

## **Travail de fin d'études et stage[BR]- Travail de fin d'études : Energy Return on Investment of Synthetic Fuels[BR]- Stage d'insertion professionnelle**

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**Faculté** : Faculté des Sciences appliquées

**Diplôme** : Master en ingénieur civil électromécanicien, à finalité spécialisée en énergétique

**Année académique** : 2021-2022

**URI/URL** : <http://hdl.handle.net/2268.2/15914>

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# Energy Return on Investment of Synthetic Fuels

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Université of Liège

Thesis presented for obtaining a Master's degree in

**Electromechanical Engineering**

**Title:**

Energy return on investment of synthetic fuels – An analysis adapted for EnergyScope

**Theme:**

Electromecanical engineering

**Project Period:**

December 2021 - August 2022

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**Copies:** 0

**Page Numbers:** 86

**Date of Completion:**

August 22, 2022

**Abstract:**

The interest in synthetic fuels is rising and is seen as a new technological challenge for the upcoming years. Synthetic fuels can be based on two primary sources, biomass or electricity, but no technologies stand out. These fuels produce a small amount of  $CO_2$ , which is not negligible for the future. The literature does not offer many compilations of  $CO_2$  emissions for those fuels. Moreover, Energy Return On Investment is a factor that comprehensively analyses the possible implementation of these fuels in the energy system. The use of EROI at a societal level is not analyzed in depth. This report aims to establish  $CO_2$  emissions and EROI values for different synthetic fuels. The data created is then implemented in the EnergyScope model to see how the world adapts to the addition of synthetic fuels. Finally, estimate the lowest emissions level reachable for 2050 and which synthetic fuels will be the more important in 2050. Determining the  $CO_2$  footprint has been conducted by looking up different life cycle assessment studies of different synthetic fuel productions. By using Simapro software, the decomposition of each process is done for energy production, production, liquefaction and transportation. The EROI is calculated using the efficiencies and the energy invested in the different inputs needed for the process. The most accessible synthetic fuel to produce is hydrogen from both analyses. The values created are given to the EnergyScope model adapted to the Belgian case. In 2050, the model reaches a  $CO_2$  reduction compared to the 2015 level of 83% using mainly synthetic fuels. In this scenario, synthetic natural gas (SNG) is the leading synthetic fuel used. Using SNG depends mainly on the balance between the efficiency of the process and transportation. The synthetic fuel used in the future depends on which technology is developed the most.

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# Introduction 1

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## 1.1 Introduction

More and more natural disasters happen worldwide, and climate change plays a big part in it [78]. Intergovernmental Panel on Climate Change (IPCC) shows that the different impacts on the environment are already rising due to greenhouse gases. If the greenhouse gas emissions are not reduced, the impacts on the environment will be even more irreversible [35]. Therefore, the need to reduce greenhouse gas emissions is required. Thus, the European Union aims to reduce greenhouse gas emissions by at least 55% in 2030 compared to the levels of 1990 and reach carbon neutrality by 2050 [26]. To reach those objectives, efficient policies must be decided to direct the different sectors of society. To help the decision-makers, models are used to define what the different energy sectors could look like in the future. Thus, several multi-energy models already exist in the literature such as TIMES [54], GENeSYS-MOd [53] and METIS [71]. TIMES is a multi-sector model capable of generating various scenarios. However, it is not open access. GENeSYS-MOd only models an energy model for heat and electricity and is a flow-based cost optimisation model. METIS is a heat and electricity sector model that optimises the energy market and electricity demand. A model representing all aspects of society, such as heating, electricity, transportation and the rest, is necessary. Unfortunately, a perfect model does not exist. Compared with previously stated energy models, EnergyScope is a model developed by Limpens [50]. It allows computing rapidly, hourly and other indicators. Limpens [50] has studied several energy systems, most of which consider cost-based objective functions. Cost-based functions do not encompass all the complexity of the future energy system, such as the technical, societal, and environmental problems. EnergyScope has been developed to analyse several indicators, including obviously cost indicator. Limpens [50] proposed a new multi-sectoral model to answer the increasing complexity of the incoming future energy system. This model, EnergyScope (ES), is open-source and optimises the investment and operation of the different energy sectors (electricity, heating, mobility, and non-energy demand).

The main indicator studied in this work is the Energy Return On Investment (EROI). EROI is a ratio of the energy produced by fuel or technology and the energy needed to produce it [38]. Using EROI rather than a cost-based function better represents the technical and social challenges [40]. The EROI also represents the link between the well-being of the society and EROI [48]. It shows the link between the human development index and the EROI. Since the lower the EROI is, the more input energy is needed, EROI allows to grasp the quality of an energy model due to the facility to understand this indicator.

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The EnergyScope model can be optimised on EROI or cost. When the model is optimised for an almost neutral carbon world, the model imports only synthetic fuels. Those have been defined to 0  $CO_2$  kg-eq, and the EROI values have been defined only using the *ecoinvent* database. Therefore, this report aims to establish new coherent values for  $CO_2$  and EROI and to give open access to them. Afterwards, the model analyses those values to see how those data change the future energy system.

### 1.1.1 Organisation of the report

The report is organised as follows:

1. In this first section, the introduction lays out the different aspect approaches and presents the rest of the report.
2. In the second section of this report, the literature review is conducted to present the state of the art in the EROI and the assessment of greenhouse gases. The gap in the literature is highlighted, and a solution to it is presented
3. In section 3, the methodology of conducting both an LCA and EROI calculation is detailed
4. In section 4, the analysis starts by collecting all the different processes of producing synthetic fuels. Then, their greenhouse gas emission is computed, and their EROI values for different scenarios. Those scenarios are for an optimist, a realistic, and a pessimist. In addition, projections for 2035 and 2050 are proposed with minimal global warming potential.
5. In section 5, the different scenarios using EnergyScope are presented and analysed.
6. In section 6, a discussion is conducted as a function of the results and the different scenarios.
7. Finally, in section 7, the conclusion is summarised all the work.

All this layout can be seen in the following Figure 1.1:



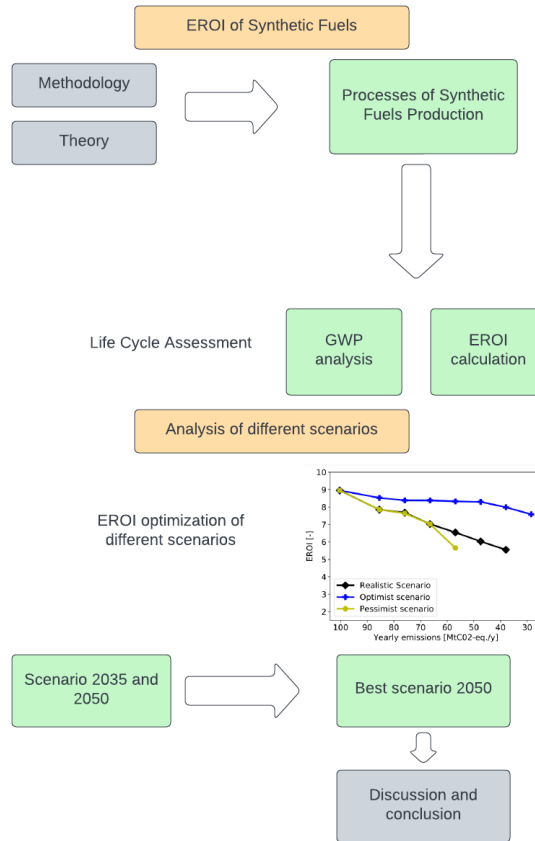


Figure 1.1. Work skeleton with the main contributions

## 1.1.2 Definitions

### Electrofuels

#### kg $CO_2$ eq

When emitting greenhouse gases, several gases has to be taken into account. Therefore, all those gases received a multiplicative factor to put them in term of  $CO_2$  equivalent. Then all those emissions are added to have an emission that can be compared between all the different processes.

### Technologies

This is the power plant used that consumes and/or produces a resource. This is an infrastructure, a mean of transport or a production unit.

### Resources

It is fuels, electricity or chemical products. It is important to make the distinctions between technologies and resources.

### Synthetic fuels

It is a fuel that is produced from a resource. Those synthetic fuels can be of any sources either from fossil fuels or renewable products.

### Bio-fuels

Bio-fuels are synthetic fuels with biomass as source.

### Electrofuels

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Electrofuels are synthetic fuels with electricity as source. Some electrofuels are called like this since they use hydrogen as a source. This hydrogen is produced most of the time through electrolysis.

**Energy Payback Time** Often referred as EPBT, this value is expressed in years. It represents the amount of time need a technology to give back the energy that has been used to create it.

# Literature review 2

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## 2.1 Literature review

The  $CO_2$  emissions are still rising every year of 400 Mt $CO_2$ -eq even if a slight slow down happened during the covid crisis [35]. Therefore, to reach the value of carbon neutrality in 2050, those emissions must be estimated correctly. The global warming potential of a product is evaluated by summing all its greenhouse gas (GHG) emissions with a specific weight, usually referred to as greenhouse gas potential. It is, for example, 25 for methane [8] which means that the methane has an impact 25 times more in terms of greenhouse gas potential than  $CO_2$ . Therefore, those GHG emissions are throughout the report expressed in  $CO_2$ -eq.

A method called life cycle assessment was developed to evaluate the global warming potential of a product in the US, first commissioned by the Coca-Cola company [29]. Then it gained much popularity during the oil crisis [6] to disappear till the beginning of the 90s when ecological awareness started to rise again [29]. The LCA has been developed and has a well-defined approach by ISO 14040 [57]. The ISO 14040 is the international standard that defines the framework of LCA into four main steps defined in SimaPro. In this project, LCA is used to determine emissions of synthetic fuels. Several times, LCA on renewable technologies has been conducted, and the values are well known [79, 33, 62]. The GHG emissions for those technologies are widely available in the literature. They are around 4-100g  $CO_2$ -eq per kWh for wind turbines and 20-300g per kWh for PV panels [27]. Those technologies are vital for producing electricity-based synthetic fuels [76, 13]. The other main mean of synthetic fuel production is biomass [46]. However, according to a recent literature review, very few papers compare biomass and electrolysis for hydrogen production [5]. For the other synthetic fuels, LCA studies are abundant but very specific. In this project, due to the number of different papers on the subject, they are stated at the moment of their utilisation.

Furthermore, Al-Breiki and Bicer [9] has looked into many synthetic fuel processes. It has studied production, transformation and transportation. This article lays a methodology used in this report even if the studied synthetic fuels. Moreover, this article does not investigate different capacity factors for renewable energy production. While compiling those different processes, the different elements required for the production are known, such as a factory, a means of transport, PV panels and wind turbines. All those elements required energy to create them, and by estimating the energy output given by the synthetic fuels the EROI can be calculated.

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Energy return on investment (EROI) is the ratio between the energy delivered to the society divided by the energy needed to receive this energy. It is a dimensionless factor, for example, an EROI of 30 represents a ratio of 30:1, where for one amount of energy given, the resource gives 30 back to society. The concept of EROI was first stated by Cleveland et al. [17] after the 1970s oil crisis when the question of how much energy is consumed by society started to gain relevance. The goal was to understand how much energy was needed to have a usable energy output. Therefore, the higher the EROI, the better the society [48]. If the EROI is under 1, it is irrelevant to use that fuel since more energy is required to produce it than it can give back. Hall, Balogh, and Murphy [38] states that the EROI is the parameter they prefer to look into in different fuels. They advocate that it allows looking more precisely than the economic market does. Sometimes the concept of energy payback time (EPBT) is used in the literature. EPBT is the time needed for a technology to give back the energy used to produce it [31]. It represents the same idea as the EROI, and their equation is as follows:

$$EROI = EPBT \times Lifetime \tag{2.1}$$

where Lifetime is the life expectancy of a power plant. Furthermore, The EROI of the oil has been decreasing since the 1900's [38]. So the EROI of the society varies proportionally even if [38] stated that it had not decreased since the 1970s. Moreover, [38] demonstrates that the minimum EROI of the society is 5. [82] propose an EROI of 7 for the good functioning of the society in first-world countries. Furthermore, [28] concludes that the EROI of the US society should be around 11 for economic growth. [48] showed a link between the Human Development Index (HDI) and the EROI. If the EROI is high, the HDI rises. When the EROI is higher than 20, the HDI reaches a maximum. To conclude, assumptions are numerous and there is no consensus about the value of EROI that the society should have to continue this way of living, but the highest the EROI is, the better it is.

Therefore, assessing the EROI from a larger perspective is necessary. Few studies have been studying the EROI at a societal level. Dupont, Germain, and Jeanmart [20] estimated the EROI on a societal level and reached the value of 8.5 for 2018. The method followed was a simple macroeconomic model with an energy sector and one regrouping the rest of the economy. The problem is that it is only evaluating the EROI at a given time and not assessing the evolution through time. Thus, Dumas et al. [19] proposed a methodology to study the EROI of an energy model for different global warming potential scenarios while considering the input's uncertainty. It allows evaluating the EROI for a whole energy system for a different configuration. In this work, since the focus is on synthetic fuels, Murphy and Hall [58] proposes that the minimum EROI for fuels is 3 to have good transportation. Chiriboga et al. [15] developed a study for bioethanol and found an EROI between 0.7 and 2.8. They still concluded that it was feasible to use bioethanol. Hacatoglu, Rosen, and Dincer [36] studied synthetic fuels for transportation and showed that the EROI at the end of use for car utilisation is between 0.8 and 1.5 for hydrogen. Once again, the EROI for synthetic fuels are very low, but there is no consensus on methodology. In addition, several examples for synthetic fuels in the literature exist [15, 39]. Unfortunately, none proposes all means of production for synthetic fuels at once. Most of the articles focus on one synthetic fuel at a time. To estimate the value of EROI of processes, Connolly, Mathiesen, and Ridjan [18] has laid down a methodology

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followed in this study. This study aims to link the analysis of a whole energy system with a multi-sectorial model and the EROI values of synthetic fuels.

