabulary using feed-forward and feed-backwards mechanisms. This especially helps creating more mutual understanding of key focus points, however, it does not strongly include more understanding on the level of terms, jargon, or equations. The shared vocabulary is scored with a +/- for concept three. The shared language is present in concept three with a red button that can be pressed. This allows for direct intervention and clarification, however, it does not aid in the development of a shared vocabulary over time.

Concept one is scored with a + for the design criteria relating to interaction between the members since the platform stimulates finding new connections and allows for interaction via the note-boards. However, the platform does not involve offline interactive sessions, these should be set-up with the initiative of the members themselves. Concept two is also scored with a + for this design criteria. This concept encourages members to come together and form interactions. However, this concept does not focus strongly on the PhD students involved, while this is the group that especially needs these interactive sessions. Concept three is scored with a ++ since this concept encourages the members to come together physically and to plan an interactive session.

Concept one is scored with +/- on the design criteria of collective development of goals. This concept has the potential to include this design criteria in the platform, however, it is a very difficult criteria to fully integrate in the platform. Concept two is scored with a ++ on this criteria, since this concept is build around the collective development of goals. It is fully integrated in the road-map. Concept three is scored with a - for this criteria since the collective development of goals is not so much integrated in the role-defined card game.

Design criteria	Concept 1	Concept 2	Concept 3
Sharing of concerns	++	+	+
Development of shared goals	+	+	+
Shared vocabulary	++	+/-	+/-
Interaction between members	+	+	++
Collective development of goals	+/-	++	-

Figure 63: Scores on each design criteria for all three concepts

The concept that is chosen for further development is the virtual platform. This concept integrates all five design criteria that were listed at the beginning of this chapter: (1) sharing of concerns, (2) development of shared goals, (3) shared vocabulary, (4) interaction between the members, and (5) collective development of goals. Furthermore, this concept allows all members to participate. Since especially the PhD students mentioned a need for more interaction and and this was also the group that is currently less involved in the collective development of goals, it is important that they are also able to use the tool. For this reason, it was decided to not further proceed with concept 2. Furthermore, the online aspect is quite strong within the e-Refinery institute. Currently there are not many options to meet physically due to the COVID-19 pandemic, but also when the pandemic is over, the virtual aspect of the institute will still be prominent. The different groups and researchers connected to the institute do not have a physical place to meet and are scattered around campus in different faculties. Due to this, and also taking into account that the e-Refinery institute is currently developing a website for the institute, it is decided that the virtual platform is the most suitable and appropriate concept for further development.

6.5 Feedback sessions

To come to the final tool design, an iterative process with four feedback sessions is used. The first session is done after the concept was chosen and held with a recently graduated Science Communication student. The tool is further fine-tuned based on this section. Afterwards, a second session is held with a PhD student involved in the e-Refinery institute. After iteration, a third session is held with a Science Communication student. In the fourth session, with another graduated Science Communication student, focused more on the visualization of the current structures in e-Refinery and the translation of that to the tool.

6.5.1 Session 1

After the concept was chosen, feedback on the chosen concept was asked from a recently graduated Science Communication student. This feedback included the following attention points:

- How do you stimulate the use of the tool? How do you make sure the members are intrinsically motivated to use the platform?
- How do you guide the tool? Do you need a facilitator? Does it run on itself?
- The technology acceptance model can be used in the designing of the tool: the members have to accept a certain (new) technology, what factors influences the acceptance of this technology?

6.5.2 Session 2

In this session, the current status of the website is first discussed. The website is currently under development, but a first concept is already shown to the e-Refinery members. This concept currently involves an overview of the full-professors and assistant professors, their background and the research they are performing.

The functionalities of the tool were explained to the PhD student and of each functionality the perceived added value was questioned, as well as the motivation to use this functionality. Regarding the platform itself, the PhD student was positive of the idea and motivated to go to the platform. The platform would especially be useful as open discussion platform to interact with more than one person. For one-on-one interaction, emailing or in-person contact was preferred, but for open discussions with multiple people, a platform would be interesting. Regarding the note-board functionality, in which members can post their goals and connect it to concerns, the PhD student was also positive and willing to use the functionality. The language function, to define terms or jargon, was also received positively.

The PhD student was also asked which additional functions would be interesting to add to the platform. It was said that a place to store files would be a good addition. In this place, people can share (poster) presentations, participation to congresses or conferences, paper publications or relevant papers. From the interview, it also became clear that the interesting part of the platform lies in the interaction between the functionalities. The connection between goals, concerns and the link with the language feature is what makes the platform interesting to go to. Therefore, being able to click from one feature to another is important. The platform should be easy and intuitive when navigating through the different functionalities, and the functionalities should be connected and integrated with each other, in stead of separate.

6.5.3 Session 3

In the third session, the tool was presented to a Science Communication student and feedback was asked regarding the current tool. Together with the Science Communication student, the functionalities of the tool were fine-tuned.

The first remark that came up was the push to get the members to the platform. In order to get the members to the platform, it should be approachable and accessible. This can be realized by making the platform easy and intuitively to navigate through different subsections. Furthermore, the members should come to the platform regularly, on a weekly basis. In order to achieve this, there should be a need or a push to go to the platform regularly. The current concept of the tool is operating on a strategic level, focusing on the shared vision, long-term goals and concerns related to this. The tool does not have functionalities regarding the operational level, relating to the more daily and weekly practises. To ensure that members come regularly to the platform, there should also be functionalities relating to the operational level. It is suggested to have a separate page for the sub-goals connected to the collective goal. On this page, updates regarding the sub-goals can be posted regularly. Suggestions for sub-goal page include a slider that indicates progress, a timeline of the project, and a to do list. Adding these functionalities makes the page more interactive for the users and gives opportunity to use the virtual platform more frequently.

In order to increase the interaction options and to also add an option for making new connections, the option for members to connect to a sub-goal is suggested. Members of the e-Refinery institute can put their name and contact information at the page of the sub-goal. They can also add a short text regarding their connection to the goal (e.g. doing research on this goal, or expert in this field of research, etc.) to indicate whether they actively do research in this area or whether they are experts in this particular field and are open to join discussion sessions.

It is also suggested to couple the language feature with the other features, allowing to make code-books for terms and jargon at the different pages.

6.5.4 Session 4

This session was conducted with a Communication Design for Innovation graduate. The session focused on visualization of the structure within e-Refinery and the translation of this towards the tool.

A pyramid structure is proposed to visualize the structure in the goals. The top layer represents the two overall goals. The layer underneath represents the collective sub-goals, research lines or research areas. The bottom layer represents the goals of individual researchers. Concerns can be related to goals of individual researchers, but can also be related to collective sub-goals in the middle layer. When concerns are similar or have a connection, this can be represented with a line between the concerns. A visualization of this structure is shown in Figure 64.

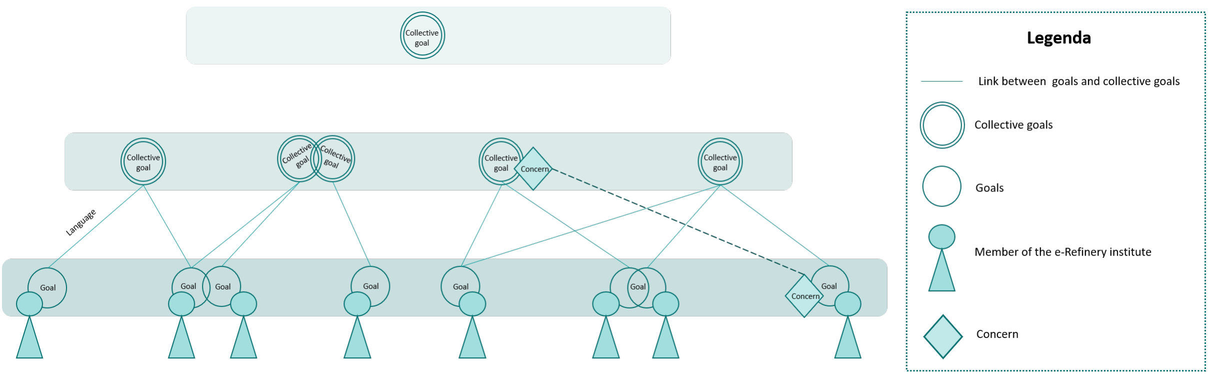


Figure 64: Structure of the goals

The second and third layer of the pyramid structure are shown in more detail in Figure 65. This figure shows how goals and collective goals are connected to each other. Each individual member formulates goals, which or often related to their research domain. There might be overlap in goals of individual researchers, which can be visualized by making the goals overlap.

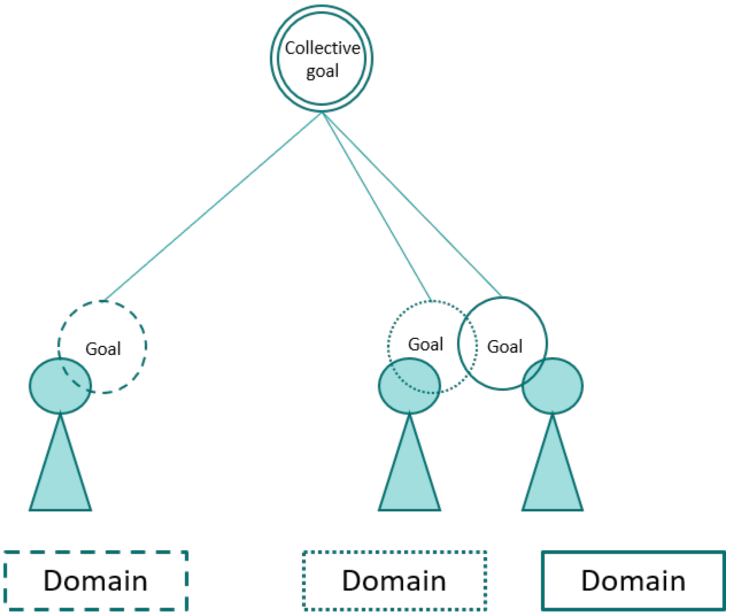


Figure 65: Connection between the members, their individual goals and collective research goals.

The relation between goals, collective goals and concerns from the perspective of the individual researcher is shown in Figure 66. A researcher is connected to their own goal, which is connected to a collective goal. In this visualization, the blue researcher has formulated one goal, connected this goal to a collective goal, and formulated one concern regarding their formulated goal. The yellow researcher formulated two goals, connected both to a collective goal and formulated one concern regarding the collective goal. The virtual platform tool forms the bridge between these researchers. The tool allows the members to visualize and make connections, based on similarities in goals of concerns.

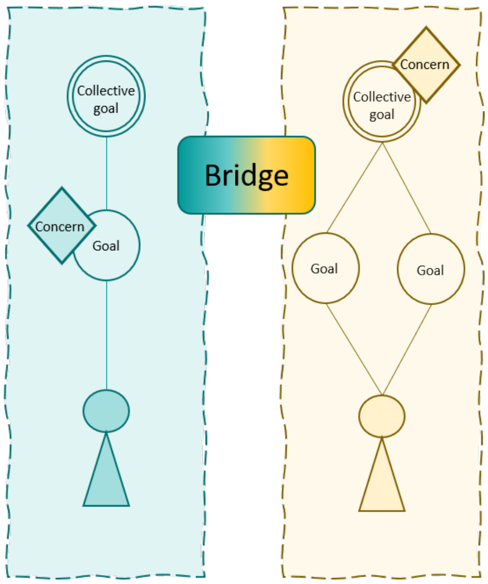


Figure 66: Relation between a collective goal, individual goal and researcher visualized. The virtual platform forms a bridge between different researchers

Members can have assumptions regarding the research and goals of others, which may or may not be correct. This is visualized in Figure 67. In this example, the blue researcher has the assumption that yellow is currently occupied with a certain collective goal. While in reality, yellow is currently more occupied with a sub-goal related to another collective goal.

The virtual platform encourages members to to make connections between goals and between concerns. This way, similarities, a connection of overlap can be visualized for the e-Refinery members. This is visualized in Figure 68. These assumptions can form the basis of discussion. If overlap is found between goals or concerns, this can be an initiator for further interaction in the form of for example brainstorm sessions or sessions relating to a shared concern.

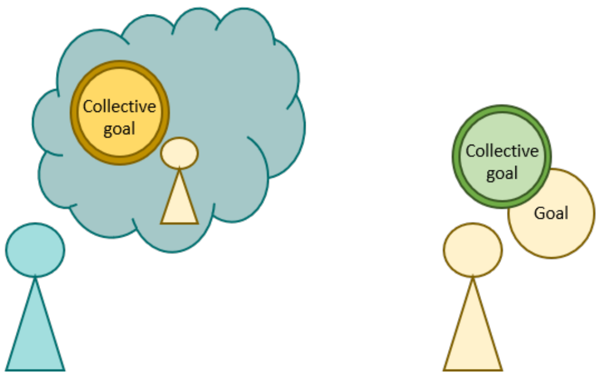


Figure 67: Assumptions regarding the research and goals of others exist between members of the e-Refinery institute.

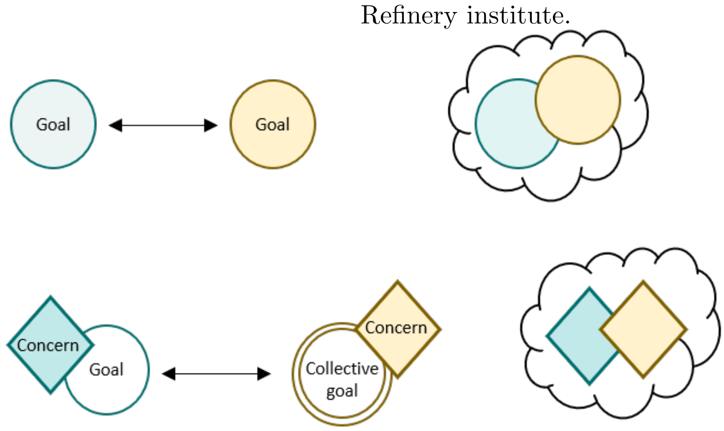


Figure 68: Connections between goals and concerns can be made

6.6 Theories relating to virtual communities

Virtual communities are defined as online social networks in which interaction takes place with the intent to share information or knowledge, which are often established on the basis of a common interest, goal or practise [13]. Virtual communities can have all different kinds of formats, known examples include Academia, ResearchGate or LinkedIN. The virtual platform developed in this chapter can also be seen as a form of a virtual community, with a format tailored to the needs of the e-Refinery institute.

Chiu et al (2006) identify knowledge sharing as a critical attention point for the success of virtual communities in professional settings [13]. In their research, they use the Social Capital Theory and the Social Cognitive Theory to evaluate the quantity and quality of knowledge sharing in virtual communities.

The social capital theory suggest that social capital influences the quality and quantity of knowledge sharing. Social capital includes the social network and the human resources embedded in this network. Social capital can be divided into a structural, relational and cognitive aspect. The structural aspect relates to the overall structure of connections between the different members. The relational aspect relates to the individual relationships between the members, including the history of the relationships. The cognitive aspect relates to shared interpretations and systems of meaning [13].

According to the Social Cognition Theory, the behaviour of an individual is shaped and controlled by the influence of their social network and the individual's cognition (expectations and beliefs). When relating this to knowledge sharing, it was seen that both expectations and self-efficiency where the two major factors for knowledge sharing. Self-efficiency relates to the level individual feel confident in their ability to share knowledge. When the confidence level is low, individuals are unlikely to share knowledge. Expectations relate to the expectations of both the individuals as well as the community. For example, strong ties with the community positively influences the knowledge exchange [13].

Figure 69 shows the relation between the Social Capital Theory and the Social Cognition Theory to knowledge sharing on virtual platforms.