The model EnergyScope takes into account the EROI as an indicator. This work follows the analysis by Limpens [50] and Borasio and Moret [7]. They analysed models comparing them between the following factors: open-source, with monthly to hourly resolution and if it takes into account the addition of electricity sector both heat and mobility sectors. In this literature review, most models use cost as an indicator, not EROI. The model MEDEAS-world is a global, one-region energy-economy-environment model [11], one of the only models that use EROI as an indicator. The EROI for this model is estimated with a life cycle analysis. For 2015 at a world level, the world states an EROI of 12 for 2015 to 3 for a 2060 complete renewable transition. In this work, the suitable model to use can be challenging to choose. Since, as Borasio and Moret [7] stated, it is almost impossible to have a model that answers all the topics and case studies, choosing the suitable model is not straightforward. Instead of creating a new model every time something specific is needed, it is better to work on existing models. The model chosen is EnergyScope TD [50]. It is an open-source, hourly resolution and low computational time model. It can be optimised on the energy system's cost and utilisation strategy for four different sectors: electricity, heat, mobility and non-energy demand. In addition, EnergyScope allows other indicators to be considered, such as the EROI.

This work is also based on what Muyldermans and Neve [59] has done previously for the EnergyScope model. Muyldermans and Neve [59] started to calculate all the different values of EROI of the different resources available in the EnergyScope model. It was mainly done using the *ecoinvent* database.

### 2.1.1 Research gaps

From there, the gap in the literature is the following:

1. Studies on EROI are specific to both technologies and resources. Therefore, it is not easy to compare those different values. Some tried to compare synthetic fuels with their fossil-based equivalent [9], but none have tried to look into a large number of processes. Concerning the  $CO_2$ -eq emission, the literature is more abundant. For synthetic fuels, works have been going on for specific applications.
2. There is no easy access to reliable data for both  $CO_2$ -eq emission and EROI for synthetic fuels.
3. no model looks at the EROI of all energy systems and how the synthetic fuels change for it.

This paper aims to complete those research gaps built on previous work of Limpens [50], Muyldermans and Neve [59], and Dumas et al. [19].

1. Collect data for all the relevant means of production of synthetic fuels and apply an LCA approach to it to determine the  $CO_2$ -eq emissions. An EROI calculation is conducted to use them in the model afterwards.
2. All the data created are open-source and used in a real case scenario for the 2035 Belgian energy system. Then those scenarios are analysed to spot the difference

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from the base case scenario.

3. Which scenario that should be followed is analysed. The goal is to find a possible  $CO_2$  reduction for 2050, which is more precise due to the determination of the GWP and EROI values to the synthetic fuels.

Moreover, all the data changes, the Simapro database [74], the spreadsheet for the EROI calculation, and the code for the different scenarios are available to help continue the work and to be transparent about the different experiments. The database can be found on this website: <https://zenodo.org/record/7014677>.

This work is to help the decision-maker use the synthetic fuels accordingly with the following questions: (1) What are the different processes for synthetic fuels production? (2) What are  $CO_2$  emissions and EROI values of those synthetic fuels following different scenarios? (3) How do those values affect the future Belgian energy system proposed by Limpens [50] and how does the model change as a function of the different scenarios?

## 3.1 Methods

This section is explaining how the analysis is carried out. Several tools and methods are necessary to analyse synthetic fuels. All processes is implemented in SimaPro with the *ecoinvent* database. The goal is to calculate each process's  $CO_2$ -eq emission and the EROI. Nonetheless, the concept of Life Cycle Assessment (LCA) is first introduced.

### 3.1.1 LCA

An LCA's goal is to collect and calculate all of the impacts that occur during the life cycle of a product and service. LCA can be applied to almost any object or event. More importantly, LCA considers all stages of the life cycle. As a result, it is possible to determine which part of the process has the most significant environmental impact. The different stages of a product emit  $CO_2$ . On the other hand, the production of synthetic fuels does not emit any  $CO_2$  since most of them use  $CO_2$  as an input or do not require it at all. Thus, it is essential to look at all the stages happening before and after the production to see if this production is  $CO_2$  neutral. The International Organisation defines the LCA with Standardisation (ISO) in the norm 14040 [57]. The norm ISO 14040 outlines the principle and framework. The main element of this norm is the four stages of an LCA. Those stages are goal and scope definition, inventory analysis, impact assessment, and interpretation. In Figure 3.1, the four stages can be explained:

1. The goal and scope is to define how the product life is taken into account and to

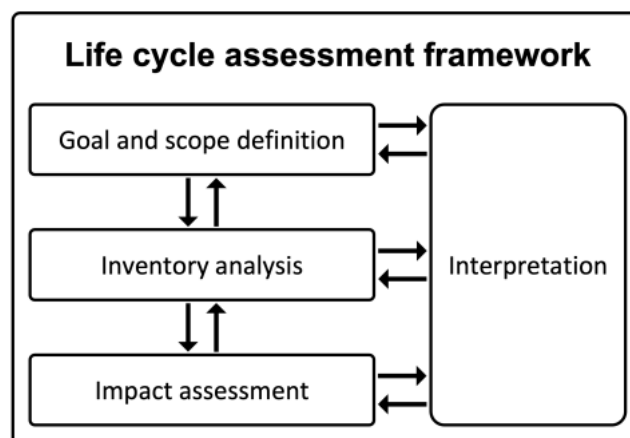


Figure 3.1. LCA stages as defined by ISO 14040 [57]

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what end this LCA is used.

2. The system inventory is the description of the material and its energy flows. It also has the different types of emissions, consumption of raw elements, and quantitative emissions to the environment. [57]
3. The data used in the inventory analysis is used for the impact assessment. It helps to determine the results of the impact categories. Those categories can be found in the definition of the SimaPro software.
4. The interpretation is quite self-explanatory. It requires critical thinking, an estimation of data sensitivity, and a good presentation of the results.

Moreover, the life cycle assessment is defined in 3 different versions:

1. **Cradle-to-Grave:** it is the LCA from the creation of the product/service through its use of it to the disposal phase of it.
2. **Cradle-to-Gate:** it is the creation of the product to the factory gate. It means that all that happens after is not taken into account. For example, in this case, it would be irrelevant to consider this scenario since the transportation of those synthetic fuels is more complex than the diesel equivalent [10].
3. **Cradle-to-Cradle:** it is a specific case of the cradle-to-grave assessment. It happens when the disposal phase is a recycle phase and produces new identical products. It can be seen as a complete loop analysis.

In the case of this project, the Cradle-to-cradle method is used as much as possible. This method is difficult to implement because the process of producing synthetic fuels, in this case, has to be incorporated into the EnergyScope model. Thus, the end of the cycle is unknown and changes at every snapshot. As a result, synthetic fuels enter the energy model directly, and the model chooses how they are used in society.

### 3.1.2 Hypothesis for synthetic fuels productions

The technologies present in EnergyScope are modelled to assess the different means of production for synthetic fuels using what has been already done in the literature. Therefore, since all the processes come from different papers, they differ from one another. Several parameters change and need to be harmonised for the sake of the comparison of the study. Different parameters are studied to handle the uncertainties:

1. The actual share of renewable energy technologies (RET) in energy production (both electricity and heat production), the various capacity factors of the RET, and the mix of means of production of the different synthetic fuels are the main elements harmonised. Each technology is presented in terms of how it is currently produced and how it may be in the future. As a result, the various processes are completed by examining what has been studied/found in the literature.
2. The various synthetic fuels are assumed to be manufactured in some locations. As a result, their transportation must be considered, as well as whether they require treatment while being transported. For example, the hydrogen must be liquefied). Producing those different fuels include a section on transitioning from one fuel to another. Furthermore, the installation is saved so that no new transportation network is created.



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3. Finally, the decided locations are essential for the fuel production from RET. Therefore, wind production is considered for countries close to Europe with a high wind potential (for example, Norway). The solar production is chosen for Morocco by being close to Europe and with high solar potential. A solar collector does the heat production.

Based on these hypotheses, the fuels studied are hydrogen, methane, methanol, ammonia, bio-diesel, and bio-gasoline. A part of the biomass is analysed for fuel production also.

### 3.1.3 EROI calculation

There are different definitions for EROI calculation. The most intuitive idea is to use cumulative energy demand (CED) that is available directly in SimaPro. Nevertheless, the CED definition in the literature and its use for EROI is unclear, as explained in Appendix A.3. By definition, the EROI of a given resource is calculated as follows:

$$EROI = \frac{E_{out}}{\sum E_{constr}} \quad (3.1)$$

where  $E_{out}$  is the energy output available in the synthetic fuel produced after all different processes, and  $E_{constr}$  is the sum of energy needed to construct and operate all the technologies used during the process and their utilisation. All those construction energies are scaled for 1 GW capacity of each process. It can be illustrated with the following example: For hydrogen electrolysis, the output is hydrogen when it arrives in Belgium, and the main input is wind electricity and water. The electricity is produced somewhere in the world, then the hydrogen is produced in a power plant, and in the end, the  $H_2$  is liquefied and transported to Belgium. So the EROI is therefore calculated as follows:

$$EROI = \frac{E_{output,WT} * \eta_{electrolysis} * \eta_{transport} * \eta_{liquef}}{E_{constr,WT} + E_{constr,Electrolyser} + E_{constr,Transport} + E_{constr,liquef}} \quad (3.2)$$

It is how the EROI is calculated throughout the rapport for all the different synthetic fuels depending on the course of their production pathways. The following hypotheses are formulated for this calculation:

1. The renewable energy technologies produce a fixed amount of electricity over time. Therefore, the capacity factor is the only factor influencing the EROI of the wind turbines.
2. It is assumed that only one technology was used for electricity production at the time. If an energy mix needs to be studied, it is created after knowing the EROI of each technology.
3. The invested energy is proportional to the energy produced by the technology as a function of its installed capacity. More precisely, once the EROI is known, this ratio is kept whatever the size of the power plant. There is no economy of scale. The EROI of one technology remains constant, whatever the size of the plant.
4. For the conventional fuels, the values in EnergyScope are used since those values are already calculated thoroughly [59].
5. It is assumed that for the transportation of those fuels, the infrastructure already exists since they existed for a long time and are being used. Since the model uses the same demand in 2050, the need for imported fuels is not going to change dramatically.

Those hypotheses are used for every synthetic fuel to be consistent throughout the report.

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### 3.1.4 Global warming potential

To estimate the  $CO_2$ -eq emissions of each process, the software Simapro was used. Simapro is explained more extensively in the following section called SimaPro. Once all the processes are defined using the database and the literature, the software provides the  $CO_2$ -eq emission and the breakdown of which input process has the most greenhouse gases impact. All the other impacts on the environment can also be calculated. The different processes are calculated for 1 kg of fuel produced. Therefore, as in EnergyScope, the resources are defined in terms of GWP per GWh. This calculation is done as follows:

$$GWP = \frac{CO_2 \text{ per kg} \times 3.6}{LHV_{fuel}} \quad (3.3)$$

where  $CO_2$  per kg is the  $CO_2$ -eq emission for 1 kg of synthetic fuels. All the data is created for the different scenarios presented before. They are used to present different scenarios of the Belgian energy system.

### Evolution of GWP and EROI in future scenarios

Several scenarios are presented for different years. The various technologies presented later are expected to be improved. As a result, each process's actual and maximum efficiencies are investigated. As technologies improve, the maximum efficiencies are considered to be reached by 2050. Furthermore, carbon footprints of electricity production from PV panels and wind turbines are likely to decrease in the future.

The IPCC projections for emission reductions in industry sectors are used to assess GWP change for material production required for these technologies [35]. The information is available in the appendix A.4. Those reductions of  $CO_2$  emission are directly removed from the production of different components necessary as input for the different processes modelled in SimaPro.

The concept of learning rate allows for assessing the change in EROI. Most of the time, learning rates link the cost of technology and its installed capacity. The learning rate is defined in a percentage representing the price decrease every time the installed capacity doubles. The same idea for the energy payback time of technology is proposed by Carbajales-Dale [12]. The learning rates are taken as 5% and 12,8% for wind turbines and PV panels, respectively [12, 45]. The evaluation of the energy invested is calculated as follows:

$$E_{inv,2050} = E_{inv,2015} * \left( 1 - LR * \text{Log}_2 \frac{cap_{2050}}{cap_{2015}} \right) \quad (3.4)$$

$E_{inv}$  is the energy invested for a given technology, LR is the learning rate, and  $cap_{year}$  is the capacity installed for a given year. Following that, the total installed capacity of wind turbines and PV panels for 2020, 2035, and 2050 must be determined and are taken in the IPCC projections [35]. The energy produced by wind turbines and PV panels is assumed to be proportional to the installed capacity to use the learning rate in the calculation of EROI directly. The change in efficiencies and learning rates from 2020 can then be used to estimate the evolution of EROI for 2035 and 2050.

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### 3.1.5 Creation of the different scenarios

For the different calculations of EROI and Global Warming Potential, several scenarios for 2035 are created. The scenarios are the following:

1. The realistic scenario: the goal of this scenario is to propose a transition that could be a possible scenario given the current technologies. It is composed of a mix of PV panels and wind turbines as the mean of production for synthetic fuels.
2. The pessimist scenario: it is used to show the worst case possible. Therefore, electricity production comes from PV panels with low capacity factors representing a poor or inefficient system. Moreover, this scenario does not consider the reduction of  $CO_2$  in the industry and the improvement of the technologies. This scenario has the highest GWP values and the lowest EROI.
3. The optimist scenario: it is the best case scenario when electricity production comes only from high capacity factors of wind turbines. This scenario has the lowest GWP values and the highest EROI.

## 3.2 Tools

### 3.2.1 SimaPro

SimaPro is a software that has been used all around the world for more than 30 years. It allows everyone to do Life Cycle Assessment (LCA) studies and changes product life cycle. SimaPro was designed to have science-based sources, providing full transparency and avoiding black-box processes [74]. Therefore, it is used for collecting, analysing, and monitoring the performance data of products [74]. In addition, SimaPro helps to model and analyses complex life cycles systematically and measures the environmental impacts. It allows access to a database called *ecoinvent* that contains several thousands of processes and their data inventory. The data inventory is the different input-output needed to produce one product. Sometimes, those products are also processed. Therefore, it creates a process tree from products to primary resources. Different methods of analysis exist. The one used in this project is called ReCiPe one and was developed between RIVM, Radboud University Nijmegen, Leiden University and PRé Sustainability [67]. This method aims to reduce the long list of life cycle inventory indicators to a manageable number. There are 18 midpoint indicators and three endpoint indicators. The midpoint indicators are investigated in this project because they allow for observing a wide range of exciting values, such as the impact of global warming impact. All the impacts can be seen in 3.2:

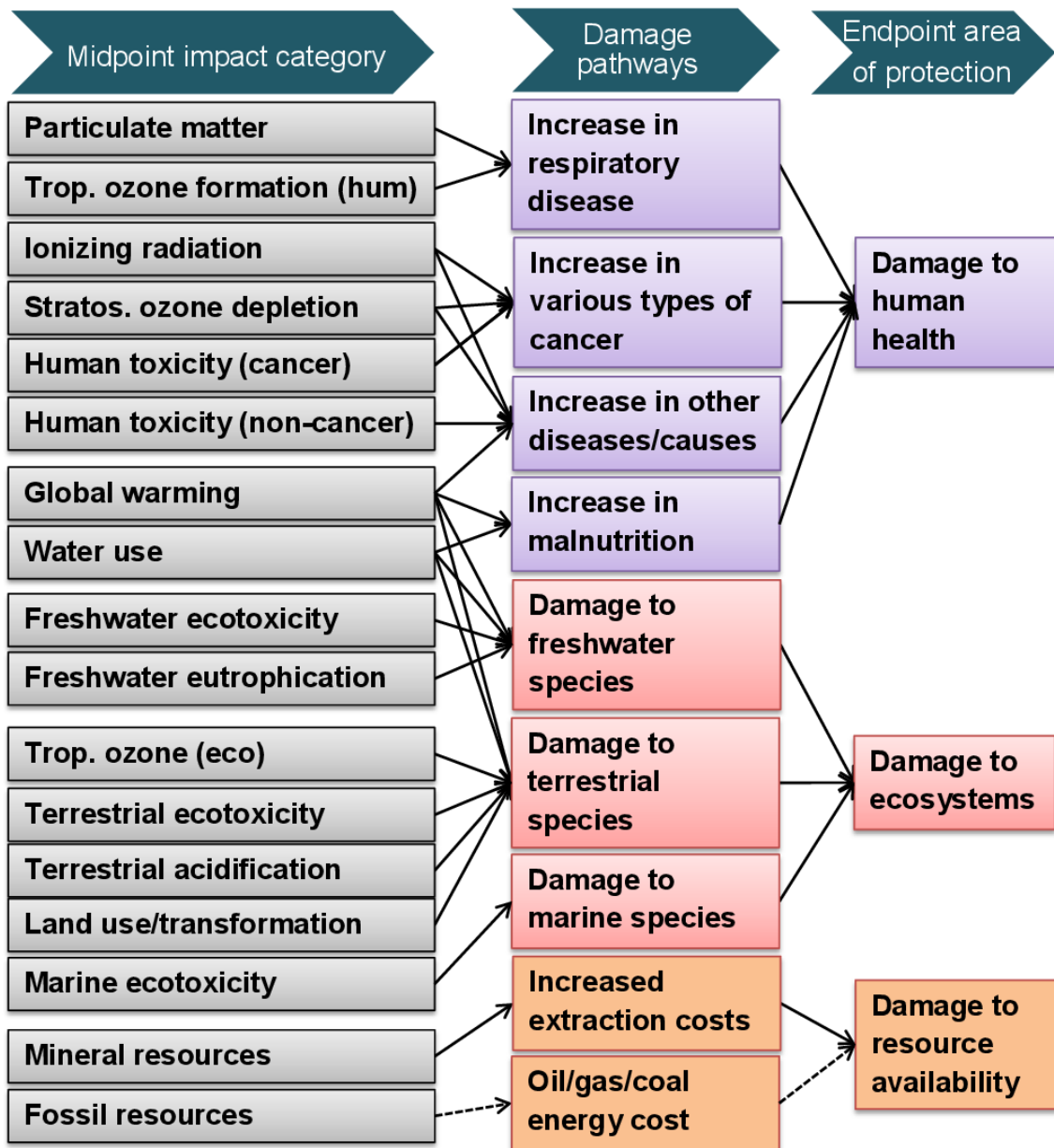


Figure 3.2. The Midpoints and Endpoints impact used by ReCiPe method [41]

In Figure 3.2, the midpoint impacts narrows down to 3 endpoint impacts. Those three endpoints impacts are useful for a rapid overview of a process and allow easily comparing two different processes. In this case, the global warming potential is the only thing considered as it is the only value that EnergyScope can consider. All the other midpoint impacts can be retrieved in SimaPro if necessary. A study in SimaPro is done by creating a process by following the four steps of the life cycle assessment as presented in SimaPro. An assembly is the combination of transportation and a process. For example, one kg of wood is transported over a certain number of kilometres. This assembly is studied by using the ReCiPe method. An example of LCA is proposed in the appendix.

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### 3.2.2 *ecoinvent*

In the LCA assessment, the *ecoinvent* database is proposed into 3 different situations called system models [22]. Choosing the right model is necessary for the good study of one process. The three main models are the following:

1. Substitution, consequential, long-term approach (consequential)
2. Allocation at the point of substitution (APOS)
3. Cut-off / recycled content approach

The consequential system model evaluates the effects of a change in an existing system using basic assumptions. This model can be used to forecast future changes. Simply put, it looks for processes that use the by-products of the investigated process. In this system model, by-products that replace another way of production bring credits to the process that produces them. It does so because it prevents using other technologies directly producing the same product. The use of co-generation plants is the best example of this. It produces heat and electricity that would have been produced by other means of production either way. Therefore, the model credits the co-generation of the other technologies' electricity that is not produced. This system model is complex and needs lots of studies to use correctly. Moreover, it requires a thorough understanding of the market, which is not the goal and scope of this study.

The idea behind allocation at the point of substitution is that the producers and users who benefit from waste by using by-products share the burdens. This system model is simple to grasp; it attempts to avoid allocations with the treatment system. For example, if waste can be burned afterwards and used to generate heat, it can be recycled. The issue with this system model is that it can be difficult to quantify all of the benefits of waste, such as the cost-benefit analysis. This system model is not used because the processes investigated produce little meaningful waste.

The cut-off approach follows the idea that the producers pay its emissions. Therefore, the waste is the producer's responsibility, and the recycled products are burden-free (cut-off). For example, if a process uses recycled paper, this system model is not taking into account all the forestry works but only the collection and the process of turning waste into recycled paper. Furthermore, waste producers do not get any credit if their wastes are reused or treated. For example, if waste is burnt for heat production, the burden goes to the one that created the waste, not the one burning them.

As a result, the system model used in this work is the cut-off approach because the first processes studied have little waste. It is also easier to use and understand for the reader.

### 3.2.3 EnergyScope

EnergyScope is an open-source energy system tool that can optimise investment and the energy system related to an area. The model is a single node model developed by Limpens [50] in a collaboration between UCLouvain and the EPFL university. It is a multi-sectoral

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model designed in a linear programming formulation. It also has an hourly resolution, thanks to the use of typical days. The typical days are defined later in this section.

### **Typical days**

First, the model works with an hourly resolution and has to balance the demand for every hour of the year. So for every hour, the demand has to be met with a mix of production. The mix of production is mainly done in two parts intermittent energies such as wind and solar panels and energies that can be deployed at any time. In addition to this, the energy demand varies during the day and throughout the year. Therefore, EnergyScope uses an hourly times series to describe all the time-dependent variables, such as the production curve of the intermittent energies and the End-use Demand. The demand is explained later in another section. Since the numbers of hours in a year are high, EnergyScope TD, to reduce the time of computation, uses those times series to create 12 typical days. It groups the 365 days into 12 days representing the year the most. 12 TD is the optimal trade-off between computational time and precision [50]. Therefore, EnergyScope optimises a year made of 12 TD instead of a whole year.

### **The model**

Three blocks are used to create an energy system, resource, technology, and demand. The model uses all those blocks to create the optimal energy system to meet the demand at any time. The blocks are the following:

1. The resources account for all the primary energies that are available. These are either produced locally, such as wind, solar energies, biomass or waste, or imported, such as natural gas, oil, hydrogen, and electricity imports.
2. The technologies make the links between the resources and the demands. In EnergyScope, the layers are using technologies to balance resources and demands. They include both the resources and the demand. The layers can be used to transform energy from a resource layer to another or a demand layer or finally to store energy. For the storage, the energy is localised in the same layer and can be put or removed at any time.
3. The demand in EnergyScope is defined as end-user demand (EUD). It differs from most models. Those models use the final energy consumption (FEC). The difference between those two is that the EUD is the energy demand expressed in terms of services. So as an example of mobility, the unit for the EUD is a passenger-kilometer. In the FEC, mobility is defined as the quantity of diesel the EUD needs for its number of passenger-kilometer. There are four sectors of EUD: electricity, heating, mobility, and non-energy demand. Finally, there is even a breakdown in the EUD, which is called the End-use Types (EUT). For the heating sectors, those are the high heat demand and the low heat demand in district heating and low heat demand decentralised.

### **Optimization problem**

The model uses EUD as input parameters. The EUD is a non-energy parameter. Then the FEC is used as the denominator of the EROI calculation. Therefore maximising the EROI

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is equivalent to minimising the denominator, which corresponds to the energy invested. It is trying to minimise the energy invested for both technologies and resources. The objective function to minimise is the following:

$$\min E_{in,tot} = \sum_{j \in TECH} \frac{E_{const}(j)}{lifetime(j)} + \sum_{i \in RES} E_{op}(i) \quad (3.5)$$

where TECH and RES are the lists of all the technologies and resources and lifetime(j) is the lifetime of a technology. It is calculated to have the system's annual energy consumed as input. The  $E_{const}(j)$  and  $E_{op}(i)$  are defined as follows and represent the annual energy invested in the system:

$$E_{const}(j) = e_{const}(j)F(j) \forall j \in TECH, \quad (3.6a)$$

$$E_{op}(i) = \sum_{t \in \mathcal{T} | \{h, td\} \in T\_H\_D(t)} e_{op}(i)F_t(i, h, td)t_{op}(h, td) \forall i \in RES \quad (3.6b)$$

Where  $e_{const}(j)$  in [GWh/GW] is the fixed value of energy invested in the construction of the technology j, this is a cumulative energy demand for a 1 GW powerplant. This value is multiplied by F(j) [GW] or GWh for storage technologies which is the installed capacity of the technology. For  $e_{op}(i)$  in [GWh/GWh<sub>fuel</sub>] is the fixed value of the energy invested in operation of the resource i for 1 GWh<sub>fuel</sub>.  $F_t(i, h, td)$  [GWh] is the quantity of fuel used during the hour  $h$  of the typical days  $td$ .  $t_{op}(h, td)$  is time period duration (normally one hour).  $\mathcal{T}$  is the set for all a year (8760 hours),  $T\_H\_D(t)$  is the hour  $h$  and the typical days  $td$  associated with the period  $t$ . Summing all the different typical days and the hours of those using  $T\_H\_D(t)$  is equivalent to the 8760 hours of the year.