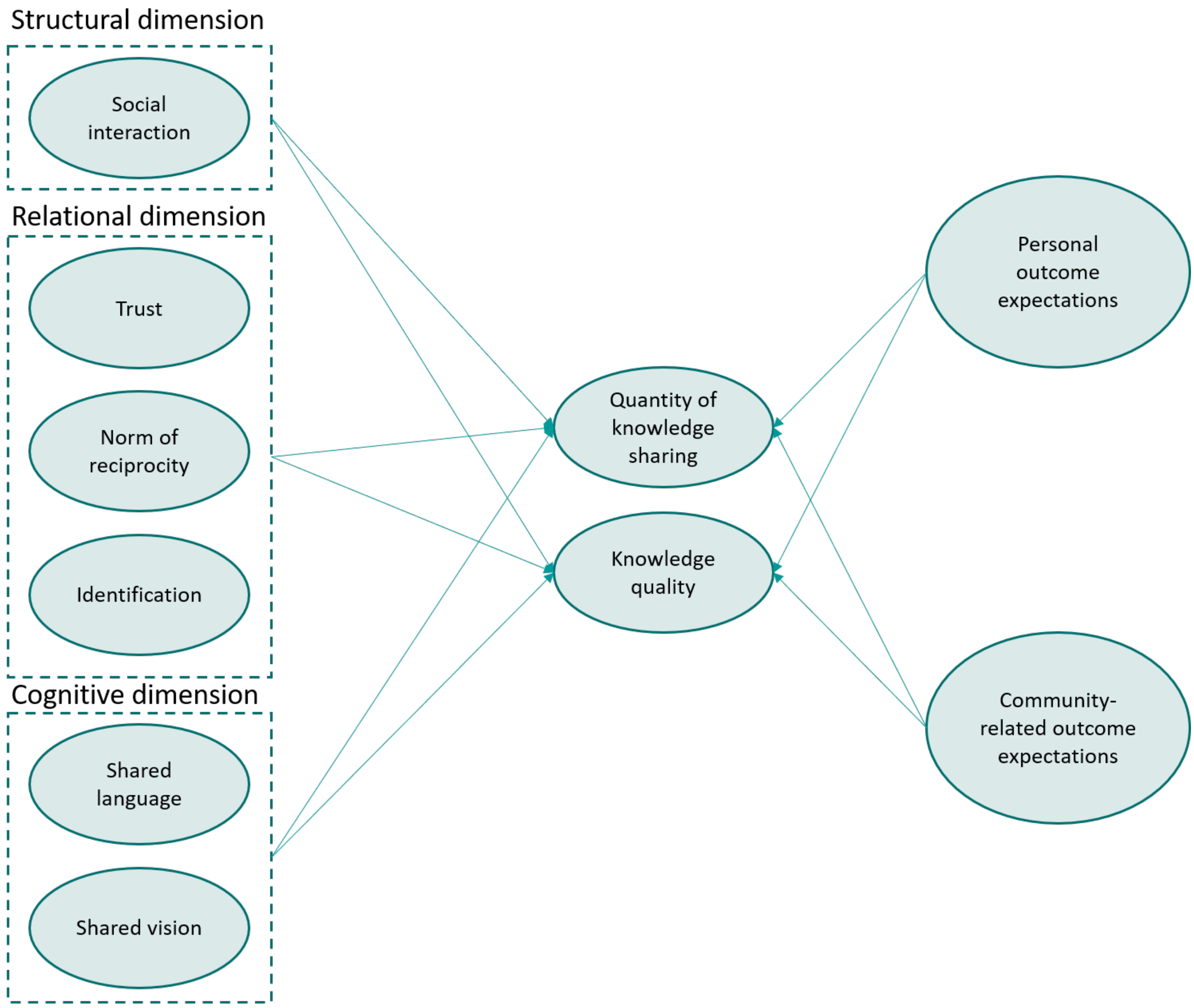


Figure 69: Model relating the Social Capital Theory and the Social Cognition Theory to quality and quantity of knowledge sharing on virtual platforms (Adapted from Chiu et al (2006) [13]

Another related theory is the Technology Acceptance Model, relating to the acceptance of users towards a new technology. An extended version of the technology acceptance model is shown in Figure 70 [86]. This model shows the interaction between the perceived usefulness of a technology, the ease of use and the willingness to use the technology. Both the perceived usefulness and the perceived ease of use influence the attitude of the user, leading to more or less willingness to use a certain technology. For the final tool design, this means that both the perceived usefulness and the perceived ease of use should be high. The members of the e-Refinery institute should understand the usefulness of the tool and also perceive it to be useful for them and their work. Furthermore, the should also be easy and straight-forward enough in use.

The technology acceptance model is adapted by Teo et al (2003) to include characteristics of the virtual community, e.g. the information accessibility and the community adaptivity. Information accessibility refers to the type and amount of information that is available via the platform. Furthermore, it also refers the the availability and accessibility of the information, e.g. the way the information is presented and the ease of finding information. There should be a balance between the amount of information available, too little information does not serve the purpose of knowledge sharing, while too much information causes an overload [86]. Community adaptivity refers to the extend in which the members of the virtual community are able to adapt to the platform, e.g. the structure, the information content and related their needs to the platform. Community adaptivity allows members to have more control over the usage of the platform [86].

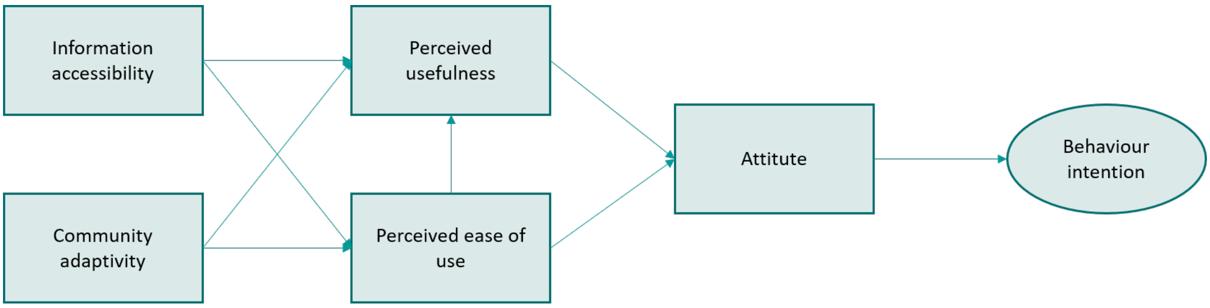


Figure 70: Extended technology acceptance model (adapted from Teo et al (2003) [86])

6.7 Testing of the tool

The tool is tested by asking two PhD students to fill in the sub-goal and concern feature of the virtual platform, in a similar manner as shown in Figure 80 and Figure 81. The PhD students are both connected to the e-Refinery institute and doing research that falls within the institute. The PhD students are referred to as 'PhD student 1' and PhD student 2' later on in this section.

The PhD students received a PowerPoint with the sub-goal and concerns format where they can fill in the two pages. The PowerPoint also included the guidelines for using the tool and the given example given in Figure 80 and 81. Afterwards, their feedback is asked in a feedback session where they mention positive and negative aspects of the tool. They can also mention which parts of the tool are very strong and which are the weak parts of the tool.

The filled in pages by PhD student 1 are shown in Figure 71 and 72. The names in the figures are changed to 'PhD student 1', 'PhD student X' and 'PhD student Y' to mark the notes of different people and to make the figures anonymous, however, the notes and other persons mentioned in the figures are real-life people working for the e-Refinery institute. The notes and concerns posted in the figures are also real-life examples of concerns, notes and remarks that have been made in the course of the project.

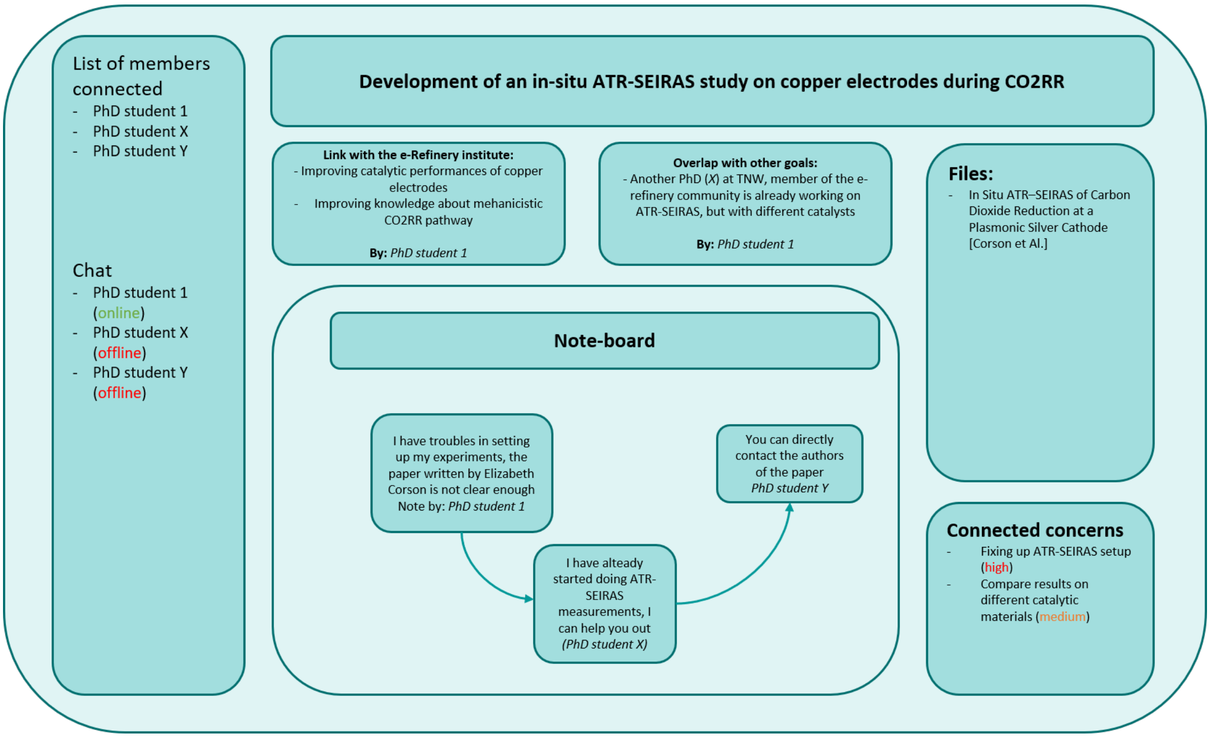


Figure 71: Sub-goal part of the virtual platform filled in by PhD student 1.

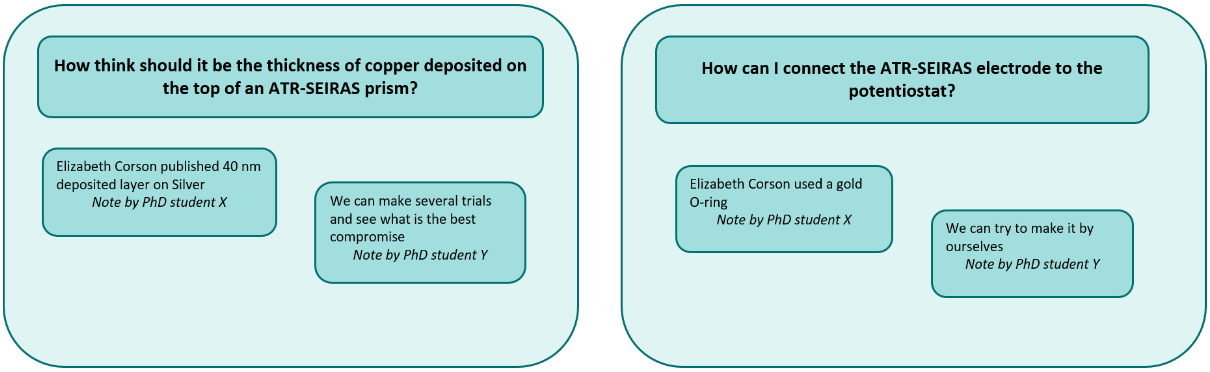


Figure 72: Concerns page of the virtual platform filled in by PhD student 1.

The filled in pages by PhD student 2 are shown in Figure 73 and 74. The names in the figures are changed to 'PhD student 2', 'PhD student X' and 'PhD student Y', and 'Prof' to make the figures anonymous and to indicate the notes of different e-Refinery members. The notes and other persons mentioned in the figures are real-life people working for the e-Refinery institute. The notes and concerns posted in the figures are also real-life examples of concerns, notes and remarks that have been made in the course of the project.

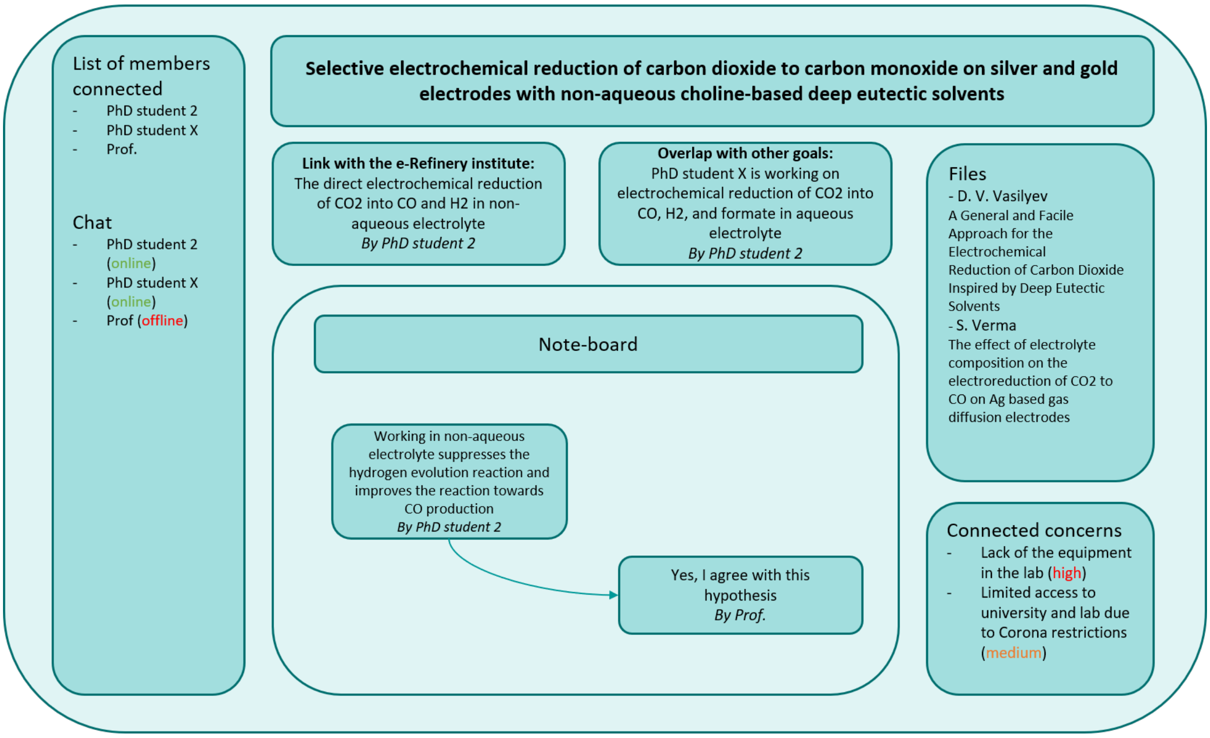


Figure 73: Sub-goal part of the virtual platform filled in by PhD student 2.

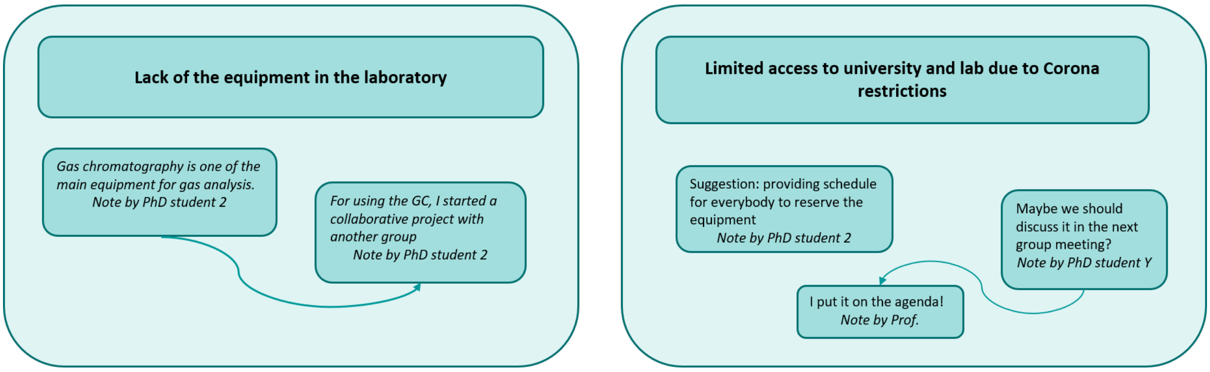


Figure 74: Concerns page of the virtual platform filled in by PhD student 2.

6.7.1 Feedback

Both PhD students were able to fill in all the boxes of the figures without too much trouble. With the instructions and the provided example, both PhD students were able to successfully fill in the sub-goal page and formulate related concerns. Both PhD students appreciated the example that was given and acknowledged that this helped them in filling in the figures.

Both PhD students found this platform to fit the e-Refinery institute. PhD student 2 mentioned the greatest benefit of the tool for the institute as followed: *when we define our sub-goals, we can find similar projects which are carried out within the e-Refinery institute. It could be a good starting point to become familiar with other projects and start collaborative projects with other members of the institute.*. PhD student 1 agreed that the virtual platform fits the e-Refinery institute, however, one concern regarding intellectual property was raised. The virtual platform should be something within the community itself rather than open to anyone, in order to protect the knowledge that is shared.

When asked if there were any missing functionalities or options, PhD student 1 mentioned that a list of everyone's projects, that is updated regularly, would be a great addition to the platform. PhD student 2 would like to have a list of equipment, material or software used to reach the sub-goal integrated in the virtual platform. This would include for example equipment that is used in a project, such as gas chromatography or lithography, or a list of used software, such as Aspen Plus or MATLAB, added to the sub-goal page of the virtual platform. This was suggested in order to facilitate collaboration and finding connections within the institute.

The strong points of the platform according to PhD student 1 are the ability to share ideas and projects, as well as the interconnection between other PhD students. PhD student 2 especially liked the concerns part of the platform. Both PhD students mention time-consumption as a potential weak point of the platform. When it becomes too time-consuming, it might be hard for PhD students to implement it.

Both PhD students were personally interested in using the platform. Especially because they think it's a great way to become more familiar with the projects of others within the institute. Both PhD students also think that the platform would be used by other members of the institute. However, this is also dependent on whether the platform is easy and clear enough to use and the platform should not be too time consuming.

6.8 Final Tool - virtual platform for interaction

This section describes the final tool that is developed. The tool that is chosen as most suitable is a virtual platform. This platform is not developed, since that is out of the scope of this thesis, but guidelines on what features this platform should have are developed, as well as visual representations of how this features could look like.