The global warming potential is examined in EnergyScope TD to assess climate change. The annual greenhouse gas emissions [MtCO<sub>2</sub>-eq./y]  $GWPt_{tot}$  is calculated as the sum of two factors. First, the emission of technologies during construction, operation and maintenance, and decommissioning is reported to be for one year. Second, there are emissions associated with the operation of the resources. These emissions are described below.

$$GWPt_{tot}(j) = \sum_{j \in TECH} \frac{GWP_{const}(j)}{lifetime(j)} + \sum_{i \in RES} GWP_{op}(i) \quad (3.7a)$$

$$GWP_{const}(j) = gwp_{const}(j)F(j) \forall j \in TECH \quad (3.7b)$$

$$GWP_{op}(i) = \sum_{t \in \mathcal{T} | \{h, td\} \in T\_H\_D(t)} gwp_{op}(i)F_t(i, h, td)t_{op}(h, td) \forall i \in RES \quad (3.7c)$$

Therefore, it is the same idea as for the EROI. The emissions for technologies are the constant value times the installed capacities F. The emissions for the resources are the for fuels from cradle to consumption multiplied by quantity used  $F_t(i, h, td)$  and the duration  $t_{op}(h, td)$ . Finally, the optimisation is defined by a target  $gwp_{limit}$  on the annual emission  $GWPt_{tot}$  as follow:

$$GWPt_{tot} < gwp_{limit} \quad (3.8)$$

The goal is to put an upper bound on the system to have a limit to work with. It allows the model to optimise while constraining the CO<sub>2</sub> emissions. In the end, the EROI that

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is shown in different graphs of this report is computed after the simulation with:

$$E_{out} = FEC \tag{3.9a}$$

$$E_{in} = \arg \min E_{in,tot} \tag{3.9b}$$



# Analysis 4

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## 4.1 Energy conversion pathways and processes

The following section presents several processes. The goal is to have a better understanding of the different technologies that exist for synthetic fuel production. First, the different means of production are presented. Secondly, different processes existing in EnergyScope are modelled. Then the liquefaction and transport of those fuels are analysed. From there, the EROI is calculated. Finally, discuss the results and see if the data created is coherent with the literature.

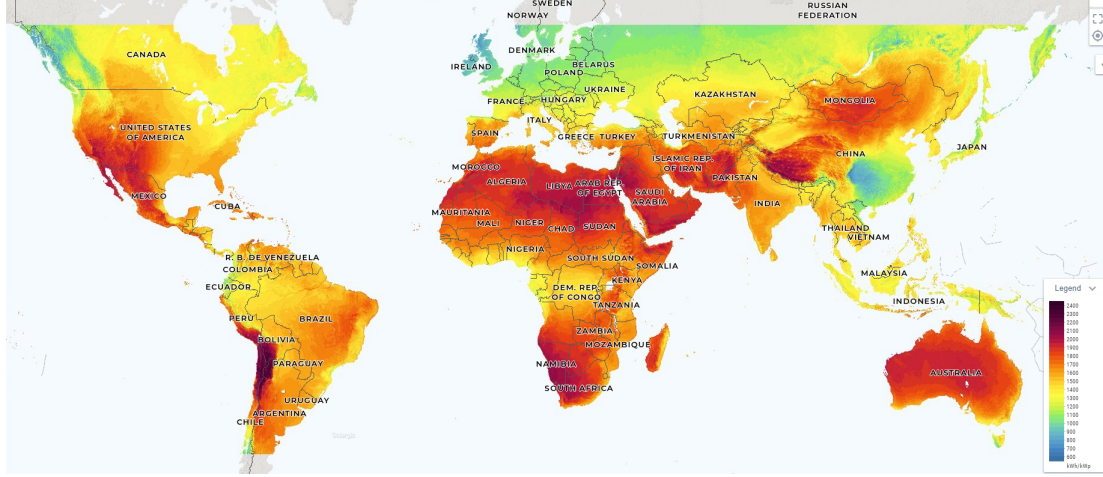
### 4.1.1 Energy Production

This section shows the different means of electricity production. Those electricity productions are primarily used as input for synthetic fuels such as hydrogen through electrolysis. First, wind power production is looked into for Norway. resources and (NVE) [66] in 2013 showed that wind power capacity factors in Norway are between 36 and 50%. Therefore, the LCA of production for 1 kWh can change a lot in function of the capacity factor, and  $CO_2$  emission also varies accordingly. The  $CO_2$ -eq emissions are as follows in Norway:

| Capacity factor (%)           | 30   | 40   | 50   | 60   | 70   |
|-------------------------------|------|------|------|------|------|
| g $CO_2$ -eq emission per kWh | 16.1 | 12.1 | 9.73 | 8.14 | 7.01 |

**Table 4.1.**  $CO_2$ -eq emissions of a wind turbine in Norway as a function of the capacity factor

Then, the PV panels production is analysed for the Morocco region as an example which is a region with high solar potential, as can be seen in the following map:



**Figure 4.1.** Solar potential map [3]

In Figure 4.1, the regions of the world with the highest solar potential are the African Saharan region, the middle east, the north of Chile, and Australia. The significant regions studied are Chile, Morocco, and Australia for their political stability compared to the others in the region [23]. In this project’s scope, Morocco is taken into account as the first assumption since it is the closest to Europe. Table 4.2 show how the capacity impacts the  $CO_2$ -eq emissions of PV panels:

| Capacity factor (%)      | 10  | 15   | 20 | 25 |
|--------------------------|-----|------|----|----|
| $gCO_2$ emission per kWh | 130 | 86.6 | 65 | 52 |

**Table 4.2.**  $CO_2$  emission as a function of the capacity factor for a PV placed in Morocco

The tables 4.1 and 4.2 indicates that the  $CO_2$  emission ranges from 7g per kWh to 130g per kWh, which makes rather a wide range to base the production of fuels on. As Muyldermans and Neve [59] used in their work, the energy mix used for the synthetic fuels energy input consists of 80% of high-quality PV panels and 20% high-quality wind turbines. It is considered that the wind turbines and PV panels are installed in efficient locations. Therefore, a capacity factor of 25% corresponds to PV panels in Chile and Morocco, and for wind turbines, a capacity factor of 60% is kept. Therefore, the mean emission for electricity production is 43g per kWh or 12g per MJ.

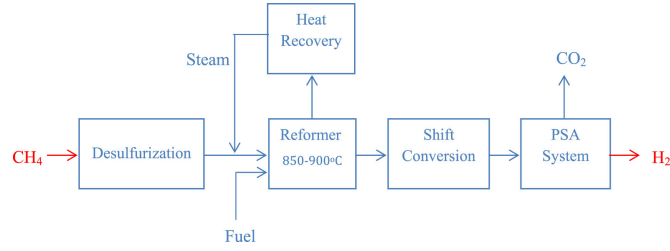
#### 4.1.2 Hydrogen Production

In this project’s scope, hydrogen production is taken into account for several different technologies. For hydrogen production, in EnergyScope, four of them are listed, one from methane, one from electrolysis, one from biomass and one from ammonia. Therefore, the main current mean of production is hydrogen production from steam methane reforming (SMR) [47].

#### Steam Methane Reforming

This process accounts for 96% of the actual production. [60, 47] It consists of a steam reformer that produces from a given gas with a  $C_nH_m$  structure into CO and  $H_2$ . After

that, a water-gas shift reactor (WGS) transforms the CO and water into  $CO_2$  and  $H_2$ . A simple schema can be seen underneath:



**Figure 4.2.** Flow diagram of the SMR process

Figure 4.2 shows that the process requires fuel and heat. Nikolaidis and Poullikkas [60] stated that the process has an efficiency of 74 to 85% and a capacity factor of 90%. The data inventory of the process is available [43]. The model presents the input-output for a process and can be remade in SimaPro by recreating the process.

| Inputs                | Values | Outputs              | Values |
|-----------------------|--------|----------------------|--------|
| Water ( $m^3$ )       | 0.46   | Wastewater (kg)      | 90     |
| Natural gas ( $m^3$ ) | 3.03   | Carbon dioxide (kg)  | 5.18   |
| Heat from steam (MJ)  | 24.5   | Carbon monoxide (kg) | 0.2632 |
| Steam (kg)            | 6.4    | Hydrogen (kg)        | 1      |

**Table 4.3.** The input/output values for SMR for 1 kg of hydrogen

The process produces 5.18 kg  $CO_2$  eq per kg of hydrogen produced. The total actual life cycle assessment is of 10.5 kg  $CO_2$  eq which also what Spath and Mann [73] observed. The LCA mainly considers the global warming potential from natural gas extraction and the heat needed for the process. All the inputs and outputs are taken for Morocco since it is one of the locations studied. As shown in Figure 4.2, this way of producing hydrogen is a carbon incentive. Therefore, alternatives like using green gas for this process or electrolysis must be explored.

## Electrolysis

Since the rise of RET and the need to phase away from carbon-based fuels, the use of electrolysis for hydrogen production seems possible in the future. The electrolyser modelisation is not that complicated since the technology has existed for a long time and has been established [47]. The idea is quite simple to use water to produce hydrogen. The water is decomposed into oxygen and positive hydrogen ions, and the hydrogen is formed at the cathode. This process has an actual efficiency of 60 to 80% [47]. Therefore, the electrolyser model taken into account in SimaPro is given in table 4.4

| Inputs            | Values | Outputs       | Values |
|-------------------|--------|---------------|--------|
| Water ( $m^3$ )   | 0.018  | Oxygen (kg)   | 16     |
| Electricity (kWh) | 79     | Hydrogen (kg) | 1      |

**Table 4.4.** The input/output values for electrolysis for 1 kg of hydrogen

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The Life Cycle Assessment shows a  $CO_2$ -eq emission of 1 kg per kg of  $H_2$ . In addition, the process does not produce any  $CO_2$  since there is no carbon included in the process. Therefore, electrolysis is mainly dependent on the emissions due to electricity production.

### Hydrogen from Biomass

Hydrogen production from biomass (ex: pine) is studied in Kalinci, Hepbasli, and Dincer [46]. This paper studied two different types of biomass gasification for hydrogen production. It removes the hydrogen from the syngas produced through a PSA unit. The system is modelled as follows using the data available from Kalinci, Hepbasli, and Dincer [46]:

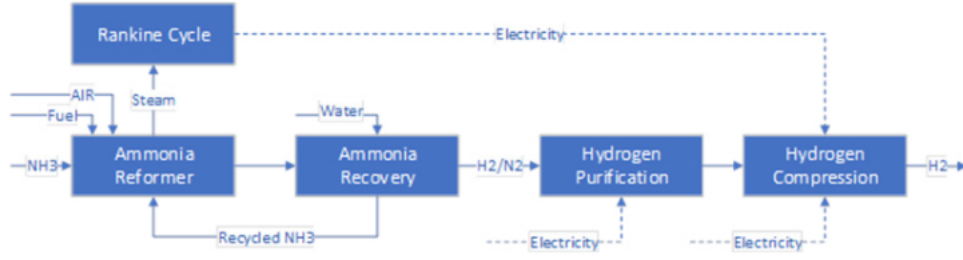
| Inputs          | Values | Outputs           | Values |
|-----------------|--------|-------------------|--------|
| Wood chips (kg) | 22     | $CO_2$ (g)        | 22.5   |
|                 |        | Electricity (kWh) | 10     |
|                 |        | Hydrogen (kg)     | 1      |

**Table 4.5.** The input/output values for wood with gasification for 1 kg of hydrogen

The  $CO_2$  presented in Figure 4.5 accounts for the embodied energy of the power plant. The embodied energy is the  $CO_2$  and energy needed for the power plant's construction, maintenance, and decommissioning. Therefore, this is 1kg of hydrogen emission, considering that it is a part of the lifetime production. It is important to note that this means of production is made for small applications. Without accounting for the transport and only the hydrogen production, the  $CO_2$ -eq emission is -2.91kg per kg of hydrogen. Simapro considered that the electricity produced from the process equals the  $CO_2$  emission of the current electricity mix in Europe. Therefore, it allows to not produce  $CO_2$ . In reality, this  $CO_2$  emitted is equal to 0.795 looked with removing the electricity produced by the process. To conclude, hydrogen production in the future is probably done using electrolysis since the values of  $CO_2$  emissions are already relatively low. If the efficiency of the different processes is compared, electrolysis is less efficient than hydrogen by biomass production. In the future, this may change since the electrolysis is underdevelopment. Finally, biomass is used to create different products (other biofuels) and is already limited in EnergyScope.

### Hydrogen from ammonia

Ammonia is seen as a possible way of energy carrier. Therefore, the possibility to transform ammonia into hydrogen has to be studied. The ammonia is decomposed into hydrogen and nitrogen. The process is as follows:



**Figure 4.3.** process to produce hydrogen from ammonia [24]

Figure 4.3 is a simpler process than the one used in Cha et al. [14]. The process consists of an ammonia reformer, but an ammonia loop is necessary since the Sabatier reaction is not efficient enough. Since high purity of hydrogen is necessary, purification is done, followed by the compression of this hydrogen. The process is, therefore, as follows [14]:

| Inputs           | Values | Outputs       | Values |
|------------------|--------|---------------|--------|
| Ammonia (kg)     | 43.177 | Nitrogen (kg) | 4.67   |
| Natural gas (kg) | 6.042  | Hydrogen (kg) | 1      |
| Air (kg)         | 193.17 |               |        |

**Table 4.6.** The input/output values for ammonia transformation through Sabatier reaction for 1 kg of hydrogen

The LCA here does not take into account the power plant use. Therefore, the  $CO_2$  emissions are a bit underestimated. This process produces if the ammonia comes from a green source 81 kg of  $CO_2$ -eq and if the ammonia comes from an actual source 141 kg of  $CO_2$ . This high production of  $CO_2$  is since the heat needed for the process comes still from natural gas.