The final tool consists of multiple features. Those features are discussed and explained in this section. The features included in the virtual platform are:

- Shared vision visualization
- Virtual note-board
- Language feature

6.8.1 Shared vision visualization

The basis of the virtual platform is the visualization of the shared vision. The concept with the five different aspects of the tool is used for this. This should be integrated in a page where these aspects of a shared vision are visible for each member. The timeline below the shared vision is interactive and includes a slider which shows how the circles of a shared vision have changed over time for the e-Refinery institute. Show for example sliding from April to June could show an increase in awareness around the concerns (the circle becomes bigger) and a decrease in the awareness around the goals and ambitions (the circle becomes smaller). This feature could help the e-Refinery members to become more aware of how a shared vision is currently existing in the institute, making it easier and more straightforward to guide the direction.

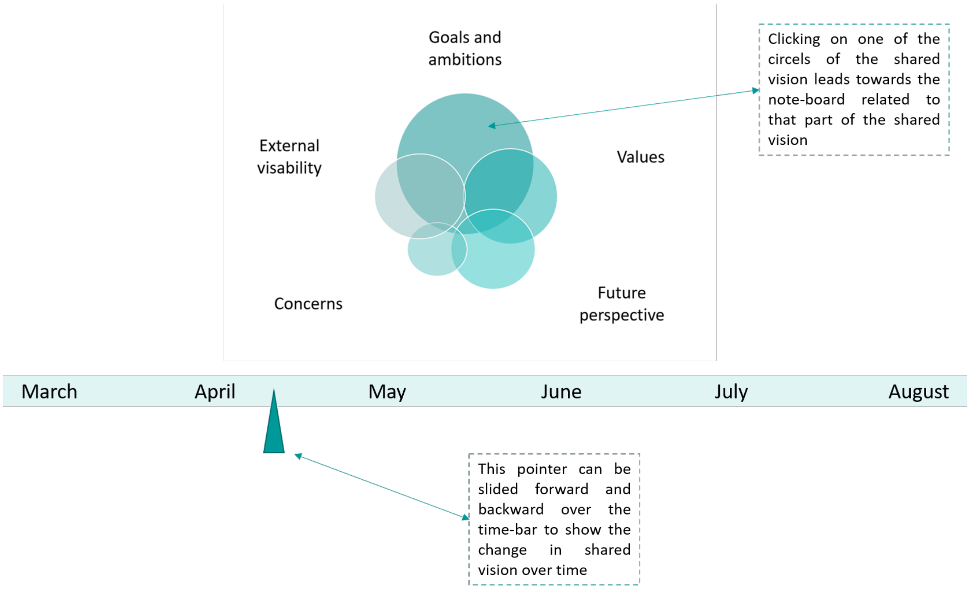


Figure 75: Shared vision visualized on the virtual tool

6.8.2 The virtual note-board

Clicking on one of the circles on the shared vision page leads to the first note-board, which gives an overview of the two main goals of the e-Refinery institute.

The e-Refinery institute formulated two collective goals [65]:

1. Design and construction of a 100-kW electrochemical testing device for the selective conversion of CO_2 into ethylene.
2. To develop a 100-kW thermal bench scale set-up of a Sabatier reactor for continuous methane production from CO_2 and H_2.

These two goals are the beginning page of the virtual platform. This overview forms the basis for the addition of collective sub-goals, which could also be formulated as research lines or research areas. It is up to the board and the principal investigators to add these collective sub-goals, research lines or research areas. A set-up for this is shown in Figure 76.

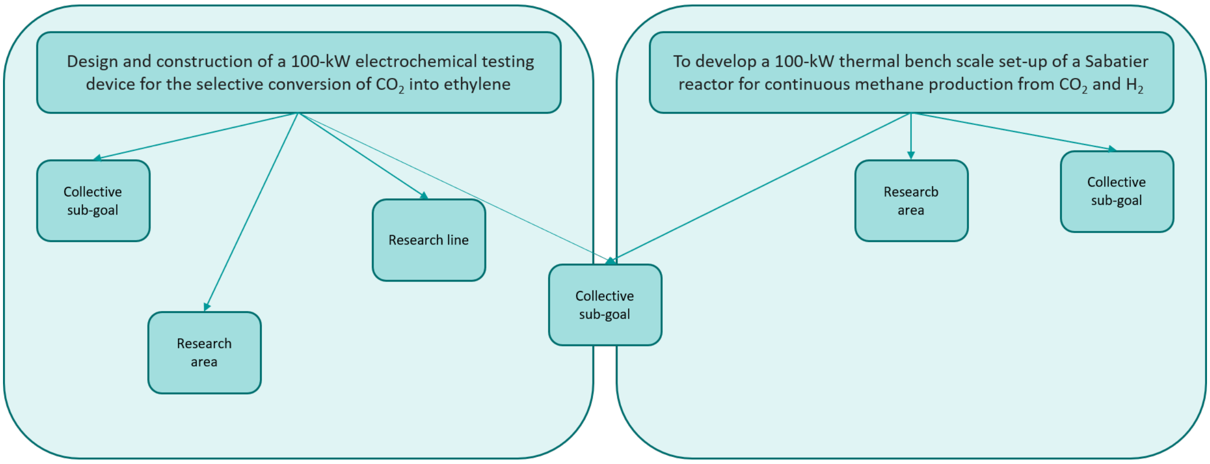


Figure 76: Overview of the first page, the beginning page, of the virtual platform

Individual research goals can be connected to the above mentioned collective sub-goals, research lines or research areas. This can be done by clicking on the block, which opens a new virtual note-board with a similar structure. This feature allows the e-Refinery members to post notes around this topic. In this note-board, concerns regarding the overall goal and regarding individual goals, could be posted as well. With arrows, the members are able to connect concerns to goals. This way, it is also possible to connect one concern to multiple goals, or multiple concerns to one goal. Clicking on the concern note leads to another page, a note-board related to that particular concern. In this note-board, members are again encouraged to post notes regarding this concerns, giving other's feedback or indicate whether they share this concern or not. Via both the note-boards related to the sub-goals and the concerns, members can find each other and connect with each other.

A visualization of how the collective goals note-board and the note-board for concerns could look like is shown in Figure 77.

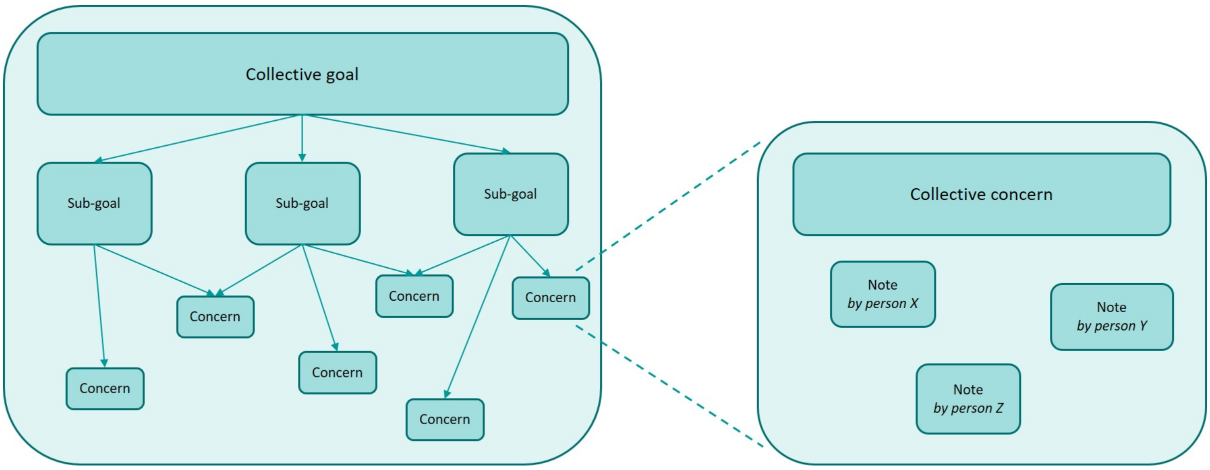


Figure 77: A visualization of how the note-board feature could look like on the virtual platform

It is also possible to click on one of the post-its with a sub-goal on it. This leads to a next page dedicated to the sub-goal. This page has a list of connected members. Members of the e-Refinery institute can put their name and contact information at the page of the sub-goal. They can also add a short text regarding their connection to the goal (e.g. doing research on this goal, or expert in this field of research, etc.) to indicate whether they actively do research in this area or whether they are experts in this particular field and are open to join discussion sessions.

The sub-goal feature also includes a progress bar, in which the progress of the goal can be updated. The files related to the goal can also be found on this page, as well as the concerns that are connected to this sub-goal. Clicking on one of these concerns leads to that particular page. The sub-goal feature also includes a box in which the link with the e-Refinery institute is described. Furthermore, a box with other related sub-goals is also included. In this box, other sub-goals that have a connection with this goal are listed. So when a line is drawn between two sub-goals in the overview page, shown in Figure 77, the connected goals pop up in this box.

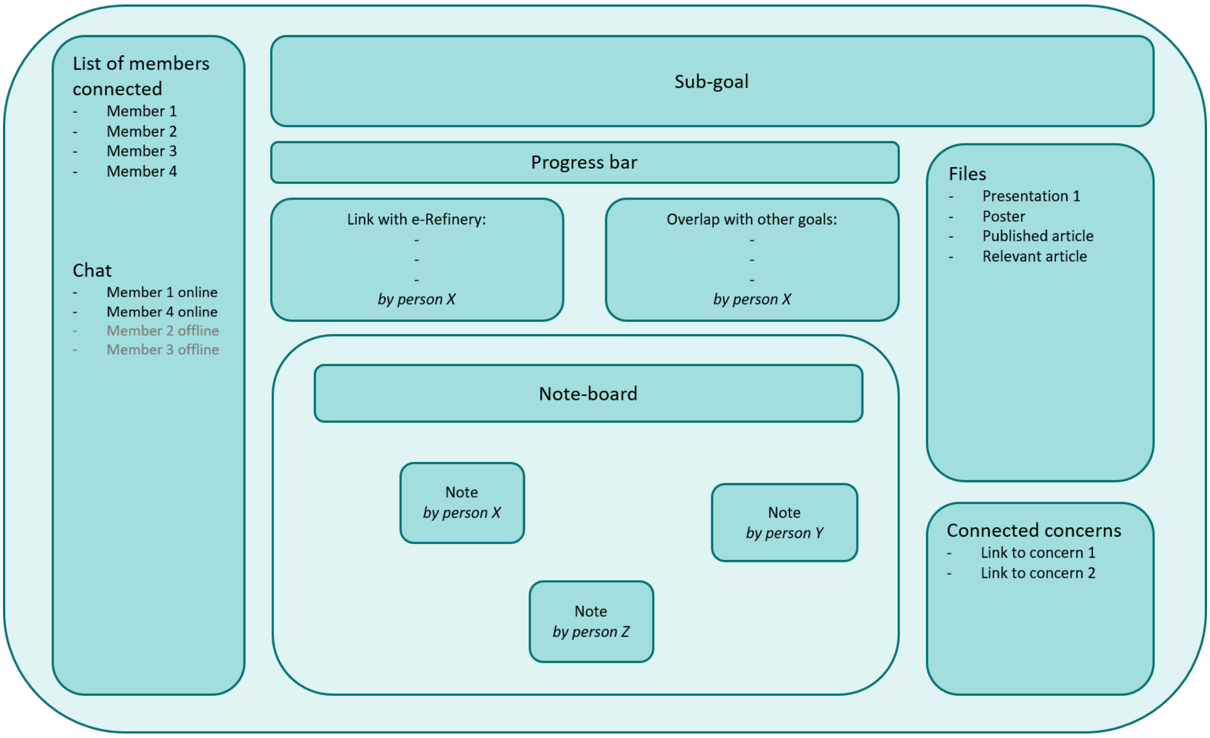


Figure 78: A visualization of the sub-goal feature on the virtual platform

6.8.3 Language feature

In order to develop a more shared language and to make the members aware of the language they use, the virtual platform also includes a language feature. The members are able to select words or parts of sentences of others if they are unfamiliar with the term or if something is not fully understood. This word or part of a sentence then changes colours, so it becomes clear that there is a misunderstanding there. In this case, other members that are familiar with this word, are able to give a definition or explanation.

An example of how this language feature works is shown in Figure 79. In this case the word 'catalyst' is selected by one of the members are a word that is not fully understood. Another member sees this and adds his or her own definition or explanation to this word, the word changes color and When you now hover over the word with your cursor, the definition or explanation becomes visible.

This feature could also be expended towards an online dictionary, in which all words or parts of sentences are kept in an overview. This could be an additional feature of the virtual platform.

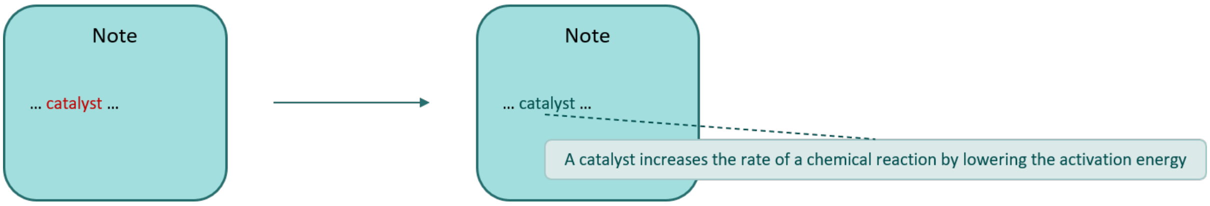


Figure 79: Language feature in the virtual platform

6.8.4 Tool guidelines

The setting-up of the boards include the follow steps:

- Two collective goals related to the direct and indirect route are already put in the note-board
- Board (maybe together with PI's) set up the research lines, collective goals or research areas.
- PhD students log in the virtual platform. They formulate individual research goals they are currently working on and add concerns related to their goal.

The guidelines for adding individual goals and concerns:

- Formulate a research goal that you're currently working on. When formulated a goal, try to make it a specific goal within the context of your whole PhD project.
- Put the goal in one or two sentences at the top of the note-board
- On the left, a list of members is shown. Here you can connect yourself to the goal. Other members can connect themselves to your goal as well.
- Describe how the goal relates to the e-Refinery institute in the box 'link with e-Refinery'.
- In the box 'overlap with other goals' the goals that have a link with your goals are placed, this is based on the connections made in the overview page.
- The note-board box can be used to place notes regarding this sub-goal. Each member, even when they are not connected to the goal, are able to place notes here or to react to notes.
- The box on the right allows to upload files related to the goal, including for example papers or presentations.
- The 'connected concerns' box shows the concerns that are connected to the sub-goal.

Figure 80 shows how the sub-goal note-board can be filled in, using one of the goals of the Chemical Engineering part of this research as an example.

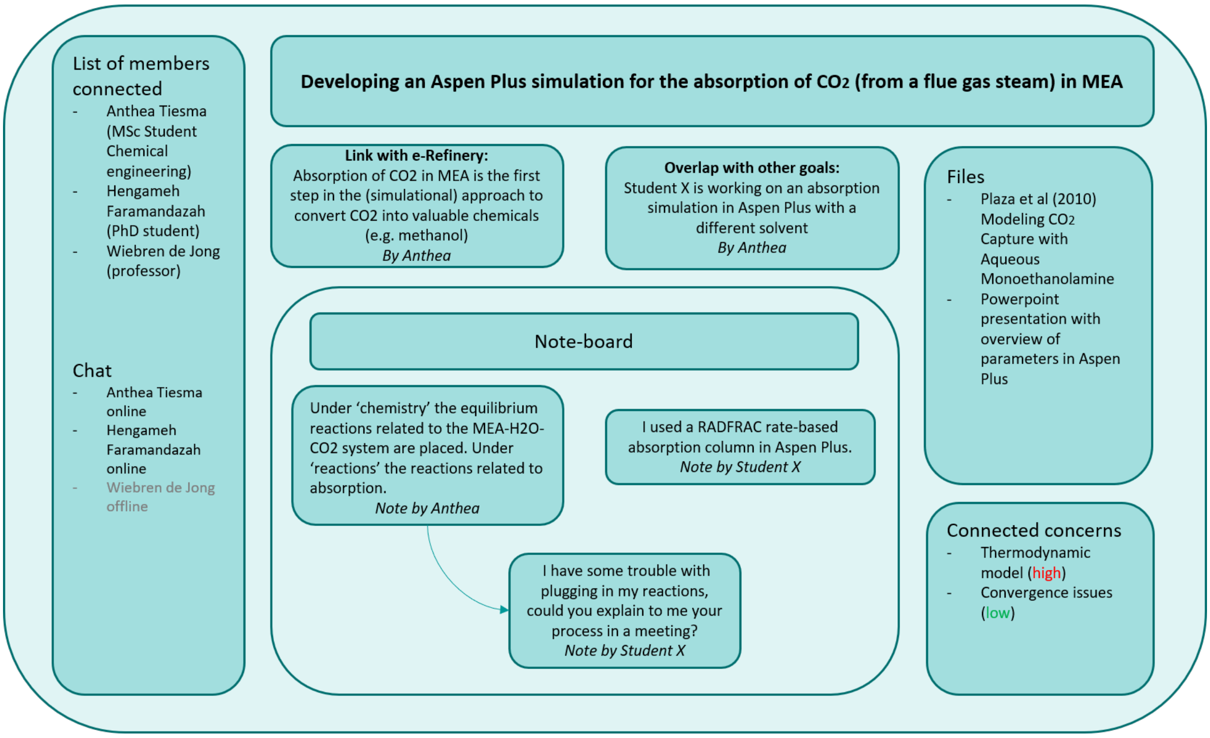


Figure 80: Sub-goal note-board filled in by the author of this thesis to give an example of this functionality.