### 4.1.3 Ammonia Production

Nowadays, the use of ammonia is already widely used in the industry. The power plant already exists, and the systems of transportation exist also. More than 96% of the ammonia is produced through this route [72]. Therefore, for ammonia production, the hypothesis made is that for ammonia production, there is a need for hydrogen and nitrogen. Therefore, the Haber-Bosch process is adapted to have an electrolyser to avoid  $CO_2$  emissions. The actual Haber-Bosch process is as follows:

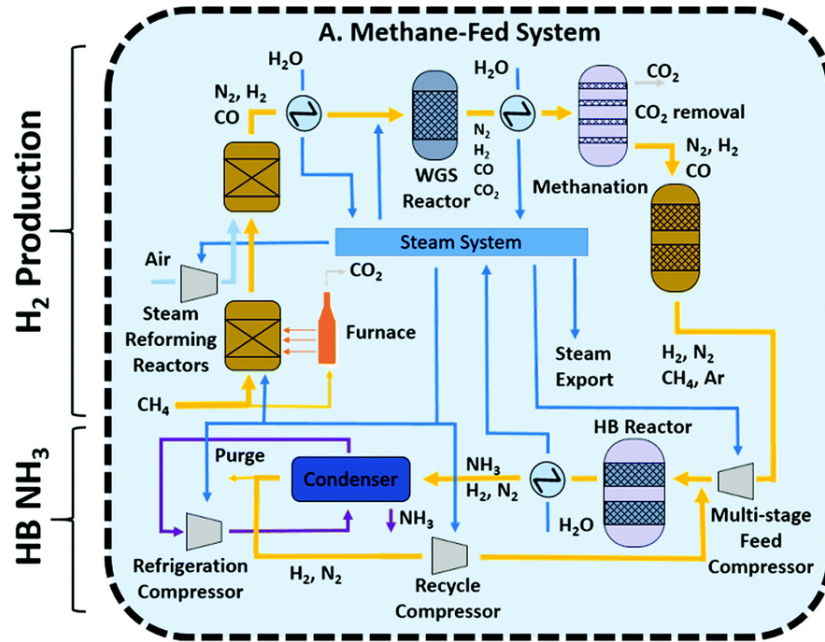


Figure 4.4. Typical Haber-Bosch Process [72]

In Figure 4.4, it can be seen that the process uses an SMR to produce the hydrogen as shown in Hydrogen Production. Moreover, ammonia production consists of the Haber-Bosch process, which uses nitrogen and hydrogen to reform ammonia. Therefore, since the reaction is endothermic, a high temperature is needed. The process already exists in Simapro and is as follows:

| Inputs                | Values  | Outputs             | Values |
|-----------------------|---------|---------------------|--------|
| Water ( $m^3$ )       | 0.14    | Carbon dioxide (kg) | 1.44   |
| Natural gas ( $m^3$ ) | 0.625   | Nitrous oxide (kg)  | 0.0007 |
| Nickel (kg)           | 0.00035 | Water ( $m^3$ )     | 0.0544 |
| Solvent (kg)          | 0.0007  | Nitrogen (kg)       | 0.0012 |
| Heat (MJ)             | 15.66   | Ammonia (kg)        | 1      |

Table 4.7. The input/output values for Haber-Bosch process for 1 kg of ammonia

It produces 2.78 kg  $CO_2$  eq. emission for 1 kg of ammonia. This process is already efficient since it has existed for a long time and is also responsible for 1.8% of worldwide greenhouse gas emissions.

### Green ammonia

To avoid natural gas as input of the process, the SMR can be replaced by an electrolyser and PSA for both nitrogen and hydrogen production. This process can be seen in the following figure:

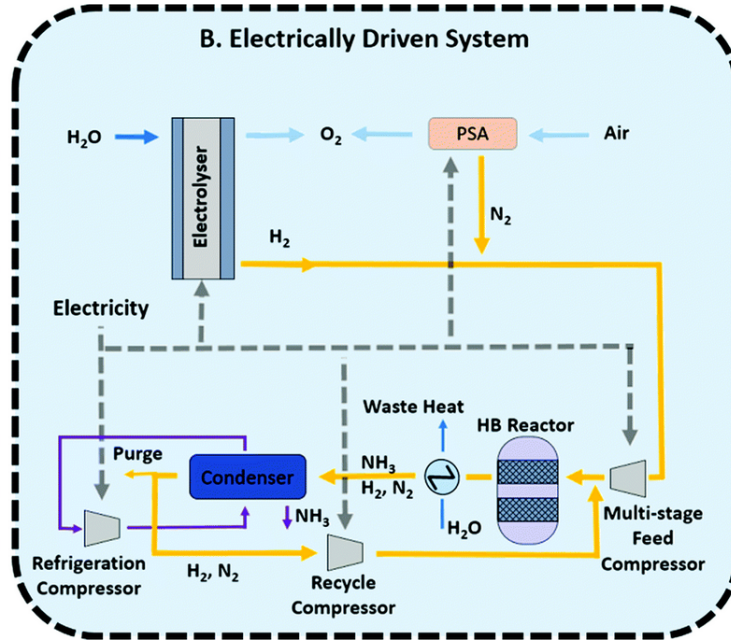


Figure 4.5. New generation of Haber-Bosch Process [72]

As seen in Figure 4.5, the process is fully electrified, and the ammonia production process stays the same. This process is modelled in Simapro, considering that the heat required stays the same because the SMR does not consume much heat compared to the Haber-Bosch process. This process is modelled as follows:

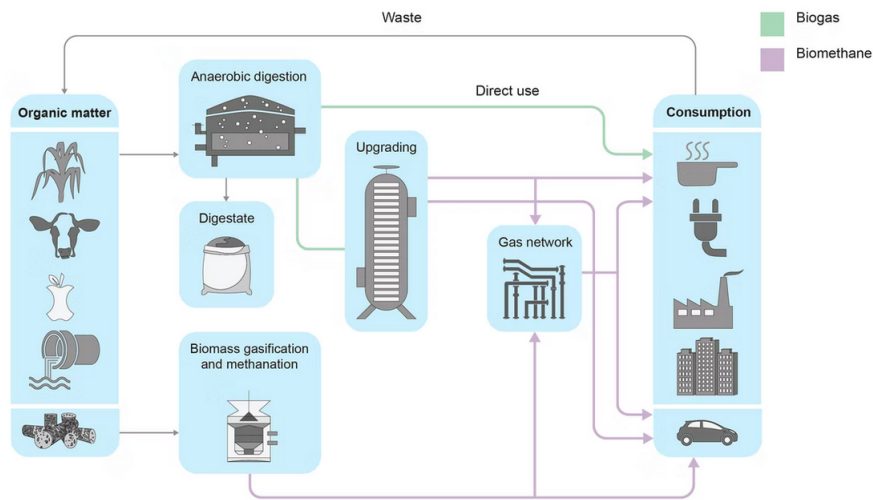
| Inputs          | Values  | Outputs            | Values |
|-----------------|---------|--------------------|--------|
| Water ( $m^3$ ) | 0.14    | Ammonia (kg)       | 1      |
| Hydrogen (kg)   | 0.117   | Nitrous oxide (kg) | 0.0007 |
| Nickel (kg)     | 0.00035 | Water ( $m^3$ )    | 0.0544 |
| Solvent (kg)    | 0.0007  | Nitrogen (kg)      | 0.0012 |
| Heat (MJ)       | 15.66   |                    |        |
| Nitrogen (kg)   | 0.823   |                    |        |

Table 4.8. The input/output values for Haber-Bosch process for 1 kg of ammonia

This process produces twice less  $CO_2$  than the methane-fed process (in Morocco). In the literature, Smith, Hill, and Torrente-Murciano [72] states that today's best technology requires 30MJ/kg of ammonia and that the theoretical best electrical is 48MJ per kg. Therefore, at first glance, the EROI of green ammonia production is lower than the actual ammonia production. This system is, therefore, less efficient than the actual Haber-Bosch process.

#### 4.1.4 Biogas Production

The production of biogas is the production of a synthetic fuel composed of natural gas and  $CO_2$ . Other elements can be present as oxygen and nitrogen, but this is not a generality [49]. The biogas is not used directly in Energyscope. Biogas gas is often necessary to produce other synthetic fuels such as biomethane from a biomass source. The process of biogas production is the following:



**Figure 4.6.** Multiple types of biogas and biomethane production [42]

In Figure 4.6, there are different ways of production and different sources for carbon and hydrogen. Europe’s primary means of production are crops, animal manure, and waste[42]. The way to produce biogas is through anaerobic production, which transforms glucose into methane and carbon dioxide.

### Biomethane

From there, the biogas can be upgraded to biomethane through different processes. The different processes are pressure swing adsorption, membrane separation, cryogenic separation, and absorption techniques. This process exists in Simapro; therefore, the modelling of it is kept as it is:

| Inputs            | Values | Outputs              | Values |
|-------------------|--------|----------------------|--------|
| Water ( $m^3$ )   | 0.577  | Carbon dioxide (kg)  | 5      |
| Wood (chips) (kg) | 3.8    | Carbon monoxide (kg) | 0.0035 |
| Electricity (kWh) | 0.835  | Biomethane (kg)      | 1      |
| Heat (MJ)         | 0.0061 |                      |        |

**Table 4.9.** The input/output values for biomethane production from wood for 1 kg of ammonia

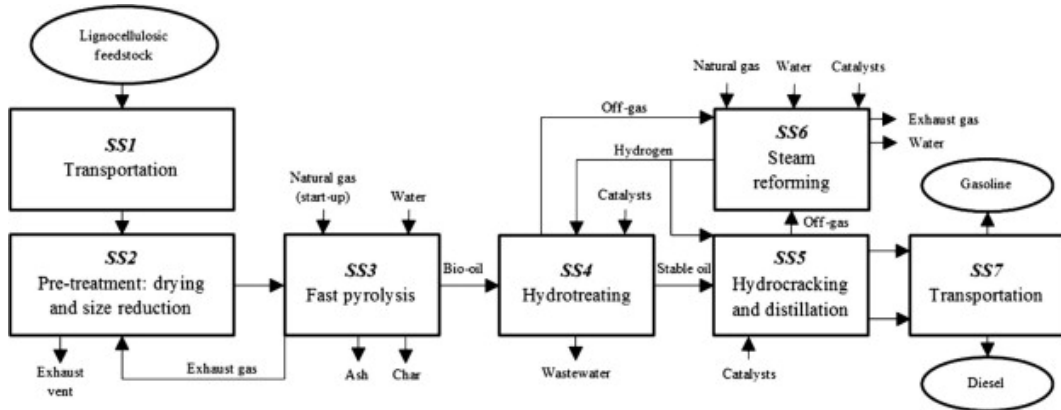
This way of production was chosen because it is already implemented in EnergyScope. It is producing of biomethane with an LHV of 25 MJ/kg. The efficiency is changed to model the future technologies and the use of the electricity needed for the process. The  $CO_2$ -eq emitted is 0.58 kg per 1 cubic meter of natural gas produced. This process seems efficient, but since it is based on an existing process and in the *ecoinvent* it is reliable.

### 4.1.5 Biodiesel and Biogasoline

The bio-oil production is based on different types of biomass. The pyrolysis of wood can be a way to produce biodiesel and biogasoline. This process produces a bio-oil then



hydrogen is needed to create vehicle-grade oil. Therefore, the production is following the process proposed by Iribarren, Peters, and Dufour [44]:



**Figure 4.7.** Biodiesel and biogasoline process [44]

As seen in Figure 4.7, the all process is quite complex, but the hydrogen production could be replaced by electrolysis to emit even less  $CO_2$ . Unfortunately, the process is so complex that it would be too difficult to determine since what is happening inside is not clear/unknown. The process input/output is as follows:

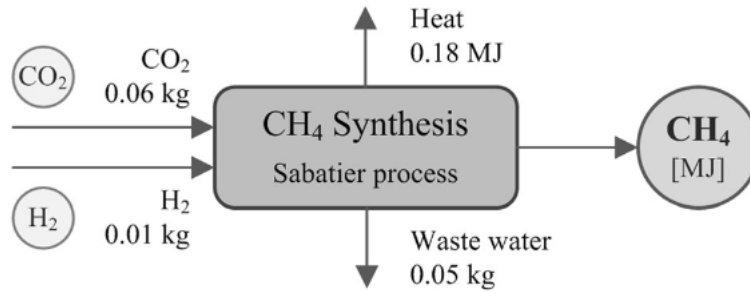
| Inputs                  | Values | Outputs               | Values |
|-------------------------|--------|-----------------------|--------|
| Cooling Water ( $m^3$ ) | 0.843  | Carbon dioxide (kg)   | 1165   |
| Natural gas ( $m^3$ )   | 329    | Water (to air) (kg)   | 427.14 |
| Electricity (kWh)       | 134.4  | Water (to water) (kg) | 287    |
| Metal catalyst (kg)     | 1.52   | Biogasoline (kg)      | 427    |
| Bio-oil (kg)            | 2265   | Biodiesel (kg)        | 573    |

**Table 4.10.** The input/output values for biogasoline and biodiesel production from wood [44]

The results are that 52.8 kg of  $CO_2$ -eq emitted for both fuels since it is the same process. The main reason for the pollution is due to the catalyst requirement. The energy invested is high due to the number of wood chips necessary.