Figure 81 shows two concerns related to the sub-goal and some notes that have been posted for this concern. The two concerns linked to the sub-goal were real-life concerns during the author's thesis and the notes posted in this note-board were ideas or solutions discussed in meetings.

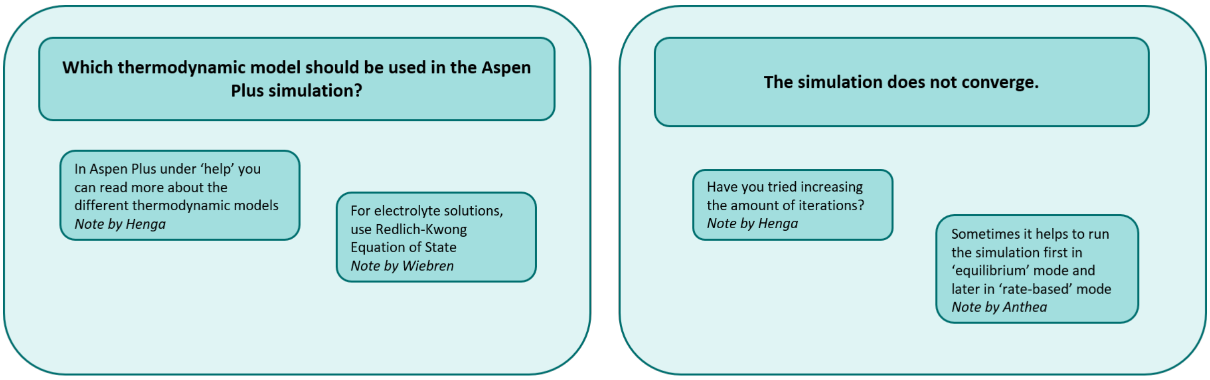


Figure 81: Two concerns note-boards filled in by the author of this thesis to give an example of how this functionality could look like.

7 Discussion

This chapter discusses the results of this research. First the research methods of the three phases are discussed. Afterwards, the results of the three phases are discussed.

7.1 Discussion of the research methods

The research is conduced using a Triple diamond research method, an extended version of the Double diamond research method [14]. The Double diamond research method integrates both theory and practise and alternates diverging and converging stages, giving structure to the research and aiding in making decisions. A third diamond has been added to this research method to extend the Double diamond to a Triple diamond method, allowing to discover and explore the case before choosing a problem direction.

The added value of using a triple diamond research method in this research is the continue evaluation from both a theoretical and practical point of view. The addition third diamond that is added to this research method allows to explore and discovers the case from a more broad perspective, without already having chosen a problem direction. This way, a problem direction can be chosen with the integration and input from practise. Furthermore, this preliminary discovery phase allows to researchers to grasp the full complexity of a certain case. After the discovery phase, a problem direction is chosen for further research.

7.1.1 Discovery phase

In the discovery phase, the e-Refinery institute as a whole is researched with the aim to define a problem direction for the rest of this research. This is done by interviewing three members of the e-Refinery institute, all full-filling a different role in the institute, including an assistant professor, full professor and a board member. The discovery phase can be seen as a preliminary research to the rest of the research.

The e-Refinery institute consists of over 40 researchers in total, with all kinds of different backgrounds. In the discovery phase of this research, three members are interviewed, which is a small selection of the total members related to the institute. Therefore, it is possible that selecting three other members for the preliminary interviews, may have yielded in a slightly different problem direction. Therefore, the reliability could have been increased by interviewing more members in the discovery phase. The different roles and background of the three interviewees. Looking back, especially the addition of a PhD student in this round of interviews would have been beneficial for the research. In a later stage of the research, the development of the tool, the emphasis shifted more towards the PhD students involved in the e-Refinery institute. In the first phase, no PhD student was interviewed.

7.1.2 Deepening phase

The deepening phase consisted of two parts: a literature review and interviews with e-Refinery members. In the literature review, a deeper understanding of the concept shared vision is created, leading to an adaptive definition of what a shared vision entails within the context of research institutes. Furthermore, drivers and barriers for the development of a shared vision are obtained.

A total of 24 articles have been reviewed for the systematic literature review. These articles included different fields of research, including social sciences, (public) health care, and education. The e-Refinery institute is an interdisciplinary research institute with the focus on developing (technological) solutions for the energy transitions. The drivers and barriers for the development of a shared vision within research institute in this particular field that e-Refinery plays in, is of course a very narrow subject. Therefore, for the systematic literature review, articles have been selected that contain information that can be translated to this particular field. Therefore, there was not always a direct connection between found drivers and barriers and the field e-Refinery is in.

7.1.3 Design phase

In the design phase, a virtual platform has been developed as a communication tool to aid the e-Refinery members in the development of a shared vision. The design phase focused on five design criteria: (1) sharing of concerns, (2) development of shared goals, (3) shared vocabulary, (4) interaction between members, and (5) collective development of goals.

In the design phase, a morphological chart has been developed with the help of an education expert (during the brainstorming sessions) and the drafting of the concept has been done with the help of a recently graduated Communication Design for Innovation student. In order to further improve the morphological chart and the concepts, this step could have integrated input from the e-Refinery members as well. This has been done in a later stage of the research, where a PhD student of the e-Refinery institute, a Communication Design for Innovation student, and a communication expert have been asked for feedback sessions regarding the development of the tool.

Involving the e-Refinery members earlier on in the design process might have been beneficial in the development of the tool, by tailoring the tool more towards the institute. Earlier integration of theory and practice might have lead to valuable feedback and critique on the tool in an earlier stage. Earlier engagement of the practise, in the form of interviews and feedback sessions with e-Refinery members focused on the tool development, would have increased the validity of the final tool.

In a later stage, when the final tool concept had already been chosen, feedback sessions were conducted. These sessions were used to gain insight in the e-Refinery institute, with particular more insight around the five design criteria, and to further improve and fin-tune the final tool. The first session was conduced with a PhD student that currently performs research within the e-Refinery institute, this session is described in Section 6.1.1. Even though it was just one student, the results from the interview matched what was already said regarding the five design criteria in the deepening phase interviews and could therefore be assumed to be valid for the e-Refinery institute in general, especially for other PhD students within the institute. Besides, this feedback session did not aim to gain completely new information, the main aim was to obtain more details and background information about statements and results already found in the deepening phase interviews. Therefore, having one interview already was sufficient to reach this goal. However, the validity of this feedback session could have been improved by performing multiple feedback sessions with different PhD students, in order to further improve the reliability of the statements made in the feedback session. It was chosen to only have one feedback session regarding this subject due to time constraints and to use the sparse time available for other feedback sessions regarding the functionalities of the tool.

Furthermore, four feedback sessions where in the iterative process of the tool development, discussed in Section 6.5. These sessions included Science Communication students and graduates, as well as one PhD student involved in the e-Refinery institute. The main goal of these sessions were to evaluate the tool in general, the functionalities of the tool, and to improve upon them. These feedback sessions helped to bring the tool to the next level by fine-tuning the functionalities of the virtual platform. The first three sessions were solely focused on the tool and its functionalities itself. The fourth session was different in nature and did a step back from the tool to look at the structures within e-Refinery. This session helped to get a more clear overview of the connection between the five design criteria. Making these connections and visualizing them, allowed to integrate these connections better in the tool as well.

7.2 Discussion of the results

This session discusses the results of the three phases, the discovery phase, deepening phase, and design phase.

7.2.1 Discovery phase

In the discovery phase, a problem direction is obtained from 3 interviews with e-Refinery members. In the problem direction, two observations are highlighted: (1) the difference in interpretation of research goals amongst the different individuals, and (2) the difference within the e-Refinery institute regarding collaboration and cooperation between the different parties. From these two observations, a problem direction is stated as followed: *There is a difference in insight amongst individuals within the e-Refinery institute about the vision, goals, and means of the e-Refinery institute.*

The results are based on the 3 interviews with different e-Refinery members, all having different roles in the institute. The different roles allowed to look at the e-Refinery institute from multiple angles and viewpoints, giving a broader overview of the institute. However, the total amount if interviews in this phase is limited.

7.2.2 Deepening phase

The concept shared vision has been defined in this research as an adaptive and time-dependent concept. This is done based on the definitions found through the literature review in the deepening phase of this research, in combination with the author's perspective of how this could be translated into an adaptive, time-dependent concept. This lead to a definition of a shared vision based on the following five aspects: (1) goals and ambitions, (2) values, (3) future perspective, (4) concerns, and (5) external visibility. Furthermore, a visualization is presented where each aspect is displayed as a circle. The size of the circle indicates to which extend this aspect is present in a collaboration.

In other literature, a shared vision is not often described in literature as a time-dependent concept. As mentioned by Robertson (2006): *The critical component to the success of this collaboration was the creation of a shared vision. Although this vision was broad in scope and somewhat vague at the start of the collaboration, it developed into a much more defined and truly shared vision through negotiation and experience [77].* Even though it is acknowledged that a shared vision is not something 'set in stone' at the beginning of a project, it grows and develops over time, the definition of the concept does not include this time-dependent component explicitly. Furthermore, literature does not provide concrete descriptions of how a shared vision develops over time. The definition by Robertson (2006) implies that a shared vision is at the beginning less defined or ill defined (*'somewhat vague at the start'*). In this thesis, I wanted to move away from the idea that a shared vision cannot be fully defined at the beginning of a collaboration. Therefore, this thesis presented a description and visualization to evaluate a shared vision as an adaptive concept. The main difference compared to the description given by Robertson (2006) is that in this thesis a shared vision is not seen as something that is '*growing and developing*' over time, but as a concept that is '*adapting*' over time. Therefore, the definition presented in this thesis moves away from the idea that a shared vision is ill-defined and somewhat vague at the beginning of any collaboration.

In the second part of the deepening phase, 9 interviews are performed. The interviewees were all members of the e-Refinery institute. The group of people that were interviewed was rather diverse, in terms of function as well as the role they fulfilled in the institute. There were PhD students interviewed, as well as principal investigators and board members. Some interviewees performed research that falls within the institute, other had an advisory role. This allowed to gain a deeper understanding of the differences within the institute and allowed to look at the institute as a whole.

7.2.3 Design phase

One of the main questions regarding the implementation of the tool is whether the e-Refinery members feel the need to go to the platform and to use the tool. It is important that the tool clearly portraits the added value it posses in relation to the e-Refinery members. Furthermore, the perceived need of the members also play an important role. It is important to keep reflecting on the virtual platform to make sure the needs of the e-Refinery members are met.

Another discussion point is the bridge between virtual and physical interaction. The tool gives a virtual platform which allows interaction between members. However, the virtual platform is not a replacement for interactive sessions with other members, such as brainstorming sessions, idea generation session or sessions relating to issues. The virtual platform aids in finding and making connections with other members to brainstorm with, to generate ideas with or to discuss issues with. Furthermore, the tool also visualizes and makes connections between goals and concerns that may previously have been unknown. However, the actual setting up of those interactive sessions is still up to the members themselves.

According to the extended technology acceptance theory by Teo et al (2003) the amount of information available on the platform should be balanced. Too little available information available on the platform does not serve the purpose of information and knowledge sharing, while too much information causes an overload and clutters the platform. Therefore it is important to keep track of the amount of information available via the platform. At the first instance, when developing and when the platform is launched, members should be encouraged to share information and knowledge to make sure enough information is available. After a certain amount of time, the filtering and keeping track of information becomes more important. Information that is not relevant anymore should be deleted or archived, to make sure the platform is not cluttered, and an overview is maintained.

8 Conclusion

In the conclusion, the main question and the sub-questions are answered.

8.1 Answering the sub research questions

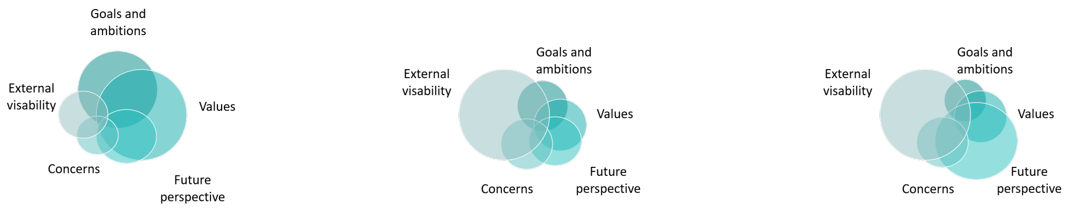
> *How can a problem direction be defined for the e-Refinery institute, taking into account the uncertainty that is inherently integrated in research projects?*

The problem direction is therefore stated as followed: *There is a difference in insight amongst individuals within the e-Refinery institute about the vision, goals and means of the e-Refinery institute.* This contains both the underlying issue of a difference in shared vision between the individuals in the e-Refinery institute on what the overall goal of the institute is, as well as the difference in which means should be deployed in order to reach there.

> *How can the concept 'shared vision' be defined as an adaptive concept?*

The concept 'shared vision' has been defined as a concept depending on the phases existing in a research project. A model has been developed based on the definitions of a shared vision from the literature review. The aspects of a shared vision include: (1) goals and ambitions, (2) values, (3) future perspective, (4) concerns, (5) external visibility.

A model has been developed to visualise the shared vision. This model includes five circles. These circles can be enlarged or reduced, based on whether a certain aspect is more or less present in a research project. It is argued that a shared vision is an adaptive concept that changes over the course of a research project. The visualization is shown in Figure 82.



(a) (b) (c)

Figure 82: Shared vision illustrated as a concept that is dependent on time.

Figure 82a shows a proposed model for a shared vision for the initial phase of a research collaboration. In this phase the shared values and shared goals are enlarged and perceived to be more important. Figure 82b shows a later stage of the collaboration, where external visibility is enlarged. In a later stage, external visibility becomes more prominent in order to establish resources. Figure 82c shows an end stage of the collaboration, where goals are mostly reached, and external visibility of the results and the future perspective of the project become more prominent.

> *What are the drivers and barriers for developing of a shared vision within an inter-disciplinary research institute?*

The drivers and barriers for the development of a shared vision have been identified with a systematic literature review. These drivers and barriers include the following aspects:

- Shared goals: sharing goals is both a sub-aspect of having a shared vision, as well as a driver for the development of a shared vision. Having shared goals aids in the development of a shared vision. Misalignment of goals and members that do not share an overall goal, hinder the development of a shared vision.
- Collective development of goals: relating to the development of goals as a collective. Allowing members of an institute to develop goals in a collective manner increases the level of shared vision. A lack in the collective development of goals does not directly form a barrier for a shared vision, however, developing goals in a collective manner increases the alignment of shared goals and therefore aids the shared vision.
- Mutual expectations: clear expectations of what the role and goal of each individual within the collaboration. The alignment of mutual expectations helps the development of a shared vision by having clear defined roles and expectations of each other.
- Financial and human resources: the availability of financial and human resources. When financial resources and social capital are perceived to be plenty, it aids in the development of a shared vision.
- Knowledge sharing: the quantity and quality of the knowledge that is shared between the individuals in the collaboration, when the quantity and quality is high, the development of a shared vision is facilitated. Too little knowledge sharing or knowledge sharing of low quality hinders the development of a shared vision.
- Caring about similar issues: the level of sharing and overlap between issues. The care for similar issues part of a having a shared vision. Furthermore, sharing concerns and issues within collaboration also aids in the development of a shared vision. When issues and concerns are not shared, this forms a barrier for the complete integration of a shared vision in a research team.
- Motivation: motivation to join the research project and to work on collective goals is a driver for the development of a shared vision. A lack of motivation is a barrier for a shared vision. Especially in the e-Refinery institute, where members are voluntarily connected to the institute, motivation is a strong driver for the connection to the institute and to their goal.
- Interaction: interaction between members drivers the shared vision. This influences directly and indirectly the shared vision. A lack of interaction forms a barrier in the development of a shared vision
- Shared vocabulary: the level of shared vocabulary in the collaboration, including terms, jargon and equations, but also mutual understanding about how research is performed.
- Communication on the same wavelength: the ability of individuals to relate to each other when talking about research.
- Previous relationships: existing previous relations can aid in the development of a shared vision. The lack of previous relationships does not have to be a barrier for the development of a shared vision.
- Trust: trust between members of a project group has a positive effect on the development of a shared vision. A lack of trust can hinder the development of a shared vision. This

can be both directly or indirectly, e.g. a lack of trust can for example lead to a lack of knowledge sharing.

- Appreciation for work: when the work of the individual members is appreciated in the group, this can aid in the development of a shared vision by for example increasing the motivation of members.
- Positive experience: the collaborative environment as a whole also influences the development of a shared vision.

How can a tool be designed to aid the e-Refinery members in the development of an adaptive shared vision?

An adaptive tool has been developed based on brainstorming sessions and a literature investigation and is further fine-tuned with feedback sessions. Based on the interviews in the deepening phase, the tool was developed to aid in the following five areas of the development of a shared vision:

- Caring about similar issues
- Collective development goals
- Sharing of goals
- Interaction between members
- Development of a shared vocabulary

A virtual platform is developed as a tool to aid the e-Refinery members in the development of a shared vision. The platform visualizes the structure of the goals within the the institute. Furthermore, the platform integrates note-boards that can be used to add additional information regarding individual goals and concerns. The platform is interactive, therefore, all members can react to each other and form new network relations as well.

8.2 Answering the main research question

The main research question for this research is defined as followed:

How can members of the e-Refinery institute be enabled to develop a shared vision to deal with uncertainty in the project?

In this research, a virtual platform has been designed in order to aid the members of the e-Refinery institute in the development of a shared vision. The platform integrates the following five design criteria: (1) sharing of concerns, (2) development of shared goals, (3) shared vocabulary, (4) interaction between members, and (5) collective development of goals.

The tool allows the members to connect with each other and interact with each other on a day-to-day basis via a virtual platform with note-board functionalities. The note-boards of the platform relate to shared goals and shared concerns, both aspects of a shared vision. Furthermore, the tool allows the members to visualize the structure between different individual and collective goals and concerns. By making these connections and links, the process of developing shared goals in a collective manner is facilitated.

Part III

Integration

Final note

In this last section, a final note about the research is given. This includes answering the overall research question that has been posed in the general introduction of this thesis. Furthermore, the generalization of the results from the Communication Design for Innovation part are discussed, showing to which extend the results can be used and translated to other case studies apart from the e-Refinery institute. The significance of this research and the contribution to the science communication field is also discussed. This section wraps up with showing how the integration between both fields and the advantages this had.

Answering the overall research question

The overall research question that is posed in this thesis is:

How can technical solutions be developed for the capture of CO_2 and subsequent conversion of CO_2 into CH_3OH with renewable based H_2, while managing uncertainty in the development of technical solutions?

In the first part of this thesis, a technical solution has been found for the capture of CO_2 and the subsequent conversion of CO_2 into CH_3OH with renewable based H_2. This has been done by performing simulations in the Aspen Plus. With the simulation and a sensitivity analysis for the absorption, stripping and conversion step, the operating conditions of the blocks have been evaluated. This research falls within the activities of the e-Refinery institute. The e-Refinery institute has as main goal to develop and implement technologies for the sustainable development of chemicals and fuels.

In the second part of this research, the development of a shared vision has been used in order to evaluate how uncertainty can be managed. This parts evaluated collaboration in interdisciplinary research institutes and takes a more general approach. The final product of this part is a virtual platform that can be used to help research institutes in the development of a shared vision. The virtual platform is tailored to the e-Refinery institute and its specific needs.

Generalization and significance of the results

The communication design for innovation part of this research used the e-Refinery institute as a case study. This institute is a interdisciplinary research institute, dealing with a complex project in an uncertainty rich environment. The development of a shared vision has been used to evaluate and improve the collaboration. The results of this research can be useful for other research institutes as well.

The drivers and barriers that were found in the systematic literature review do not only apply to the e-Refinery institute, but are valid for interdisciplinary research institutes in general. The articles that were used in the systematic literature review all reviewed complex cases with an interdisciplinary approach. The cases described in the articles used for the systematic literature review cover a range of different research fields, including amongst others interdisciplinary collaboration in health care teams, governance of watersheds, and energy transition projects. Some cases are characterized by the complexity in their technology development, while other cases have a stronger focus on society or societal embedding. The e-Refinery research institute as it is currently operating, has a stronger focus on the development of complicated technologies, however, the goal described by the institute also includes the implementation of these technologies, in which the embedding in society becomes more prominent. Since the institute is relatively young, the shift to focus more on the societal embedding is not yet there. The theoretical framework that is constructed in Section 4.1 can be applied to a range of different research institutes.

The framework would be most fitting to research institutes with the characteristics of complex problems and institutes that are interdisciplinary in nature, meaning that researchers in the institute have different backgrounds and therefore also might have different world-views, using different research methods and do not yet have an established shared vocabulary.

The tool that is designed in this research, the virtual platform that aids in the development of a shared vision, is tailored to the current needs of the e-Refinery institute. The main focus of the tool consists of the following five design criteria: (1) caring about similar issues, (2) collective development of goals, (3) sharing of goals, (4) interaction between members, (5) development of a shared vocabulary.

In order to tailor the virtual platform to fit other institutes, it is recommended to research the institute in a similar manner as done in Section 5. With a combination of interviews and surveys, the focus points for the tool, the design criteria, are found. The virtual platform is developed around these focus points. However, the virtual platform can easily be tailored to other needs as well. The interviews and survey focus on the five aspects of a shared vision: (1) goals and ambitions, (2) values, (3) future perspective, (4) concerns, and (4) external visibility. The virtual platform as it is developed for the e-Refinery institute has the main focus on the goals and ambitions and the concerns in order to aid the shared vision development, since these two aspects are currently the main bottleneck for the e-Refinery institute. For other institutes, it is possible that the focus would have to be more on for example values or external visibility. The virtual platform can be tailored in order to make these aspects more prominent. In order to do this, it is suggested to use the shared vision visualization shown in Figure 75 as a starting point.

Since a shared vision is in this thesis defined as a time-dependent concept as well, changing over the course of a project, the concept of a versatile virtual platform fits the goal of developing a shared vision. This research adds to the current literature that is already available on the development of a shared vision. One of the main new insights in the definition of a shared vision is the time-dependent component that is introduced in this research. A shared vision as a time-dependent concept is a new way of looking at this concept and not yet as such described in existing literature.

Synergy between the two fields

Doing research on both the technology development as well as the collaboration aspect of this technology development allowed to have a more broad understanding of how technologies can be developed in interdisciplinary research projects. The first part of this research had a strong focus on technology, which allowed to be fully submerged in the world of complex technology development. This allowed to understand the e-Refinery institute better. Besides, it helped in gaining insight in which struggles might come up for other researchers, leading to a broader understanding and a change of perspective as well. Having this broad understanding improved the second part of this research by having a stronger basis of understanding of the technology side and therefore a higher ability to relate to the researchers that were interviewed.

1 References

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Part IV

Appendices

A MEA make-up stream

Table 75 shows the input and output of the calculator block.

Table 75: Defintions of the variables for the calculation block

Variable	Information flow	Definition
RECYCLE	Import variable	Stream ID: RECYCLE, Component: H_2O, unit: kg/hr
MU	Tear variable	Stream ID: MU, Component: H_2O, unit: kg/hr
PREHEAT	Export variable	Stream ID: PREHEAT, Component: H_2O, unit: kg/hr
RECMEA	Import variable	Stream ID: RECYCLE, Component: MEA, unit: kg/hr
MUMEA	Tear variable	Stream ID: MU, Component: MEA, unit: kg/hr
PREMEA	Export variable	Stream ID: PREHEAT, Component: MEA, unit: kg/hr

The following calculations shown in Equation 55 to 58 are plugged into the calculator block.

$$PREHEAT = 921.022 \tag{55}$$

$$MU = PREHEAT - RECYCLE \tag{56}$$

$$PREMEA = 394.084 \tag{57}$$

$$MUMEA = PREMEA - RECMEA \tag{58}$$

B Explanation of the correlations

The information for the correlations is retrieved from the Aspen Plus help guide [3].

Mass transfer coefficient and interfacial area method

The correlation by Bravo et al. (1985) is used to predict the mass transfer coefficient and the interfacial area for structured packing. The equations used in this correlation to calculate the mass transfer coefficient are shown in Equation 59, Equation 60.

$$k_{i,k}^{L} = 2\sqrt{\frac{D_{i,k}^{L}}{\pi t_L}} \tag{59}$$

$$k_{i,k}^{V} = 0.0338\frac{D_{i,k}^{V}}{d_{eq}} Re_v^{0.8} Sc_{V\ i,k}^{0.333} \tag{60}$$

In which $k_{i,k}$ is the binary mass transfer coefficient for the liquid and vapor phase in m/s. $D_{i,k}$ is the diffusivity of the liquid and vapor in m^2/s, t_L is the residence time for the liquid in s. The equivalent diameter is given by d_{eq} in m. Re_v and $Sc_{V\ i,k}$ stand for respectively the Reynolds number for the vapor and the Schmidt number for the vapor.

Equation 61 shows the relation used to calculate the interfacial area.

$$a^I = a_p A_t h_p \tag{61}$$

In which a^I is the total interfacial area for mass transfer in m^2, a_p the specific area of the packing in m^2/m^3, A_t the cross-sectional area of the column in m^2 and h_p the height of the packed section in m.

The correlation is based on the parameters that define the dimensions of the corrugation of the packing, shown in Figure 83.

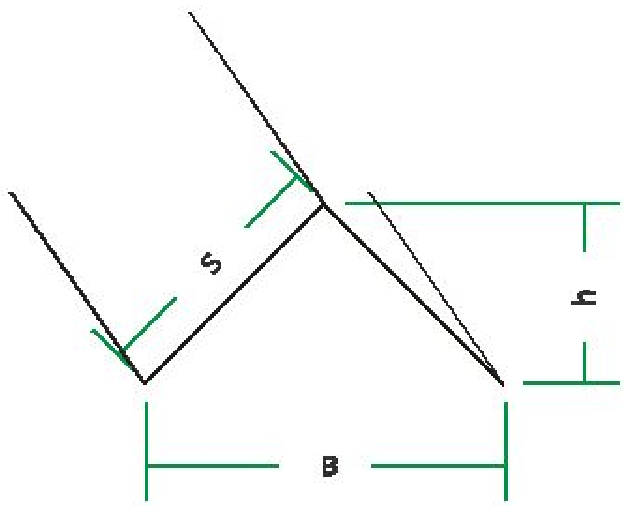

Figure 83: Corrugation (retrieved from Aspen help guide [3])

The parameters used in the correlation are shown in the table below.

Variable	Parameter	Unit
B	Base width of a corrugation	m
S	Slant height of a corrugation	m
h	Height of a corrugation	m

Heat transfer coefficient method

The correlation by Chilton and Colburn is used to calculate the heat transfer coefficient. The heat transfer coefficients are calculated from the binary mass transfer coefficients. Equation 62 and 63 are used in these calculations.

$$h^L = k^{-L}\rho^{-L}C_P^L\left(\frac{\lambda^L}{\rho^{-L}C_P^L D^{-L}}\right)^{2/3} \tag{62}$$

$$h^V = k^{-V}\rho^{-V}C_P^V\left(\frac{\lambda^V}{\rho^{-V}C_P^V D^{-V}}\right)^{2/3} \tag{63}$$

Where h is the heat transfer coefficient in liquid and vapor phase in W/m^2K, k the mass transfer coefficient in m/s. C_P stands for the specific molar heat capacity in J/kmol·K, ρ is the molar densitity in kmol/m^3 and λ the thermal conductivity in W/m K.

The Chilton and Colburn method is based on the Chilton-Colburn analogy, providing a relationship between the Stanton number for heat transfer, the Prandtl number, the Stanton number and the Schmidt number. The analogy is shown in Equation 64.

$$St_H Pr^{2/3} = St Sc^{2/3} \tag{64}$$

In which St_H is the Stanton number for heat transfer, shown in Equation 65. Pr stands for the Prandtl number, shown in Equation 66. The equation for the Stanton number is shown in Equation 67. Sc represents the Schmidt number, shown in Equation 68.

$$St_H = \frac{h}{\rho C_p u} \tag{65}$$

$$Pr = \frac{C_p\mu}{M\lambda} \tag{66}$$

$$St = \frac{k}{u} \tag{67}$$

$$Sc = \frac{\mu}{M\rho D} \tag{68}$$

In which D is the average diffusivity in m^2/s, M the molecular weight in kg/mol, u the average flow velocity in m/s and μ the viscosity in Pa s. Solving the heat transfer coefficient for each phase leads to the relation presented in Equation 62 and Equation 63.

Hold up method

The correlation by Stichlmair et al. (1989) is used to predict the liquid holdup for all kinds of packing. The equations for these calculations are shown in Equation 69 and 70.

$$h_L = h_t h_F A_t \tag{69}$$

$$h_t = 0.555 Fr_L^(1/3)(1 + 20\mathit{\Delta} P^2) \tag{70}$$

In which h_L is the volumetric liquid holdup in m^3 and h_t the fractional holdup, h_F the height of the packed section in m and A_t the cross-sectional area of the column in m^2. Fr_L is the Froude number for the liquid and $\mathit{\Delta} P$ the pressure drop in Pa.

The parameters used in the correlation are shown in the table below.

Variable	Description	Unit
a_F	specific area of the packing	m^2/m^3
C_1, C_2, C_3	Stichlmair constants	-
η	Void fraction of the packing	-

C Explanation of parameters

The following table with explanation is retrieved from the Aspen Plus help guide [3].

Parameter	Explanation
Chilton-Colburn averaging parameter	Weighting parameter used in average diffusivity and average mass transfer coefficient calculations by the Chilton-Colburn analogy. This parameter provides stability when compositions change, especially in reactive systems when some compositions may go to zero at the boundary. When the value is small, mass transfer coefficients and diffusivities are weighted by composition. When it is much larger than 1, the impact of composition on weighting diminshes, as was the case in RateFrac. See Chilton-Colburn Method Details for details. The default value of 0.0001 is recommended. This averaging technique is used in calculations for the number of transfer units.
Transfer condition factor	Weighting factor for compositions in calculating mass transfer coefficient. The composition and temperature used are given by $F \cdot \text{bulk} + (1 - F) \cdot \text{interface}$, where F is this factor. see note
Reaction condition factor	Weighting factor for bulk and interface compositions in calculating film reaction rates. The composition and temperature used are given by $F \cdot \text{bulk} + (1 - F) \cdot \text{interface}$ where F is this factor. see note
Film discretization option	Indicates whether the thicknesses of the film regions vary in a Geometric or Arithmetic sequence.
Film discretization ratio	Ratio of thicknesses of adjacent discretization regions when film discretization is used with the Geometric option. If the regions are numbered from 1 at the bulk to N the interface, then ratio $= \frac{d_1}{d_2} = \frac{d_2}{d_3}$ where d_k is the thickness of region k. The same ratio is used to discretize the film for both liquid and vapor phases. See Film Reactions for details about discretization.
Film discretization increment	Increment between thicknesses of adjacent discretization regions when film discretization is used with the Arithmetic option. This increment is specified as a fraction of the region closest to the interface. If the regions are numbered from 1 at the bulk to N the interface, then increment = d1 - d2 = d2 - d3 = ... where dk is the thickness of region k. A positive value means the region closest to the bulk fluid is thickest. Negative values are possible, but limit the total number of film regions. The same increment is used to discretize the film for both liquid and vapor phases. See Film Reactions for details about discretization.

Flow model condition factor (top) and (bottom), Flow model transition factor	The condition factors are weighting factors used to adjust the flow model for stages near the top and bottom of the column when using a non-Mixed flow model. A value of 0.5 implies no change from the specified flow model while a value while a value of 1 implies the Mixed model is used at the top or bottom. Values between this imply intermediate flow models. This change applies only to a portion of the column indicated by the Flow model transition factor. Its default, 0.2, means that the top and bottom 20% of stages have these adjustments applied. The actual adjustment factor at each stage is interpolated between 0.5 at the transition factor point and the specified value on the top or bottom stage.
Mixed flow model on intermediate feed stages	If selected, then the Mixed flow model is used on stages where feeds enter, other than the top and bottom stages.

Note: For each stage, the mass transfer flux and reaction rates are calculated based on an average condition of the bulk phase and the film. If there are very fast kinetic reactions, the composition inside the film will change drastically. The Transfer condition factor and Reaction condition factor (default 0.5) control the weighting of these respective averages and should be set closer to or equal to 1 in these cases in order for the averages to be more realistic. See Film Reactions for more details.

D Reactor dimensions

The data of the reactor provided by VanBussche et al. (1996) is shown in Table 76.

Table 76: Reactor data from VanBussche et al. (1996)

Parameter	**Value**
Inflow	m = 2.8 $\dot{1}0^{-5} kg/s$
Diameter	d = 0.016 m
Height	h = 0.15 m
Volume	I = $\pi \cdot r^2 \cdot h$ = 3 $\cdot 10^{-5} m^3$

The inflow in the Aspen Plus simulation equals $8.25 \cdot 10^-3$ kg/s, and is therefore 295 times larger compared to the bench scale reactor of VanBussche et al. (1996). The volume of the reactor is also increased by the same factor, leading to a volume of I = $8.84 \cdot 10^{-3}$ m^3.

The diameter:height ratio used by VanBussche et al. (1996) equals $h = 20d$. Using the same ratio and the calculated volume gives reactor dimensions for the Aspen Plus simulation of d=0.104 m and h = 1.04m.

E Interview protocol discovery phase

Introduction

Thank you for participating in this interview. This interview is part of my Science Communication master thesis project. The results of the interview will be made anonymous before using it for my research. Is it okay if I record this session?

Questions

1. What is your role in the e-Refinery project group?
2. Can you explain more about the research you are doing?
3. Can you tell me more about the individuals working in the e-Refinery project group?
4. Can you identify the different parties the institute cooperates with?
   a. Universities, industry, government companies, other parties?
   b. Who is responsible for communication between the parties?
5. Do you have regular contact with other members from the institute outside the TU Delft?
   a. How often do you talk to them?
   b. To which extend is the research discussed?
   c. Are discussions based on (scientific) content or are also dynamics within cooperation discussed?
   d. Are there official meetings or formal agreements regarding meetings?
6. How would you describe the cooperation between different parties within the e-Refinery instutute?
   a. How often do different parties meet?
   b. How often do you meet with other people from the institute?
   c. With whom do you meet?
   d. How do you feel about the cooperation?
   e. Are there friction areas within cooperation?
7. Can you explain to me the hierarchical structures within the e-Refinery project group?
   a. What is your place?
   b. What are the decisions made in your position?
   c. How do decisions made in other places affect your research?
8. Who was/were responsible for defining the goals of the institute?
   a. What was the process of defining them?
   b. To which extend has the group identified uncertainty in reaching certain goals?
   c. Has uncertainty been a factor in defining research goals and overall goals?
9. Do you have personal goals int he research project?
   a. How do these goals relate to the overall goal of the e-Refinery institute?

b. How does it affect the overall goals if your goal is not met in the end?

c. In what way is uncertainty noticeable in your personal goals?

d. How does this affect overall goals of the institute?