#### 4.1.6 Methane

It is possible to create methane using hydrogen and  $CO_2$  using the Sabatier reaction. This reaction allows producing natural gas for the actual power plant and the transport of methane since the infrastructures already exist. The process is as follows:



**Figure 4.8.** Sabatier process for 1 MJ of  $CH_4$  [64]

In Figure 4.8, the reaction takes as input hydrogen and carbon dioxide to produce methane. In Simapro, since every process works with 1kg of fuel, those values have to be scaled to the following:

| Inputs              | Values | Outputs      | Values |
|---------------------|--------|--------------|--------|
| Carbon dioxide (kg) | 3      | Water (kg)   | 2.5    |
| Hydrogen (kg)       | 0.5    | Heat (MJ)    | 9      |
|                     |        | Methane (kg) | 1      |

**Table 4.11.** The input/output values for Methane Production from hydrogen for 1 kg of methane

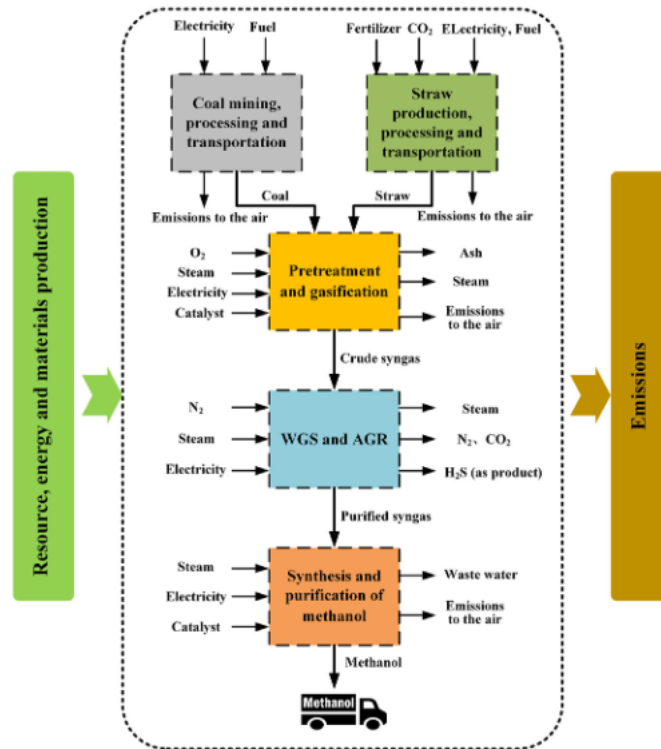
The  $CO_2$  necessary in this process has to come from somewhere, either from industry or from biomass [64]. The hydrogen can be produced from electrolysis. This process produces 0.6  $CO_2$ -eq per kg of methane which is not a lot, but it depends a lot on how the electricity is produced to deliver the hydrogen. Heat production can be seen as a way to economise  $CO_2$ . Nevertheless, like hydrogen production from biomass, negative  $CO_2$  emissions are not considered.

#### 4.1.7 Methanol

Methanol can be used for transportation purposes [10]. It can also be necessary for non-energy demand products. Therefore, several means of production of methanol are studied.

##### Methanol from wood

Methanol can be produced from wood pyrolysis. It is the method that can be used for biomass in order to produce methanol. The process is as follows:



**Figure 4.9.** Methanol production from wood (life cycle assessment) [52]

The process, in Figure 4.9, on the right side of the picture, is the one studied. The biomass is first gasified and passed in a water gas shift reaction. Then the synthesis and purification are performed. Since the process in [52] is based on straw, another process from Yadav et al. [84] is used:

| Inputs                | Values | Outputs        | Values |
|-----------------------|--------|----------------|--------|
| Water ( $m^3$ )       | 22.87  | Calcium (kg)   | 1.11   |
| Sodium Carbonate (kg) | 1212   | Magnesium (MJ) | 0.46   |
| Oxygen (kg)           | 1051   | Methanol (kg)  | 1000   |
| Wood chips (kg)       | 1430   | Potassium (kg) | 1.22   |
| Electricity (MWh)     | 0.94   | Sodium (kg)    | 0.25   |
| Heat (MWh)            | 0.84   |                |        |

**Table 4.12.** The input/output values for Methanol Production from wood for 1000 kg of methanol

The process presented in 4.12 produces 80g of  $CO_2$ -eq, which principally comes from the electrical and heat needed for methanol production.

### Methanol from methane

Methanol can also be produced using the natural gas route. Therefore, the process is as follows:

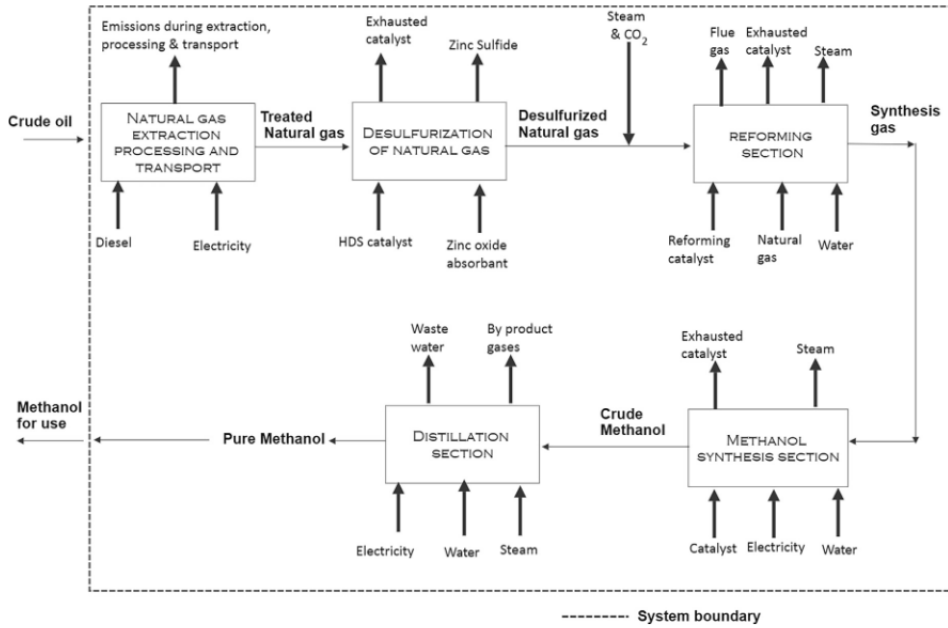


Figure 4.10. Methanol production from methane [75]

In Figure 4.10, the steps from the crude oil to the methane are not taken into account and considered Simapro already does that. From there, an SMR is done, then a methanol synthesis. Methanol is purified to achieve a high quality. The process is therefore modelled as follows [75]:

| Inputs            | Values  | Outputs           | Values |
|-------------------|---------|-------------------|--------|
| Air (t)           | 23962   | Waste Water (kg)  | 176    |
| Water ( $m^3$ )   | 7776    | Carbon oxide (kg) | 176    |
| Methane ( $m^3$ ) | 1712000 | Methanol (t)      | 1000   |
| Electricity (MWh) | 539.136 |                   |        |

Table 4.13. The input/output values for methanol production from natural gas for 1000 tons of methanol

In the table 4.13, this process produces 2 kg of  $CO_2$ -eq emission, mainly from the production of methanol in itself. The process is also quite efficient, more or less 50%.

### Methanol from hydrogen

Methanol can also be produced from hydrogen and requires a  $CO_2$  source. The process in itself is not that different from the picture 4.13 since it is the same idea to have a steam reforming reaction [68]. The process is as follows:

---

| Inputs              | Values  | Outputs           | Values  |
|---------------------|---------|-------------------|---------|
| Carbon dioxide (kg) | 1441    | Waste (kg)        | 578     |
| Hydrogen (kg)       | 203     | Carbon oxide (kg) | 66      |
| Electricity (kJ)    | 1188000 | Methanol (kg)     | 1000    |
|                     |         | Heat (kJ)         | 1400000 |

**Table 4.14.** The input/output values for methanol production from hydrogen for 1000 kg of methanol [68]

The process in table 4.14 produces 0.226 kg of  $CO_2$ -eq per kg of methanol. This emission is principally due to the hydrogen electrolysis and the  $CO_2$  that does not react during the process. In addition, the process requires 45.3 MJ of energy which makes the process in terms of invested energy the same as the production of natural gas.

### Electricity import

Instead of importing fuels, the model could import electricity directly and considers it to be from a mix of different countries:

| Country       | Percentage of importation |
|---------------|---------------------------|
| Netherlands   | 0.2                       |
| Luxembourg    | 0.1                       |
| France        | 0.4                       |
| Great Britain | 0.1                       |
| Germany       | 0.2                       |

**Table 4.15.** Proportion of the imported electricity for Belgium as a function of the countries

Those values have been estimated using the different transfer capacities installed with Belgium and surrounding countries [25]. The emission is of 0.252 kg  $CO_2$  eq. per kWh of electricity. In comparison with the other process, this is quite high. However, this value is lower and lower since the  $CO_2$  emission due to electricity production in those countries will decrease due to the rising share of renewable energy.

### 4.1.8 Results

The results from the different technologies using the scenario that is considered the most plausible are as follow :

| Means of production                     | Synthetic fuels | $CO_2$ emission (kg $CO_2$ eq.) |
|---|-----------------|---------------------------------|
| Steam Methane Reforming                 | $H_2$           | 10.5                            |
| Electrolyser                            | $H_2$           | 0.898                           |
| Hydrogen from wood                      | $H_2$           | 0.795                           |
| Hydrogen from actual ammonia production | $H_2$           | 141                             |
| Hydrogen from green ammonia production  | $H_2$           | 16.2                            |
| Haber-Bosch process                     | $NH_3$          | 2.78                            |
| Electric HB Process                     | $NH_3$          | 1.27                            |
| Biomethane from wood                    | $CH_4$          | 0.325                           |
| Methane from Hydrogen                   | $CH_4$          | 0.507                           |
| Biodiesel from wood                     | Diesel          | 52.8                            |
| Biogasoline from wood                   | Gasoline        | 60.4                            |
| Methanol from wood                      | $CH_3OH$        | 0.0891                          |
| Methanol from methane                   | $CH_3OH$        | 2.01                            |
| Methanol from hydrogen                  | $CH_3OH$        | 0.226                           |
| Imported Electricity for 1 kWh          | Electricity     | 0.252                           |

**Table 4.16.** Summary of the  $CO_2$  emissions. The biomethane from wood has an LHV of 25MJ/kg, whereas the methane from hydrogen has an LHV of 50 MJ/kg.

In the table 4.16, the difference in emissions between the fossil-based synthetic fuels and the biomass or hydrogen production routes is pretty straightforward. If those values are divided by the LHV of the fuels, hydrogen is the most relevant fuel to produce. The different fuels produced from biomass produce less  $CO_2$  emissions since there are from a source that is considered by simapro  $CO_2$  neutral. From there, the transport of these fuels is studied.

#### 4.1.9 Transport of synthetic fuels

It is assumed that the transport of synthetic fuels is liquefied due to the different potential locations chosen for electricity production. The transport of liquefied fuels is a technology used for long-distance transport as stated by Wulf and Zapp [83]. The process for hydrogen is as follows:

| Input              | Values   | Output                  | Values |
|--------------------|----------|-------------------------|--------|
| Steel (kg)         | 1.63E-3  | liquefied H2 (kg)       | 0.983  |
| Concrete ( $m^3$ ) | 0.055E-3 | Hydrogen as losses (kg) | 0.0162 |
| Aluminium (kg)     | 3.84E-4  |                         |        |
| Hydrogen (kg)      | 1        |                         |        |

**Table 4.17.** Input and outputs for the process of liquefaction of hydrogen

This process has an efficiency of 80 %, which cannot be neglected. The  $CO_2$  emission rise to 0.904 kg $CO_2$ -eq. which is equivalent to a rise of 15% in comparison to normal hydrogen electrolysis. Concerning the process of liquefying methane, since it is a technology already used, the process present in SimaPro is used directly. In addition, the liquefaction of methanol and ammonia are not be considered as the process are efficient at 99.15% and 99.94% respectively [10]. Therefore, the liquefaction of those two fuels is neglected for their transportation. For transportation overseas, those fuels are transported by boat. In

SimaPro, those processes already exist for transport by sea. Transportation represents 10 to 15% of the  $CO_2$  emission of all processes, which is not enormous but not negligible.

#### 4.1.10 $CO_2$ calculation

From there, all the processes are defined and now the  $CO_2$  evaluation can be done as explained in Global warming potential. Therefore the results here are presented for the fuels produced with a base of hydrogen electrolysis. It allows changing the capacity factors of the electricity factors. As presented during the analysis of the processes, the emission for biomass is difficult to predict since harmful  $CO_2$  emissions are not relevant. Moreover, EROI values cannot be validated by the literature. Here are the  $CO_2$  emissions for the wind turbines with the change of capacity factors.

| CF       | Emission in (kg $CO_2$ eq/MWh) |       |       |       |       |
|----------|--------------------------------|-------|-------|-------|-------|
|          | 30%                            | 40%   | 50%   | 60%   | 70%   |
| H2 elec  | 31.5                           | 24.03 | 19.5  | 16.47 | 14.31 |
| BioCH4   | 50.61                          | 40.53 | 33.62 | 29.01 | 25.70 |
| NH3      | 54.72                          | 49.68 | 46.8  | 44.82 | 44.82 |
| Methanol | 53.64                          | 45.36 | 40.32 | 37.08 | 34.74 |

**Table 4.18.** Emissions of the different fuels as a function of the capacity factors of a wind turbine in 2015

As shown in Figure 4.18, the  $CO_2$ -eq emissions are divided by two between the worst case and the base case. Therefore, the capacity factor is one of the most impacting factors influencing the  $CO_2$ . Concerning the PV panel, the different results can be seen in the following graph:

| CF       | emission in (kg $CO_2$ eq/MWh) |        |        |        |
|----------|--------------------------------|--------|--------|--------|
|          | 10%                            | 15%    | 20%    | 25%    |
| H2 elec  | 248.4                          | 165.9  | 124.8  | 99.9   |
| BioCH4   | 383.04                         | 257.04 | 194.4  | 156.24 |
| NH3      | 187.2                          | 136.98 | 111.78 | 96.48  |
| Methanol | 291.6                          | 201.6  | 156.06 | 128.7  |

**Table 4.19.** Emission of the different synthetic fuels as a function of the capacity factors of a PV panel in 2015

In Figure 4.18, the emissions are much higher from PV panels than wind turbines. It can be ten times higher. In terms of emission as a function of the capacity factors, the emission can be 2.5 higher between the best and worst-case scenarios. Nowadays, using most wind turbines is more interesting.