Closing

Thank you so much for your time.

F Discovery phase interview transcripts

Interview Transcripts

Interview 1

- Can you define your role in the e-refinery project group?

- Of course, I'm actually an appointed assistant professor within the e-refinery, to the electrical sustainable energy department. So that is the electrical engineering part of our faculty, let's say. And my role is the electrical energy convergence within the e-refinery project. So of course the e-refinery is about converting electrical energy into molecules or the other way around,very simply put, and to do that you have these electrical chemical cells. And these electrical chemical cells they prefer to have a certain voltage or current, so a certain electrical energy and my goal is to get the energy from where it comes from, so maybe solar panels for example, to get it to the right form through the electrical chemical cells in the most efficient way obviously.

- That's always the case yes, and are you doing research on that as well?

- Yes, so, as an assistant professor I don't do much research myself, but I have two PhD'ers working on this also within the e-Refinery project, but yes I also still when I, let's say, when I have time left, I do some research as well.

- Okay, and can you tell me more about other individuals working for the e-refinery group? From your perspective, who do you see?

- So, from my perspective, I see the most, let's say a couple of colleagues from 3ME and a couple of colleagues from chemical engineering and the reason that I collaborate the closest with them is because I need to know how these cells behave and what kind of electrical energy they prefer before I can set the requirements for the components or devices that I'm trying to make. So a lot of the times I'm in calls with them or collaborating with them or negotiating with them what they need let's say

- Okay, and are there parties outside the university, because I saw that the e-refinery with industry, other universities, do you see something from that?

- I have to admit that I'm not part of this project for a long time, only a couple of months. So for me, the interactions with the companies that participate in the e-refinery is very little. But I am collaborating with some parties, companies, let's say other research institutions, on these topics. But they are not necessarily part of e-Refinery, it's just people I know that I think we can work together.

- Do you know who's responsible within the e-refinery to communicate with different parties?

- Oeh that's a difficult questions, for me, the person why I see doing that is *name*. But I'm not sure if she's also the one responsible for it. So she's the one doing it, and I don't know if she's the one responsible for that.

- Okay, and you said you had some contact with other people from the TU Delft. How often do you have contact with other people? Is it like once a week, month?

- Yeah I would say on average once a week. Sometimes it's multiple times in one week, sometimes it's not at all, but I think on average once a week I talk to one of my colleagues within e-refinery.

- And to what extend do you discuss research that is going on within the e-refinery group? You really go in-depth with people about different topics?

- That depends, there is different types of meetings. Some of the meetings are more focused on acquiring funding for research, so those are usually not that in-depth but more focused towards what approach are we going to take. What are we going to research and how can we collaborate, those types of meetings. But then there are also the meetings were me and my colleagues just have questions for each other, that goes really in-depth and it goes into the technical details. And usually than also one of our PHD's is there and we're really trying to get somewhere let's say.

- Then it's more a session in stead of a meeting

- Yes yes yes

- How would you describe the cooperating between different parties within the e-Refinery group? You said you didn't see much of the outside of the university yet?

- Yes, not yet, so that I'm not so sure about. But within the university I think it's actually working very well. People are very open to working together. Sometimes in research projects I've noticed that different faculties are not very inclined to help you out. But within the e-refinery I find that it's quite the opposite, so that was a very comfortable situation for me. And also I think for them. So the collaboration is quite close and it's working smoothly if you'd ask me.

- Okay that's really good to hear! Are there also friction area's?

- I would not say so, I think everything is working fine. Let's say the only challenge I see personally within e-refinery is that the final goal is to reach large scale applications. And I think that some faculties with there research are not at that level yet. For us it would possible, because for us it is kind of mature technologies that we are using. But for them, they are really doing new stuff and usually that is on, let's say, an extremely small scale. So that's a challenge. But I don't think, I wouldn't say that's a friction, but I'd say that's a challenge.

- More a technical challenge.

- Yes yes

- How do you deal with such challenges, since your research is more mature?

- So one thing that we're doing is talking them and seeing, let's say, anticipating on how it will be like. I can give you an example, because they are working on CO_2 electrolysis, that is on a very small scale. But then we talk to them, like what can we do, what is the most similar, how can we try to already look for the future? And basically what they said is that you also have PM fuel cells that are electrolyzers for hydrogen, and they said that that will most likely behave very similar to that what we are doing with co2 electrolysis. So that why we focused on that let's say. And then probably the step towards co2 electrolysis for us will be small.

- Okay, that's good. Can you explain me more about the hiarchial structures within the e-refinery group? Because there are some project leaders, I guess, some researchers..

- I would say, yeah of course there is always a hierarchy, but I'm not noticing it too much. People are not behaving as, I'm the boss listen to me. No I would say, it's more collaboration of equals, of course there is people calling the most of the shots, but I never felt that I had to do something that I didn't want to do or something like that so. There is a hierarchy but it's not bad.

- That's good, but how does it look like? What are the different roles that people take in the group? There is always someone that makes more of the decisions and someone that does more of the research part. How are the roles defined?

- Yeah so I think there are a couple of people making the decisions, and then again the person I had the most contact with is *name*. So to me it seems kind of like she's the one making most of the decisions. And then there are, I don't know what their official role names are, it's a part of staff within the e-Refinery, what was his name. there was this relatively new guy who started within e-Refinery, Peter I think, but I forgot his last name. So he takes up more the administrative tasks I know, and he does it actually very well. Other than that I didn't have very much contact yet with let's say the different roles that. But I'm sure there is also like PR people and things like that.

- Yeah, and someone that keeps the lines between industry and other universities open?

- Yeah yeah

- Do you know who was responsible for defining the goals of the e-refinery institute?

- Haha, you're asking all kinds of difficult questions. I will be honest with this: no I don't

- Haha okay and did you make research goals for yourself and the research?

- Yes yes I did

- How do you see that in line with the overall research goals of the e-refinery group? Does it match?

- Yes, so we tried very hard to make it match. Also with my PHD students. Although I wonder if it is possible in the relative short term. Because most of the goals are relatively large scale and for us that is very possible. So our goals are aimed towards the larger scale application, but okay I don't know from other groups if it will be possible, but we really try to fit within those goals. To make sure that if by any change it happens, that we can also contribute to the goals. It would not be a problem from our side let's say

- Okay, how did you define your goals? What was your process behind it?

- Let's say when I was applying to this position, I read all the e-refinery documents and also started thinking about "what do I think are the challenges and should be the objectives from our point of view?". So during my interview for the position I presented those thoughts and then of course you get some feedback and you read a bit more and in the end I have defined my goals within the research direction in that way. And of course that trickles down to my PHD students, but yes they have their smaller individual goals, but they fit within my larger goals, let's say.

- Okay, and what if you don't reach your goals? How does that impact the e-refinery group? Maybe not a nice situation to think about, but..

- Uhmm, it sounds very bad, maybe, but I think even if I would not achieve any of my goals, the e-refinery would still be fine. Because for us, let's say, the electrical power converges are devices you can buy. Like, they are less than ideal maybe, but you can just buy from a big company, like ABB, you can just buy these devices and it works. It's just, okay, it's not gonna be most efficient or most cost efficient, but it's fine let's say.

- Okay, do you notice some uncertainty in your goals? That you are uncertain about? Whether you're going to reach a goal? Or how to reach a goal?

- Uhmm well, it wouldn't be research if there was no uncertainty, I think

- Yeah that's true

- So, that is also reflecting the way that I define my goals usually, is that the goal is defined in such a way that there is no uncertainty, but the way that you reach that goal can be fastly different from what I think it will be now and it probably will be different from what I think it will be now. I wouldn't say there is uncertainty in the goal, but the final the final solution is very unclear, let's say.

- Okay, and do you have any idea how that effects the overall goals of the e-refinery institute?

- Hmm again I think, it wouldn't affect it that much.

- But in terms of efficiency?

- Yeah in terms of costs and efficiency you could consider that a huge impact, but uhmm, overall it would still work, let's say, so the basic principle would be the same.

- Okay, but in terms of costs and efficiency, would it still be as easy to implement in our daily lives? If it is not as efficient as we hope it would be?

- Yeah so that is where it matters, it's that... well if we are talking about these large scales, than the daily lives would not be as much effected, but it would affect the, let's say, economical feasibility of such projects, right? To actually make such systems on a large scale. Those will be massively effect. I know from, let's say hydrogen, that the components that we would design and make, make up about 30% of the whole system, it depends a bit, but yes it has a huge impact. So in terms of will it work, it has very little impact, but in terms of economic feasibility of the total project, yes it would definitely have an impact.

- Okay. And do you deal with that in any way in the e-refinery group? Are there like, for example, scenarios in which it is not as efficient and how do you deal with that in that case?

- There are people, let's say that, I haven't really talked to them much, but from TBM you have quite a few people working on e-refinery and well I think they are also working on, let's say, the economical feasibility of the system and I think that is an important assessment that has to be made. Because for us, we can make it almost as efficient as you want it to be, as long as you have enough money. So yea, there is obviously a trade off there. And at some point I can image even you'd sacrifice some efficiency so you'd have a cheaper system, that would probably be fine. Especially when we're talking about renewable energies.

- Okay, thank you so much. I think that was my last question. If you have any remarks?

- No, I don't think so.

- Oh well I have one last questions, later I'm going to do a second round of interviews to go more in-depth, would you be interested in participating later as well?

- Yes sure!

Interview 2

- So, can you explain me a bit more about your role in the e-Refinery project group?

- I am there mainly as a representative of my section.

- Which section are you in?

- I'm in the section of electrical power grids, this is part of the department of ethical sustainable energy, in the faculty of electrical engineering and mathematics and computer sciences. So in our department we have like three sections, our section is the one that works with kind of systems of systems or system integration, from an electrical point of view. It could be like a combination of neighbourhoods or margins, or micro-grids, transition systems, transmission systems. And then we tackle different issues there, like modelling for different phenomena: electromagnetic, electro-mechanical. And then we still working on co-simulations, because sometimes we have to interface for instance to have electrolyzer a chemical part, what platform the electrical part modelling the platform. And this process is happening for different time scales and they have to interact, so this are examples and then we also do something with cyber security, planning, markets applied to continuancy in the power systems, so and also protection. And my part be stabilization so resiliency against any kind of disturbance that could cause imbalances that could lead to disruptions and blackouts, so to keep a stable system, to keep the balance at any time. This could be something in a very small timescale, so milliseconds, or microseconds, we're talking about so. In this systems the scale is, the phenomena happens usually very small, so it's time to go to the speed of the light. So therefore we need to carefully study and make sure that all of the devices, and supplementary or auxiliary control systems are well designed and they work properly. And this has become a huge problem and now that we are translating to so called clean systems, or fully de-carbonized systems. Because essentially we are starting to face out all conventional technologies and conventional plants, so far we have almost 60 years of research on system interactions, thermal, hydral, nuclear, so on. And the technologies involved are very mature, they are raw washed, so we can do anything to the system and we have a blackout never, or hardly ever. But now we are removing all these matureness and we are putting new things, which are very difficult to control because, you know, for radiation we have solar radiation as main force and wind speed is very fluctuating, stochastic, and it's not the same as a hydro-power plant which can store water or fossil fuel, you can store the fuel. A problem when to use it, how to regulate. It is not so very predictable. And then therefore the high controllability and now we have to do that. On the one site a very fluctuating primary resource and on the other hand we have problems also with the device and how they connect to the system so they have to couple the little predictability because of the primary couple with converters or dis-converters for limited capability so we have the performance and they are faster in different domain. So.. eh..

- Yeah

- And then electrolizers for instance are part of these, so this is more... this is one generation this is demand. Well. The fuel cell is generation, which can be also similar kind of electrolyzers. Like P-e-m electrolyzers. We have the p.e.m. fuel cells. And then these electrolyzers are expected like to grow on a large scale. Probably up to one gigawatt, now there are different researches on. And the electrolyzers are respond to demand. So like conventional systems in which only generation was taken care and the new system demand also has a vital role, because we rely only on regulation to fully take care of the system. Because they have very limited capabilities and the most advance technologies we will not. We will never be able to just compensate any variation just by .. generation. Just that is really not possible. So demand has a role there, storage as well. Demand is especially more important because it is about consumers. So conventionally the system has been such that the consumers do whatever they want and the generation has been following and adjusting. And we have consumers doing whatever they want and the generation also. So we need to match somehow that.

- Yeah and that can be quite difficult

- Actually it can be done by generation. A lot can be done with consumers. So the prices are one of this and this is really appeal for this because the speed with which you can increase or decrease the consumption by an electrolyzers and especially in the larger scale. So we are talking about the 1 gigawatt. You can say okay you can go one gigawatt to 700 megawatt, so 300 megawatt decrease for instance in 10 milliseconds for instance. And that is fantastic for disturbances because then usually the timescale in which usually the conversion units it was doing that. So this means we are finding new sources to compensate the absence of what we have now. And so motivated by this I started some research on the use of ... and then to see how this effects this responsive demand of electrolyzers could be. And we did this project called TSO2020. So that is not exactly the full name of it. It has a very long name for this project because it is combination of different electricity carries through transmission, fast transmission, so on in the north of Europe especially around the area of Delftzijl and then north of Germany. And then there is also a very interesting case study because for our national system in the Netherlands that part is the most intensively interest of dynamic phenomena. The most intensively because there are a lot of new developments, so we have power electronic users to interconnect to Norway for instance, to Denmark. So overhead conventional over-headlines without any converter, like this cables that you see in the streets, in the highways. Just the cables who connect. Or that is the transitional solution that is our. We have this cables that are the most station with a lot of complex circuits and electronics. And this has a lot of implications on the system performance. And not only that that is as much as we have renewable power plants, of 600 megawatts, and many other developments that changed the dynamics a lot. And then we were.. for instance... you could place electrolyzers, electronics facilities for up to at least 300 megawatt by 2030.

- Yeah

- And this is is very important because it is an important actor that can modify each consumption upwards and downwards. And I want to say, okay let's see because this is a really nice case, a nice case study. Because this is really... Like, extreme a lot of new technologies. Let's see how consumers can play a role there. And then we did this for this project before we started in e-refinery. Because the work on the use of electrolyzers in the stabilizers of electrical grids are very severe, they are critical disturbances, disruption, blackout.

- Do you know more about the different individuals working for the e-refinery project? Because it's quite a big group, do you have contact with others and with whom?

- Yes it's a very big group, but, to be honest, I don't know everyone in the group. I'm a bit more familiar with some researchers, professors, PhD's, postdoc's who are a bit more or less closer to what I do. Especially the people that is working in renewable energy, from different aspects. Like for the power-electronics or the dynamics and some researchers from the faculty of 3ME. 3ME is... they work a lot on solar fuel cells and electrolyzers. From applied sciences as well, the people working with batolyzers. They have also a lot of focus on the physics of the phenomena, from an other perspective. Yeah. And a bit of the TBM faculty because they work on markets, on planning.

- And with the people that you talk to, the other researchers, how often do you talk to them? Once a week? Once a month?

- Yeah uhmm I would say at least once a month, yeah.

- And can you also identify other parties outside the university? Is there industry involved? Or government? other universities?

- So yeah, there is a lot of interest in the TSO 2020 project that is going to finish this year, in December. I told you already I finished my part in December last year, they are now doing the pilots. So they start the real electrolyzer of 4 megawatt in Saint San Ferdi. and we also build a full illustration for hydrogen and some buses and trucks that work with hydrogen. Locally we will have our ... reaction. ... and there in this project we did a lot of new networking and a lot of contact with new partners, especially outside my field. Because for electrical engineering, typical partners are mainly the manufactures are utilities field. But with this project we know more people. Also manufactures from electrolyzers and suppliers and converters. But also people working for environment, policy making, people that are more connected to the society.

- Is that new for you? That you work with those kind of partners?

- Yeah that was new for me, that was really out of my comfort zone.

- And how did you like it?

- In the beginning it was really complex, because it was more kind of traditional scientist, really focusing on physics and all these things. Usually you only talk with your peers who are more or less acquainted with the policy, so they already naturally talk with them about any complex things technically and they follow. So if you talk with the chemistry people or policy makers, from the politics sector or something like that, you say something and they show "how does this work"? so you have to improve a lot of your communication and presentation skills. Which I did. And it went okay, it went quickly. For me it was not so difficult because when I was younger, when I was in high school, I was a bit also involved in politics. In this kind of young members of a political party in my country

- So you were experienced a bit?

- We had to a lot of lobbying and speeches and such. When I started university. It is more then 10 years ago, but it's like riding a bike. You learn it and then 10 years late when you need it, you remind easily

- Yeah takes some time as well

- But that is really nice because the most important added value of that is that you present and you show what you are doing. And people to understand the value of that is really important, it can make impact. And also it is important because we need to make society more aware of the importance of the scientific challenges we really have to tackle. Which are tremendous. People think it's just connecting a wind-farm, an electrolizer.

- Yes it takes more than that

- It's not that simple, it really takes a lot of work. A lot of disciplines

- And i think people sometimes forget that these huge technological challenges also impact their live. They feel like it's something outside there life and outside society, but actually it impacts everyone in our society. And I feel like sometimes people don't realize that.

- Yes exactly.

- Do you have, with the e-Refinery project, also contact with parties outside the university.

- If I made contact or if I have contact with the members?

- Yes with the members inside the e-refinery project but outside the university, outside of TU Delft

- Hmm

- Like policy makers or . . . ?

- No not often. The policy makers I contact, more like ministries. But I think one partner also is this institute, they work on this 1 gigawatt electrolizer, I also have some contact with them. Outside the organization. We still have the discussion whether we are going to do something. but probably that will happen next month or so.

- Okay, do you know if someone else in the group is like a spokesperson to other parties in the e-refinery group?

- Uhh

- Do you know something about the communication lines?

- Yeah I think we have this ... organizational structure. We have.. I think that is *name*. We have other colleagues helping her. I think through them we can also reach other parties. So to in conversation from people from my faculty that is in e-refinery, like for instance, the head of my department.

- Do you notice that there is in e-refinery a hierchial structure? That some people are designated to do something else than other people? Is there like a structure of researcher, maybe someone that guides them and someone that keeps contact?

- Yeah to be honest I haven't gotten deeply into this.

- Okay. Do you know who was responsible goals of the e-refinery group? The overall goal?

- So yeah that is a good question.

- So are you aware of them? Do you know them?

- No not by heart.

- Yeah so there is a direct conversion goal, an indirect conversion goal and I think a bio-conversion goal. But do you know who is responsible for making those goals?

- I can image it was one of the researchers.

- Yeah probably someone in the beginning

- Maybe *name* or other colleagues or other colleagues that have been working a lot on the chemical side.

- And did you make goals for yourself? For your own part in this group?

- Well within my area yes. I have my own 10-years research plan. My contributions to the organization, the department and the faculty. And there is some alignment with what e-refinery does. If I have to continue on the research about the more advanced systems, that is much higher in the ... and more responsible users. Not only electrolizers but also look at systems like compressed air, and also the closed look. So how do we use electricity. So electrons converted into molecules into ... and fuel cells for example. I have different projects that I started to and that I see opportunities to work with and partners with e-refinery. And also partners that are also in the consortion.

- Are your goals related to the overall goals? If you don't reach your goal, does that impact the e-refinery group?

- When if I don't reach one of my goals does this if...

- Yeah maybe not such a nice question.

- Yes I'm trying to understand

- Yes if you don't reach one of your goals, does that impact the overall goal of the e-refinery project?

- Probably in some sense. For instance you would say, not reaching means probably not that we fail, but that we reached something different than we expected. Because research is about an hypothesis and then doing the studies to see if this is true or different. So we still have to do a lot, because there is a lot of discussion about this ... . but the part that has to do with e-refinery is that theoretically you see more so the renewable energy to make the chemical park greener or cleaner. Of course bio-reminder concerns and ... concerns, but for clinical concerns we have to study a lot. Because keeping a running stable system, every second, millisecond and microsecond for the long term, we are not only talking about a year but for the next years, decades. It's a huge and complex task and we still have to find out if we can, if one piece is really part of the solution, it seems that we are still in the very preliminary stage, so we can say that. So we can not already say that keep a stable system in the Netherlands, but it's more complex in Europe. But if we put electrolizers everywhere it is not good for the system so we still have to check that. So in that sense we, I think, the finals of my research will be the push to see if other system like transportation or the production of chemicals or fuels that.. this is done by electricity, by green electrons. How appealing is this also for the electrical system in a cell to keep it stable. This is an important part of the push as well, we see. What is the added value of ... also for the electrical system. We are highly dependent on electricity also, we cannot image a life without it. So we are like trying to aggregate the whole ... of an .. on the fly. We did do a lot but I think it has a huge impact because it helps to push the .. in my case from the perspective of ...

- And do you think that in your research there is a lot of uncertainty about how it will develop exactly? Like you're now here and you'll go somewhere there, sit her uncertainty on that road, like how it will develop?

- Yeah about technological development ... there is a mixture, there are different types of uncertainty that happen. When we talk about the uncertainties I always think about the timescale in which they occurs. If it is one week or one day or one hour or one second or so on. And also, in terms of days and hours in which we do the research, but also in terms of developments, policy developments, scientific developments. And crazy things like this COVID. Many things have effect. The ... changes significantly because of consumption patterns for instance. They could cover .. because we still have a nice .. system. But in the future it is more complex. But yes yes there are uncertainties. The way we define extreme situations, in which we do the research, in advance. So we can do research on the safe side and try to find solutions to what if extreme cases happen. I mean, ..

- Do you take this uncertainties in your research as a part of your research?

- Yea jup jup

- And can you identify and name some of the most important uncertainties? What do you think is the most uncertain in your research.

- I think the most uncertain is what happens politically everywhere. *laughing* because this effects everything. But do you mean that in a process we have more like established a way to deal with that? I mean in my area, my field area. Not only in my field, but also in the utilities it is done this./ from political and societal. So we have the finer mechanisms, we have the .. in the case of. Because we are talking about the .. the main thing with uncertainties, because it is this system. The transition towards a clean system, it can happen very fat or very slow. Or maybe at some point discarded. If we find out a way to .. a way to manage all the abilities as we are able to do it currently. That could happen huh. There could be there reasons outside the technological part. This shouldn't be.. we are not taking another direction. So therefore we have different scenarios, three, four, paths. We defined some case studies around these paths. I think this could be a safe practice.

- It is really nice that you work with these different scenarios

- Yes because it really is better than just working with the best and worst case. So maybe you have a worst case but now we are talking about different paths and different kinds of worst cases.

- That is really cool that you work with different scenarios. I think for my communication part I'm also going to work with different kind of scenarios about a certain technology. Let me check if I have more questions. Have you cooperated with other people from e-refinery yet? Maybe outside your normal research group

- Uhmm outside my research group. They have done some work with other people from my department not my section, but other sections. People from professor power, power electronics, solar PV a bit. And I'm starting with some master student now with people from professor Mulder with the batallizer.

- How do you think the cooperation is? is there any friction point in cooperation or is everything going smoothly?

- So far it is going smooth, because I always try to see it from how do we compliment each other. So always open and positive try to discuss, maybe it overlaps. So that is that. Nowadays it that is more common. That it overlaps in the same group or even different groups. Because at some point this energy transition has grown especially in the field of energy, which has been in electrical system, exclusive to ourselves, only electrical engineers. But now we have more people talking about that and doing something. so this is a big difference. So there is a point where it overlaps, but I think if we are open and we are looking forward to see how we can cooperate and that is the most healthy approach. So.. because we are more having overlap, but at some point we are always dealing with this overlaps from a different perspective and that's what makes the difference. So that is important to first understand, what we are aiming to, what are our interest, what are we looking at. And then we can establish a mechanism, a complimentary, an collaborative work.

- I think I asked all my questions. Is there anything maybe you want to say about the project, something about cooperation or anything? something you feel like missed?

- I don't think, I haven't missed, I said to much already.

- Thank you very much. I'm gong to do a second round of interview in a few months and is it okay to contact you again?

- Yes of course.

Interview 3

- Yes we are recording. So let's start. The interview is about the e-refinery project. You're part of that right?

- Yes yes, yes I am

- What is your role in the e-refinery project group? Can you explain it to me?

- How familiar are you with e-refinery now? Very familiar?

- Uhm I read everything I could find online and I had 2 interviews so far

- Aha. So e-refinery as you know, is an institute. And it's an institute which is composed of different faculties. And what makes e-refinery different from other projects is that we are trying to increase technology development by making information flow between different aspects of technology development really fast. And with that I mean that you do generally, you have, any process, you have first a proof of concept and then comes the people from catalysis and from applied sciences and they look and say 'oh yeah the catalysis works' and then comes TMB and the people from 3ME and then you say: "can you do a pilot" and they do the up-scaling and the project part and the pilot. And once the pilot is there they give it to TBM, the people that do system analysis, and they say "oh btw what are the impacts of this?". And once that is done, they give it to TNO or to a company who will be willing to do the demonstration and do the commercial and then at the end of the commercial, before it gets into deployment, someone will for instance do an LCA and they will say “oh oops, if implemented this technology, we will create a lot of problems with for example water or CO2” and then it goes back. And they say “oh can you do something ... “ that is a very, let’s say, comfortable, because every group works in their own expertise, one step at the time. But we think that we need technologies which are ‘kant en klaar’ within a couple of years. People say ‘oh 2050’ but 2050 is actually really, really soon, in investment cycles. So if you want to do that we cannot spend 15 years of 20 years developing technologies or expecting that doing 20 years and then deciding it was a bad idea. We can’t. so want we have been thinking is, what if the people that do catalysis, directly work, really closely, with people who do prototype. And the people doing prototype, or people system analysis I mean, already know how the system looks like from the moment people are doing catalysis work. So we can do an exploration. So we can check very early on, is this a good idea. Because if you see, well, this idea uses very much critical materials, you can very early on look at for example another catalyst or do another kind of experimental work. So the idea is, can we get faster in this way? And if it is a bad idea, can we stop soon. Can we do something else. That’s were e-refinery. So if you want to do that, you really need interdisciplinary work. You need to allow people to do the fundamental work that you need to do, because this doesn’t replace what you need to do in the different fields, but you need to also have people who are really convinced that this approach could works, so they are willing to share their discoveries before they are even published with colleagues. And the colleagues can use that in order to make an analysis and give it back to them. So you need people who are open to work, people who are not from their field, who are open their knowledge, people who say this is your knowledge and I’m not going to take advantage from it I’m going to collaborate with you. And what’s yours is yours and what’s mine is mine. Very ... and that is not straightforward to do, because that is not how people work. So that is e-refinery. In e-refinery we have people from chemical engineering, applied sciences, really looking at catalysts and co2 flow and materials. We have the group of *name* looking at prototypes, moderate kind of size. We have people from electrical engineering, from the faculty, is like, this technology fits in our new system. Have a lot of electrical intensity. They know about electrical ... intensity, so they can tell you what is the quality of the energy, the voltage, what is the stability. Than you have the people in my own faculty, tbm, there is a loooong introduction to what I do, but it’s also a long introduction to what e-Refinery is, but then I look at the whole thing from a system point of view. So it is how this plant, so I do a lot of process design as well, very chemical engineering, a lot of aspen kind of modelling. So when we look and we say, okay this concept, this prototype is like this and I give you, I don’t know ethylene at 30% or formic acid at 10% out of the reactor. I’m selling this product at 99% so I need to do a lot of purification. How would the upscale industry look like , and what would be the economic proficiency, and what would be the life cycle assessment. So is it really better than we have today, because if it is not, let’s change it. We are not going to invest a lot of money in something worse than we have today. And with that I do not mean only co2 emissions, but what about the feedstock availability, what about the water use, land use, the use of critical raw materials like palladium or gold or like some of the nice things that people from catalysis really like. But I’m looking at it not from the 5 milligrams that you would use in the lab

- But what do you need when you scale it up?

- Indeed. If you’re going to do e-Refinery and electrical conversion of co2, where do you get the co2 from. How much energy do we need to get into the co2. Can an electro-chemical reactor deal with the impurity of the co2 that would come from an industry or do we need to put a bench before. Or do we need to have only co2 from this 2 sources. What about hydrogen, or the electricity stuff. If you have this scaling, how much then, of this renewable electricity extra I would need into this system. What about the sizes, you know. A lot of this could go on.. or modular units, speaking of economy of numbers in stead of a stale (?) so you know, as a chemical engineering, we go for the bigger the better. Distillation have to be, because they work the best, they get cheaper the bigger they are. But electro-chemical processes actually do not have that law of economics of a scale. So you may have those reactors that work better as a modular unit, so you do a ... tax of a chemical reactor, but my downstream processing, which ii need in order to sell my product ,is actually continuous, or is larger scale. How do I match this into a concept. So that is the kind of work we are doing, from my group, from my faculty. There are people who also look into what are the ethical issues around this. what are we telling for instance. Are we telling that we have a lot of renewable energy power electricity. That electricity needs to go first to industry than to households? And that is, you know, where is the society. Because, however abundant renewable electricity will be, it is not infinite. You will still need to have a wind park, and a PV solar. You still need equipment, so it is not like it's unlimited. You are still bounded by companies who produce electricity. And what is the best place, as a society, to put the electricity. That is an ethical question. How do you look at this. what does it mean in terms of capacity. Maybe it's good to have the industries, but than you cannot use the kind of people that we are using today. Because this are more chemical advance, who have a different kind of jobs. What are we going to do with the people who are not qualified to do this jobs. So ethical issues, what kind of institutes you need, what kind of policies you need, that is what TBM looks at. Not my group, the other departments. So the economies, the philosophers. I keep in the system analysis and chemical engineering, but they are all symbol sin e-refinery. That is actually how it works. I hope it makes it a little bit more clear.

- Yes that makes it more clear, I heard it from other people as well. It's to hear, because I talked to someone who focuses more on electrochemistry, so it's nice to hear someone who focuses more on the whole story. There are also parties involved outside the university, right, like industries. Do you cooperate with them as well? How does it look?

- E-refinery is just, it's now an institute, but you want to call it kind of a virtual institute. It is a virtual institute. It's not like a big pot of money. It's a institute with a lot of researcher within the university, say, my research or part of my research falls in this part. So that is clear. But then it comes, how do we fund the research. And that is, it's not like an institute who is going to fund your research, it's like an institute that is going to fund your research, they don't have money for that. And if you fund it only internally, they, how do you make certain that you are taking into account the constrains and all the knowledge that is outside the university. So what we do is, we fund the research via normal research goals, so NWO, horizon 2020, European money, or even a company. and then, in this consortia, which are larger than the university, then we integrate. You speak with *name*, who is our director, she will tell you about release, we are not the only university. I think all technical universities of the Netherlands are part of this. and then you have around 2 0industries which are also part of this. and because, they have knowledge, data, that we don't have. And we have data and knowledge that they don't have. So this is also like spit(??) making communication and getting funds. So they are inside by either being a passive factor, receive communication, receiving the reports, or most of the time being active where they come with the research questions saying very interesting what you are doing, but could you also look into this? and then we say what kind of research proposal? And we go together and what kind of consortia do we need, and we need to compete and sometimes we win the proposals and sometimes we lose them. The only different is that I think to know what the people also know what faculties they are applying for and what kind of PhD's they are having. And generally you don't get to know that so easily, but you could because you have a lot of free time to call everyone. But you don't and know you know quite easily , you can also say ' oh this interesting, have you been looking into this?' and then you create collaboration.

- And do you also talk to people outside university? Do you have meetings with them

- Yeah but that is normal in science. That is not.. as I said, all research proposals are not done as only TU Delft, it's always TU Delft plus, and there comes companies but there also comes the port of Rotterdam, or comes a province or a NGO, or comes.. so you. The problem is not only whether you can develop the technology, but whether you can develop the technology that can be employed. You can develop a technology, but if you really want to get it deployed you need to look at things that go beyond. You need to look at the people who would be running, you need to look at the locations that would be running, you would need to look at whether t he public would allow you to deploy the technology. And you cannot know that unless you speak with people.

- How often do you have contact with other people? Like once a week? Once a month?

- Ah that is a difficult one, I cannot speak. My projects are, depending on the project, depending on the system, corona, pre-corona hahaha. But you have, what we call, it's not, it's no measure in amount of meetings, it's measure on whether you have meetings where real information is transmitted. People have a lot of chats with a lot of people and you arrive at the end of the day where nothing new is said, or sometimes you only have one meeting once in a while that is really . . .

- Efficient?

- Yes that is really efficient and also like friendships and acquaintances. Like you can have acquaintances and that is nice and good to keep in touch, but there is nothing fundamental in your life that you are telling them. And you meet those people once in a while and you transmit a lot of knowledge and real information. And it's important that you create those, nobody needs to be meeting meeting every week, because everyone is really busy. But you make sure you meet when it makes sense to meet, when there is new knowledge, where there are milestones in projects. When they have doubts, when you have doubts.

- Do you see that enough in e-refinery? This kind of meetigs?

- Yea

- Or could it be improved?

- That is a difficult questions. I think a lot of meetings are related to the projects, are taking the project. But yeah, the e-refinery launches that happen every month are designed for internal and external people. So once a month someone from the group would present results, or someone from outside would present results to us. So that we know what they are doing. So I think that is good. And within the project that is project dependent. So I cannot answer that, because we have so many projects and all of them have different forms of communication.

- And within your project?

- Yes I meet enough. As I said it is not the number of meetings that count. it is the possibility for me to send emails as well with the real question and get answer. Or missing the reports and getting comments. Or teleconferences. Uhm. So it doesn't, we don't quantify information like. It is very the quality of the knowledge is very important. And I'm satisfied with mine at this moment.

- The quality as well?

- Yes in this moment yes, if you ask me in one month I could say no haha. It is all depending on the problem you are facing at the moment.

- Do you see any friction areas in cooperation between the different parties?

- We are learning, it is no friction, we are learning. How to work together in a way that we are not used to work together. It is no friction, it is just learning. I think we are doing a lot of trial by doing, so sometimes you notices we are meeting to frequently. And sometimes we went the other way, let's meet more frequently. And sometimes the meetings are too general, and sometimes the meetings are too specific. It goes back and forward. So I think it's working, but friction comes form trying to work and what doesn't?

- Yes yes it's also not a bad thing to have friction, if you communicate about. Do you communicate about how cooperation is done? Do people talk about it as well?