#### 4.1.11 Creation of Scenarios

From the emission of  $CO_2$ , it is possible to create different scenarios to study different possibilities for energy system development. To define the base case scenario, a ratio of

80% of PV panels and 20% of wind turbines is determined for electricity production since most of the places used as potential production locations are using PV panels.

|          | Mean value of $CO_2$ -eq |
|----------|--------------------------|
| H2 elec  | 51.10                    |
| BioCH4   | 78.09                    |
| NH3      | 63.11                    |
| Methanol | 74.84                    |

**Table 4.20.** Mean values of g of  $CO_2$ -eq emission per kWh for the base scenario for 80% of PV panel with a CF of 25% and 20% of WT with a CF of 60%

Those values estimate the  $CO_2$  content of the synthetic fuels when it arrives in Belgium in a liquid form. Those values for the fuels are three times less polluting than their methane-based production, and it goes up to almost five times less polluting for hydrogen.

The values from the table 4.18 for 60% capacity factor are created to create the optimist scenario. It is assumed that all synthetic fuels are created by wind turbines located in the best locations, such as the North Sea or Greenland. Moreover, the reduction of 40%  $CO_2$  emissions is deduced from the actual emissions to stimulate the future as explained in Methods. The learning rates as explained in the methodology have been added. The capacity factor of 10% from the table 4.19 is taken to create the pessimist scenario. It represents the positioning of PV panels in not efficient places. Those two scenarios represent a range of possibilities to estimate where the reality is situated between those two scenarios. The summary of those values can be seen in the following figure:

|          | Optimist value of $CO_2$ -eq | Pessimist value of $CO_2$ -eq |
|----------|------------------------------|-------------------------------|
| H2 elec  | 10.53                        | 248.41                        |
| BioCH4   | 18.94                        | 283.04                        |
| NH3      | 38.34                        | 187.23                        |
| Methanol | 30.42                        | 291.64                        |

**Table 4.21.** Resume of the  $CO_2$ -eq emissions in g per kWh for the optimist and pessimist scenario

Concerning scenario 2050, as explained in the Methods, the PV panels and wind turbines emission are reduced thanks to the value of the IPCC report. The EROI is calculated using learning rates, and the efficiencies of different technologies have been updated. Then finally, the appendix A.1 shows all the values calculated for this report.

Moreover, the efficiency of the processes has been changed. In the literature, the maximum efficiency has been researched and presented in the following table:

|          | Actual efficiency (%) | Maximum efficiency (%) |
|----------|-----------------------|------------------------|
| H2 elec  | 60                    | 80-90 [32]             |
| BioCH4   | 64                    | 80 [4]                 |
| NH3      | 67                    | 80 [72]                |
| Methanol | 87                    | 87                     |

**Table 4.22.** Efficiency change of the different processes



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No clear sources were found for the efficiency of the methanol, and the process is already quite efficient energy-wise as explained by Rosental, Fröhlich, and Liebich [68] but could be improved chemically. Therefore, for scenario 2050, the efficiency is the maximum available, considering that the different processes have been mastered in the future. Moreover, renewable technologies have also been changed using learning rates as explained in Methods. For example, the energy production from PV panels will be more than quadruple in 2050. The learning rate of 12.8% is multiplied by 4. Since the learning rate is based on the energy payback time of the technology, a reduction of 50% is a multiplication of the EROI of 2. For the wind turbines, the change is less important and leads to an increase of EROI of 30 %. For the GWP of those technologies, the industry's emissions are reduced as proposed by the IPCC [35]. The emissions have been updated in Simapro, considering that all the GWP emissions before the process of synthetic fuels production are reduced by 70% for 2050. All the data created can be seen in the appendix A.1.

#### 4.1.12 EROI calculation

The values were first estimated for the electricity produced by both PV panels and wind turbines to calculate the Energy Return On Investment (EROI), [34], [81]. In this project, only the resources are studied. The calculation of the EROI is done as explained in the Methods. Therefore, an example can be shown to calculate the EROI of hydrogen electrolysis produced by wind turbines.

$$EROI = \frac{El_{WT,lifetime} * \eta_{Electr} * \eta_{lique}}{E_{const,WT} + E_{const,electr} + E_{const,lique} + E_{transp}} \quad (4.1)$$

In the Equation 4.1, the different factors are as follows:

1.  $El_{WT,lifetime}$  is the electricity produced throughout the lifetime of the wind turbines where the capacity factor is taken into account.
2.  $\eta_{Electr}$  and  $\eta_{Lique}$  are the efficiency of electrolysis and liquefaction.
3.  $E_{const}$  is the energy needed for the construction of different elements of the process.

From there, all the EROI values can be calculated using the values available in EnergyScope to stay coherent with the values used by the tool. Moreover, the EROI calculation is based on a 30 years range because most technologies have a 30 years life expectancy. For example, the electrolyser has a life expectancy of 15 years; thus, the energy used for construction is used twice. The calculations are made for all the different processes as has been done for the  $CO_2$  emissions. The values of EROI are also calculated for the different scenarios. For example, the EROI of hydrogen electrolysis changes from a value of 10.4 for the optimist scenario to 1.8 for the pessimist scenario. The range of values for the different synthetic fuels can be seen in the table 4.27. Since the model works with the invested energy, the EROI has to be input under another form. Therefore, in the model everything is scaled for 1 GWh the EROI is inverted since  $EROI = \frac{E_{out}}{E_{in}}$  where  $E_{out} = 1$  GWh.

The values for the base scenario can be seen in the following table 4.23:

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| Resources | Invested energy for 1 GWh of fuels [GWh] |
|-----------|--|
| H2        | 0.17931                                  |
| BioCH4    | 0.30770                                  |
| NH3       | 0.296625                                 |
| Methanol  | 0.188753                                 |

**Table 4.23.** Invested energy required in GWh for 1 GWh of fuels for the base scenario

The data creation for the other scenarios is the same as for the  $CO_2$  calculation. Therefore, the EROI values can be seen in the appendix A.1.

#### 4.1.13 Comparison of the results

All the data has been created and needs to see if those values are coherent with the literature. First, the  $CO_2$  values are compared with the literature Concerning renewable technologies, the results can be seen in the following table:

| Means of production | In this study (g $CO_2$ -eq per kWh) | In the literature (g $CO_2$ -eq per kWh) |
|---------------------|--------------------------------------|--|
| Wind turbines       | 7-16                                 | 5-20 [70]                                |
| PV panels           | 52-130                               | 20-300 [27]                              |

**Table 4.24.** Comparison of the emissions for wind turbines and PV panels between the study and the literature

In this table 4.24, the range for the wind turbine is much more precise since the source is studying only offshore wind turbines as it is done in this study. Concerning the PV panels, the range is less precise due to the significant difference in technologies, and the emissions vary much more as a function of the capacity factors. Nevertheless, the values created for this study seem to be in phase with reality. In the following tables, the comparison between the values created in this study and the literature:

| Fuels    | Emissions in this study (kg $CO_2$ -eq/kg fuel) | Emissions in the literature (kg $CO_2$ -eq/kg fuel) |
|----------|---|---|
| H2       | 0.47-1.05                                       | 1 [5]   |
| CH4      | 0.35-0.70                                       | 1.5 [30]  |
| NH3      | 0.25-0.30                                       | 0.38-0.53 [72]                                      |
| Methanol | 0.19-0.30                                       | 0.123 [30]  |

**Table 4.25.** Difference between the emissions calculated in this study between what can be found in the literature. This table is for wind-based synthetic fuels.

| Fuels    | Emissions in this study (kg $CO_2$ -eq/kg fuel) | Emissions in the literature (kg $CO_2$ -eq/kg fuel) |
|----------|---|---|
| H2       | 3.33-8.28                                       | 2-7 [5]   |
| CH4      | 2.17-5.32                                       | 3 [30]  |
| NH3      | 0.536-1.04                                      | 0.78 [85]   |
| Methanol | 0.715-1.62                                      | -0.12 [30]  |

**Table 4.26.** Difference between the emissions calculated in this study between what can be found in the literature. This table is for PV-based synthetic fuels.

The results obtained in this study and between the literature for ammonia and hydrogen are coherent and abundant. For the other synthetic fuels, from the research made for

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this study, no studies have shown a clear  $CO_2$  analysis as a function of capacity factors. Thus showing a range of values that can be compared with what is presented in this study. Garcia-Garcia et al. [30] studied the synthetic fuels based on  $CO_2$  as a source and made a literature review of different studies. Concerning methanol produced from PV panels, this study shows positive emissions. Overall, the literature review states negative  $CO_2$  emissions for methanol production. During the analysis of the processes, negative emissions have been studied and dismissed since methanol does not really capture  $CO_2$  but avoids emissions by producing heat during the process. Most of the articles' values between the study and the literature are coherent for biomethane. It is relevant to note that there are some LCA that states that the emission could be ten times lower than the one presented here. [30]. Nevertheless, for all the different synthetic fuels, the values seem to be in cope with the literature.

In this project, EROI values have been calculated according to the Methods. For wind turbines, the EROI is between 14 and 30, and for PV panels, the EROI is between 5.8 and 14.7. For wind turbines, Dupont, Koppelaar, and Jeanmart [21] studied an EROI for offshore wind turbines of 12. After more research, Cleveland and Endres [16] collected different studies and showed that the EROI for Wind turbines is between 8 to 70. In the literature, for PV panels, Liu and van den Bergh [51] stated that the worst EROI for the oldest technology is 3 and for the newest technology is 16. For the electrolysis from wind turbines, Mann and Spath [55] showed an EROI of 13.2.

| Fuels                | EROI in this study | EROI in the literature |
|----------------------|--------------------|------------------------|
| H2                   | 1.86-10.55         | 1-2.5 [37]             |
| BioCH4               | 1.53-11.012        | <10 [69]               |
| NH3                  | 2.19-3.88          | not found              |
| Methanol             | 2.04-9.14          | not found              |
| Biodiesel/bioethanol | 9-10.11            | 12.55 [1] 3 [15]       |

**Table 4.27.** Comparison of different values of EROI between this study and the literature

Table 4.27 shows that information regarding EROI for various conversion pathways is scarce in the literature. For biomass-based fuels, mostly biodiesel and bioethanol, much study is available. The information that can be found for the other synthetic fuels is often incomplete or very specific. Moreover, the literature tends to state that the EROI of biofuel is around 3 or below [39], [15]. Therefore, the results are sometimes in this range of value. For higher results around ten, this mainly explains that projections of EROI for WT and PV panels are used as a hypothesis, and it is not easy to compare those values to the literature.

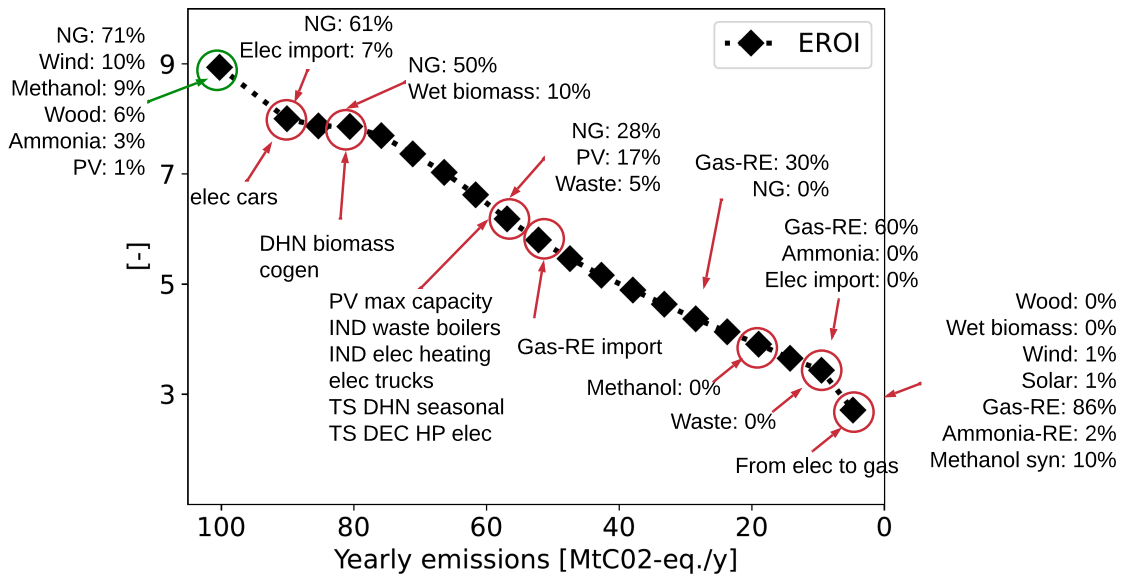
## 4.2 Scenarios

This section first presents what EnergyScope proposes before the change of data. Then the different scenarios that have been conducted thanks to the data collection presented in the previous sections are displayed and explained. Throughout this section, the reduction of  $CO_2$  is compared to the emissions of 2015, which were around 105 Mton  $CO_2$ -eq. The different scenarios with the actual values are analysed. Then, scenarios for the future

years are shown to see what could be a plausible solution for 2050.