- Yes of course, it's not like a subject of a meeting, but it is really. Now with corona, are you losing the community? As well as you are losing your community of fellows at courses, and as well as in an institute it is all about having a community. So if you don't meet physically, it is more difficult. And everyone is also tired of zooming, because we're zooming the whole day. So the solution is not 'oh let's create another zoom meeting' you know. So now it is ' okay what can we do' so it's all trial and error. And sometimes it goes better and sometimes it goes less. But you, I think, it has gone much better if you think of it as an experiments in a sense. So far nobody has left angry, nobody has accused anyone of taking ownership of their ideas. Nobody has fear of replace. So I think it has gone quite well, but can it be improved, yes, but you would expect that since it is quite new. So that is.

- It is always. You always have to find a structure that works best. It's back and forward trying.

- Yes of course. And it's a virtual institute. It's not like, we don't have any employees, everyone is there voluntary. So that makes sense right. People who don't want to join, it's no problem. You can also not join. We are not going to force you to join, no.

- Are you familiar with the goals of the e-Refinery? On the website they state 3 main goals for the e-refinery project group. Do you know who is responsible for defining those goals?

- Uhm the board? I am in the board, but we are like, we have a large board, we have 10 people. So we have representations of all the faculties and all the departments. So this has gone bottom-up, we have working sessions where we sit for 3 hours what do we want to do. And what are our targets. Do we like the phrasing, because someone phrased them. But I feel like these are mine goals as well because they come from workings sessions where I have been as well.

- Can you describe a bit more about the process of defining the goals? Because you have working sessions with the board?

- No but we have had working sessions, we call strategy sessions, where we have a board plus people, where we have an agenda and we have 3 -4 hours and you go working together or working in small groups. And you ask "what are we doing, what are our targets, what makes us different, what are ours limitations, what are our lines?". So the identification of all the lines also come from the consultations with people, do we miss somethings. What are the technologies we work on? I'm not saying this is all polder, it takes a lot of polder where in the way we approach this. and sometimes we have to take in a decision that is only supported by some and not by others. But is normal. But where are we going, what do we want to reach, how are we reaching it. Those are very common discussions. And the process, it's not like the first day, they are chancing over time. And it think it took over a year for us to get those.

- So that is quite some time.

- Yeah but we don't do this full time either.

- Do you also have personal goals for your own research?

- What do you mean with that?

- Because you have aspen research?

- Yes because the idea of analysis of systems are related to the projects I have. So I'm, you mean personal by TBM goals, not my personal personal goals?

- Yes I mean like your personal goals within e-refinery. Because the e-refinery goals are so large, you cannot reach that by yourself, you need everyone.

- No no you don't, I'm on the methodology developments. if you want to see that if you are being co2 neutral, and your job is to fuel some co2 neutral chemicals, my job is to how to create the methodology to check this is the case. Or how did you do the system analysis. So what I'm doing is allowing the 'how do we do that' and the case studies to make certain that you can actually do it. But my group alone, we are not going to produce chemicals as a group. That is 100% certain. You can't, as an university you can't, we are not an industry. We are hopefully give the methodologies. Have the prototypes, have proof of concept that would allow other to do that. So the ultimate goal is more like the direction of where we are going and why are we doing it. And a lot of what we do is how do we create the tool that would allow that to happen.

- If certain goals, for example, are not reach, how does that effect those in e-refinery? How do you see that. is there any way that people have already thought about 'how we are going to deal if certain goals are not reached'?

- Why is that a problem

- It doesn't have to be a problem

- It's science

- But is it up front that people think about this already, or is it more for a later stage? How do people deal..?

- No it's not up front that we think we are going to fail.

- Haha no that's not a good mindset

- But it's also, and that is coming from science, that you keep a critical mind and think 'is this the right thing to do' and 'is this the goal' or half way we would change it. So you cannot take the goals as draft into stone and regardless. We are developing the technologies and we notice we are not able to do A and we are never going to be able to do B, C or D, then you need to modify your goal. But a part of the problem which is a problem with the Paris agreement and the sustainable development, we need to reach there. We believe we need to do that, and we going to try to contribute through this path, this way. And if halfway we find this is not the way to contribute, we will definitely reach it, we are not going to be part of the problem. But for me it is so obvious that goals are always moving goals. You need to be very critical about it. are we able to do this. and the goals that are established there are the ultimate goals and they are going to do that for instance. Producing a 100kW electrolyezr because we think it's a nice size. But maybe halfway we decide that actually what we wanted to learn with 100, we can also learn with 25. And then 100 we are going to reduce that, but not because we can't, but because it is no point to go bigger if we already learned the lessons at this stage.

- So there is a certain flexibility

- Yes because this is not a research project, it's an institute. So in that sense, an also there are goals related to individual research projects. And once you know the answers, you can say, what is the next step. We did not already find that. we think that route A would be good because of A, B, C and D. and then you can research and maybe it's not the case and then you need to say 'oh well, why?". You know, what can we learn from this. so it's no failure if you can learn. And you say, can this be used in any way, can we still go to sustainable chemicals in this pathway. And we think we can, otherwise it would be strange, but we are open to failure. And if we are going to fail, let's fail really fast so a new option can come. So that is also, if you want to fail fast, you will have to be very critical as well. Otherwise you are gonna be 'oh no, just a couple of years' that is not the point. We are not doing this because we have other research to do

- But it's also like, people react fast to how a certain technique develops

- But they react fast in the sense of you only have 25 to 30 years to change. If the option we are proposing is a disaster, let's find it in the next couple of years and not in 2040. We do think, and there are enough evidence, this is a viable pathway for somethings, and not for others. And they would require system conditions. It would require, if we know we have a lot of clean electricity. And we have a lot of industry that only works on electricity, and if the electricity is not clean, it is going to be a disaster

- It doesn't work

- It doesn't work, so we recognize, it only fits on certain characteristics of the system. That is also what we are trying to identify, which are those. And what can we tell people about those. So if you want to have this kind of industry, someone has to make certain what kind of investment or windmills that has to take place. Or on back lines or the infrastructure, that is not established. That is not the role of the university, but we can tell policy makers what kind of conditions would work with what kind of technologies.

- Okay, that is pretty interesting to look at this form a different perspective than only research, to focus more on implementation than only development or possibilities.

- Yes that is true. Haha

- I think I have one last question, because every research deals with uncertainty, you don't know how certain technologies will develop. Is there any specific way you deal with this?

- Yes we do a lot of by-work that deals with this uncertainty. Like scaling of thinks that are not there, or systems that are not there. So deal with the part that uncertainty is in the system and it is large. So then we have the methodology. So the question is not, the answer is not a sensitivity analysis, that is just a particular part of how you look at uncertainty. We look at uncertainty in the larger, you know, what are this scenarios, what are this conditions, what are the parameters in terms of ranges. But also, how much do you know about the technology, and how much are you guessing. So you can do an aspen model and you can have 3 real data and 100 points that are assumptions. And what are you modelling then, you know. You can say okay we have this and then I'm going to assume that there are no azeotropes, that it is ideal, and I'm going to assume that I can use this thermodynamic model, that there is 100% efficiency. So how you look at and identify early on, this is what I know and this is what I don't know. Sometimes we say, we are not going to do aspen, because what we are doing is just modeling uncertainties instead of modelling data. So sometimes you need more a black box model, excel based or MATLAB based. Because the only thing we know is stoichometrics or we don't know kinetics. So why are you modelling in a dynamic way if you don't know kinetics. It doesn't mean that what you produce is no useful. You just need to say, this is useful in providing what in the size. You can do a lot with prospective assessment in technology, which is what my group does ,is try to understand what are the rawest conclusions you can draw regardless of uncertainty. So we try not to give you the size of the answer is 5,3604 to the power of -3 blablabla, that is not.. decimals, really? If you have a sample of this and you do a plant like this and you are caring about decimal. The question is, do I see orders of magnitude compared to something. when is my system really changing from positive to negative, why? So you can do aspen, you can do technical analysis, you can do life cycle assessment, but you look at it in a different way than you would look at commercial technology where you have data and knowledge. So you look at it a little bit like when is my uncertainty so high that I cannot draw a conclusion. Where the difference between option A and B is for instance form 5.4 to 5.3 there is no difference. You know, it falls within the range of uncertainty. If my answer is 5 and my other system was 20 then I say okay, it looks like, with the emphasis on looks like, this system under this condition is performing better. But that is because I, if I have the knowledge, and I can say this order of magnitude difference is robust. This order of magnitude of difference is not robust. It is the same, it's the same value, so my conclusion is that there is no evidence of difference between this system and that system. So if you do the part of all this uncertainty you can look at the results and you can do this in aspen. How you look at it is different, whether you use a qualitative assessment, a scenario assessment, parameter or no parameter uncertainty analysis, all of that departing from uncertainty.

- Okay thank you so much. - You're welcome

G Systematic literature review

Search queries

Search query 1

(TITLE-ABS-KEY ("develop" OR "developing" OR "development" OR "creating")) PRE/3 (TITLE-ABS-KEY ("shared mission" OR "Shared vision" OR "shared goals" OR "shared goal" OR "shared objectives" OR "Shared targets" OR "common mission" OR "common vision" OR "common goals" OR "common goal" OR "common objectives" OR "common targets")) AND ("research institute" OR "scientific institute" OR "academic institute" OR "academic research" OR "interdisciplinary research" OR "interdisciplinary institute" OR "research organisation" OR "scientific organisation" OR "researchers" OR "research collaboration") AND (LIMIT-TO (PUBYEAR , 2020) OR LIMIT-TO (PUBYEAR , 2019) OR LIMIT-TO (PUBYEAR , 2018) OR LIMIT-TO (PUBYEAR , 2017) OR LIMIT-TO (PUBYEAR , 2016) OR LIMIT-TO (PUBYEAR , 2015) OR LIMIT-TO (PUBYEAR , 2014) OR LIMIT-TO (PUBYEAR , 2013) OR LIMIT-TO (PUBYEAR , 2012) OR LIMIT-TO (PUBYEAR , 2011) OR LIMIT-TO (PUBYEAR , 2010)) AND (LIMIT-TO (LANGUAGE , "English"))

Search query 2

(TITLE-ABS-KEY ("develop" OR "developing" OR "development" OR "creating")) PRE/3 (TITLE-ABS-KEY ("shared mission" OR "Shared vision" OR "shared goals" OR "shared goal" OR "shared objectives" OR "Shared targets" OR "common mission" OR "common vision" OR "common goals" OR "common goal" OR "common objectives" OR "common targets")) AND ("social capital" OR "social learning" OR "collaborative learning" OR "collaboration") AND NOT ("school*" OR "education") AND (LIMIT-TO (PUBYEAR , 2020) OR LIMIT-TO (PUBYEAR , 2019) OR LIMIT-TO (PUBYEAR , 2018) OR LIMIT-TO (PUBYEAR , 2017) OR LIMIT-TO (PUBYEAR , 2016) OR LIMIT-TO (PUBYEAR , 2015) OR LIMIT-TO (PUBYEAR , 2014) OR LIMIT-TO (PUBYEAR , 2013) OR LIMIT-TO (PUBYEAR , 2012) OR LIMIT-TO (PUBYEAR , 2011) OR LIMIT-TO (PUBYEAR , 2010)) AND (LIMIT-TO (LANGUAGE , "English"))

Search query 3

(TITLE-ABS-KEY ("develop" OR "developing" OR "development" OR "creating")) PRE/3 (TITLE-ABS-KEY ("shared mission" OR "Shared vision" OR "shared goals" OR "shared goal" OR "shared objectives" OR "Shared targets" OR "common mission" OR "common vision" OR "common goals" OR "common goal" OR "common objectives" OR "common targets")) AND (TITLE-ABS-KEY ("barrier*" OR "driver*" OR "factor*" OR "Condition*" OR "variable*" OR "determinant*" OR "antecedent*") AND "framework") AND (LIMIT-TO (PUBYEAR , 2020) OR LIMIT-TO (PUBYEAR , 2019) OR LIMIT-TO (PUBYEAR , 2018) OR LIMIT-TO (PUBYEAR , 2017) OR LIMIT-TO (PUBYEAR , 2016) OR LIMIT-TO (PUBYEAR , 2015) OR LIMIT-TO (PUBYEAR , 2014) OR LIMIT-TO (PUBYEAR , 2013) OR LIMIT-TO (PUBYEAR , 2012) OR LIMIT-TO (PUBYEAR , 2011) OR LIMIT-TO (PUBYEAR , 2010)) AND (LIMIT-TO (LANGUAGE , "English")) AND (LIMIT-TO (SUBJAREA , "SOCI"))

H Interview protocol and survey deepening phase

Interview protocol

Thank you for participating in this interview. This interview is part of my Science Communication master thesis project. The results of the interview will be made anonymous before using it for my research. Is it okay if I record this session?

Introduction

1. Can you shortly tell me a bit about your background, how you got involved in the e-Refinery institute and your role in the group?

Shared vision definition

2. How would you define a shared vision within the context of a research institute or research project?

3. To what extend do you think the following aspects are important when we talk about a shared vision:

- Shared goals and ambitions
- shared values
- A shared perception of the future of the project
- External visibility of the project/institute
- Shared concerns

4. To what extend would you say that a shared vision is present in the e-refinery institute?

Shared vision drivers & barriers

5. Can you name factors that positively influenced the development of a shared vision within the e-Refinery project?

6. Are there any factors that hinder the development of a shared vision?

Questions regarding the statements

7. Could you elaborate on your answer on statement X?

8. Can you elaborate why you regard statement X as 'less important' or 'not important'?

9. On statement X you disagreed, but also thought this was important, can you elaborate on that? Do you think that if this aspect was more present in the collaboration, that it would positively influence the institute?

Closing

Thank you for participating in this interview.

Survey statements

The following statements were used in the survey. All statements were asked to be rated on a five-point Likert scale ranging from 'strongly disagree' to 'strongly agree' and 'not important' to 'very important'

1. The members of the e-Refinery institute share the same overall goal
2. The members of the e-Refinery institute developed goals collectively
3. It is clear what is expected from each member in the institute
4. There are enough financial and human resources to successfully participate in the institute
5. The members of the e-Refinery institute share knowledge and views with each other
6. The members of the e-Refinery institute care about the same issues
7. I feel like I have ownership over the part I do for the e-Refinery institute
8. I'm motivated to be part of the e-refinery institute and to work towards their goals
9. In general, there is sufficient interaction with other members from the institute
10. It feels like the members of the e-Refinery institute use similar language
11. It feels like the members of the e-Refinery institute communicate on the same 'wavelength'
12. Previous relationships with others from the institute influenced the way we shaped this project
13. I trust the other members of the institute
14. I feel like the work I do is respected and appreciated within the institute
15. In general I experience the collaboration as positive

I Instructions for the tool

Instructions for the tool

The following instructions are provided for the filling in of the sub-goal page of the tool:

- Formulate a research goal that fits in your PhD project. This doesn't have to be your main research question but can be a sub-goal within your project. Write this goal down in the 'sub-goal' bar.
- In the two boxes underneath, try to describe how this sub-goal is linked to the e-Refinery institute. In the box on the right you can whether there are other members of the e-Refinery institute working on similar goals or projects.
- On the note-board you can fill in notes related to your goal
- The bar on the right, you can list some files related to this research goal.
- Under the files bar, you can list concerns related to the sub-goal. Try to indicate whether this concern is 'high', 'medium' or 'low' in priority
- The bar on the left gives an overview of members connected to your sub-goal. This can include for example your supervisor or other's you collaborate with. It's okay if you leave this bar open if you don't want to mention names of other's.

The following instructions are provided for the filling in of the sub-goal page of the tool:

- Can you think of two concerns you have (or had in the past) that relates to the previously described in sub-goal?
- Put a description of the concern in the top box (should be 1 to 2 sentences)
- Fill in the note boxes with notes related to the two concerns (here you can provide more information)
- A note can also be added by someone else from the institute, so if you have an example of how someone else helped you with that particular concern, you can add a note of that as well

The following questions were asked to the PhD students:

- Did you have trouble filling in any of the spaces? Which?
- Do you think this platform fits the e-Refinery institute? Why / why not?
- Are there any additional functionalities/options you would like to see incorporated in the platform?
- Which aspects of the platform do you like most? Which do you like the least?
- Would you personally be interested in using this platform? Why / why not?
- Do you think other members would use the platform? Why / why not?

J Codes for the discovery phase interviews

Table 77: Codes and their explanation

Code	**Description**
Challenges	Challenges that are faced within the research (technical challenges that might hinder development of certain technologies), by working together with others (i.e. colleagues, other researchers, industries, ministries) or
Communication	Descriptions of communications within the e-Refinery institute or between members of the institute and external parties.
Cooperation	Cooperation between different parties within the e-Refinery institute.
E-Refinery	Descriptions of what e-Refinery is and how the institute works.
Goals	Related to the goals of the e-Refinery institute, or to the goals of individual researchers within the e-Refinery institute
Meeting types	Types of meetings within the e-Refinery institute
Other research	How other research outside the e-Refinery institute is perceived in relation to research within the institute.
Roles	Roles that are taken on in the e-Refinery institute
Uncertainty	Definitions and descriptions of uncertainty within the e-Refinery group

Table 78: Number of codes per interview

Code	**Interview 1**	**Interview 2**	**Interview 3**	**Total**
Challenges	3	7	2	12
Communication	2	2	6	10
Cooperation	8	15	10	33
E-Refinery	0	3	9	12
Goals	8	3	8	19
Meeting types	3	0	0	3
Other research	1	0	1	2
Roles	6	6	7	19
Uncertainty	8	7	5	20
Total	39	43	48	-