#### 4.2.1 EnergyScope base-case scenario

First, the scenario without the data change must look at to have a starting point. This analysis is necessary to understand where the problem is. This initial scenario is based on data from Limpens [50] and Muyldermans and Neve [59]. The main issue with the input data is that synthetic fuels have an emission of 0 kg  $CO_2$ , allowing the system to converge easily to a minimum  $CO_2$  emissions. The model is therefore optimised on EROI while constraining the yearly emissions of the system. The following graph shows the result of this simulation:



**Figure 4.11.** Evolution of the EROI as a function of the yearly emissions of the system. This figure also shows how the system change throughout the constraining. This figure comes directly from the work of Dumas et al. [19]

In Figure 4.11, the evolution of the energy system can be seen. The system uses first the electricity imports and then the different biomass. Then, it starts to import renewable gas. The EROI of the system is also reaching a value of 3 while constrained at its maximum. It is also relevant to note that it mainly uses synthetic gas for low emissions snapshots. The scenarios are looked into at this lowest amount of emissions. The Sankey of the base case scenario can be seen in Figure A.10. The model uses all the renewable resources such as wind turbines, PV panels and biomass since their EROI is more interesting than any synthetic fuel. Once the constraint on the  $CO_2$  is too important, the model has no choice but to import synthetic natural gas (SNG) since synthetic fuels have 0kg  $CO_2$ -eq emissions. The EROI of synthetic fuels is also really low.

#### 4.2.2 Case 2035

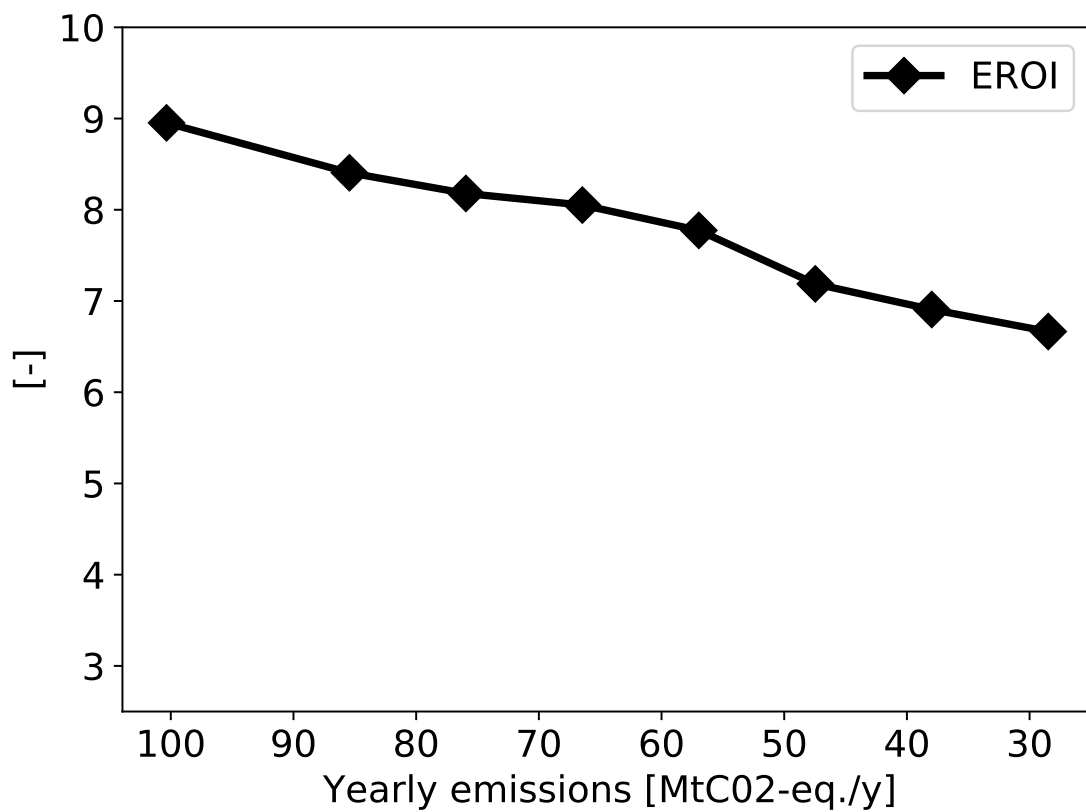
Since the values of the invested energy and GWP are changed. The input for the Energyscope model is updated. Therefore, it is interesting to look at how it affects the model and analyse how the model installs and uninstalls the different technologies. Then,

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the analysis shows the moment the model uses different technologies instead of the others. The model is optimised on the EROI, where the goal is to minimise the invested energy since it maximises the EROI as explained in the Methods. The simulation is performed for the current energy mix of Belgium without nuclear power plants. Then, every reduction of 10% of the  $CO_2$  emission is highlighted. The goal is to help understand how the Belgian energy system transitions to reach neutrality carbon.

### Best case scenario

Therefore, the case with the best scenario possible is analysed. In addition to this, the data can be found in the Altered values of the resources files of EnergyScope. This scenario uses the most efficient technologies for  $CO_2$  emissions to produce the different synthetic fuels. First, the EROI can be seen as follow:



**Figure 4.12.** EROI as a function of the yearly emissions for the best case scenario in 2035

In Figure 4.12, it can be seen that the EROI does not decrease that much between the actual situation where the EROI of the system is 9, and the final EROI of the system is 6.5. It is mainly due to the high values of renewable hydrogen in EROI. Therefore it is relevant to see how the system is for the most constrained system. The Sankey diagram where the system is the most constrained can be seen in appendix A.6.

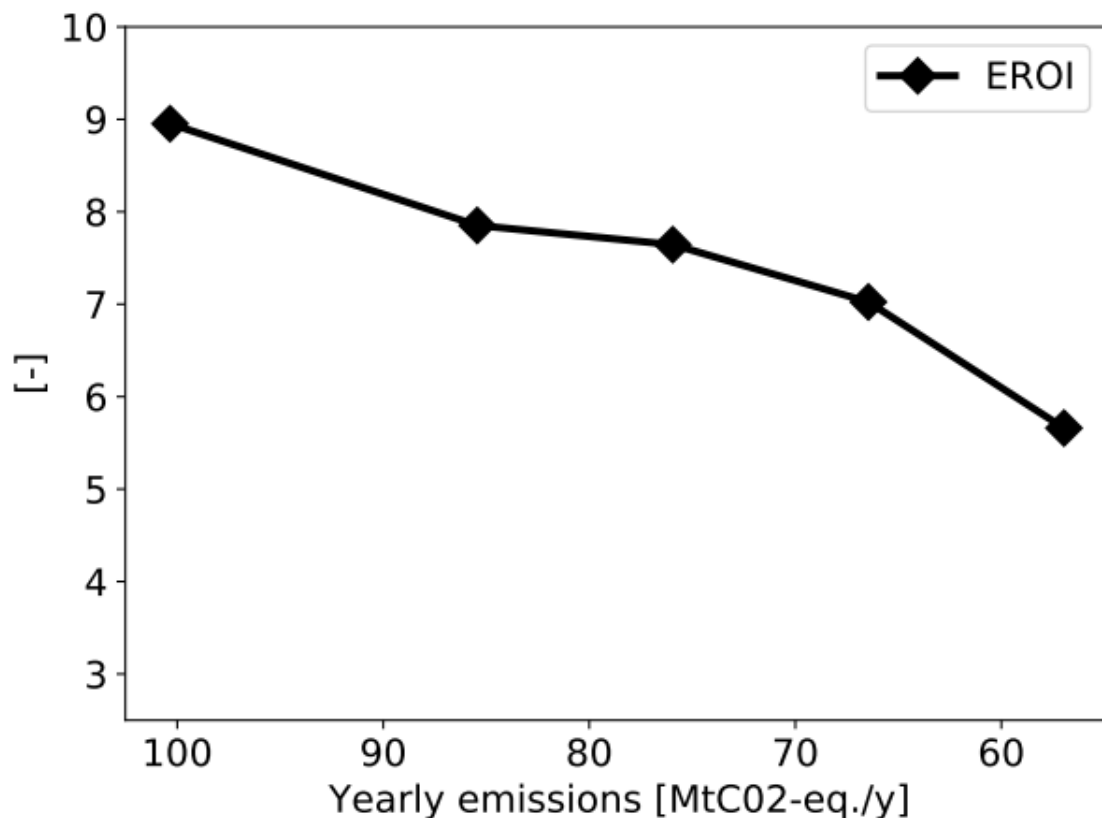
In Figure A.11, the hydrogen accounts for more than 50% of the energy required by the system. Most of it is used for high heat production and electricity production. Therefore, the rest of the system uses wind, wood, and imported electricity. The methanol that the

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model uses is for high valuable chemicals and is used all the time required. It can be observed in all the scenarios. In the end, the hydrogen is imported to be transformed into natural gas instead of importing it directly. It is more interesting to transform the hydrogen after transportation.

### Worst-case scenario

In the worst-case scenario, where most of the synthetic fuels are produced by poor efficient PV solar panels, for example, solar panels installed in Belgium. The EROI and the global warming potential of those fuels are very pessimistic. The results produced by the system are as follows:



**Figure 4.13.** EROI as a function of the yearly emissions for 2035 worst scenario

In Figure 4.13, the model can converge to a reduction of  $CO_2$  of a maximum of 40%. The reduction of EROI is almost the same as the base case of the scenario of EnergyScope 4.11. The model reaches a value of EROI of 5.5. Ultimately, the  $CO_2$  emission of the synthetic fuels is too high to be used by the model. The model's reaction to those changes can be looked into in Appendix A.6. This Sankey diagram is for a reduction of 40% of the emissions compared to 2015.

In this Sankey diagram A.12, the system imports almost a negligible amount of renewable hydrogen. It is not the primary fuel used by the model. It prefers to use all the biomass available and the solar potential. It makes sense since the system is not using synthetic fuel to produce electricity since this fuel is produced using the same PV panels. It is even more relevant for the model to use biofuel. It is also interesting to note that the system is

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a small part of bio-diesel, meaning it does not electrify all the transports. Finally, it can be seen that natural gas still accounts for 25% of the initial energy input of the system.

### Realistic case scenario

In this case scenario, the assumption is that 80% of the synthetic fuels are produced by high-quality solar panels and the remaining 20% by wind turbines. This scenario is considered the realistic one due to the potential locations presented in previous sections. Therefore, the results are the following:

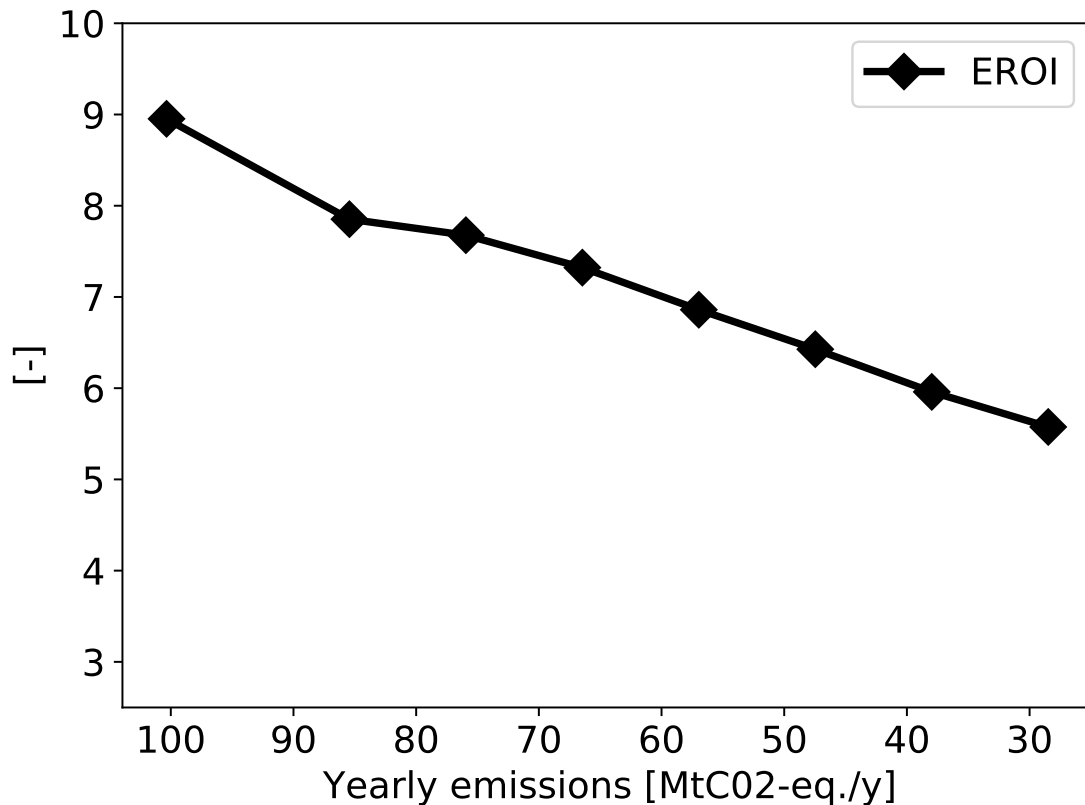


Figure 4.14. EROI as a function of the yearly emissions for the realistic case scenario

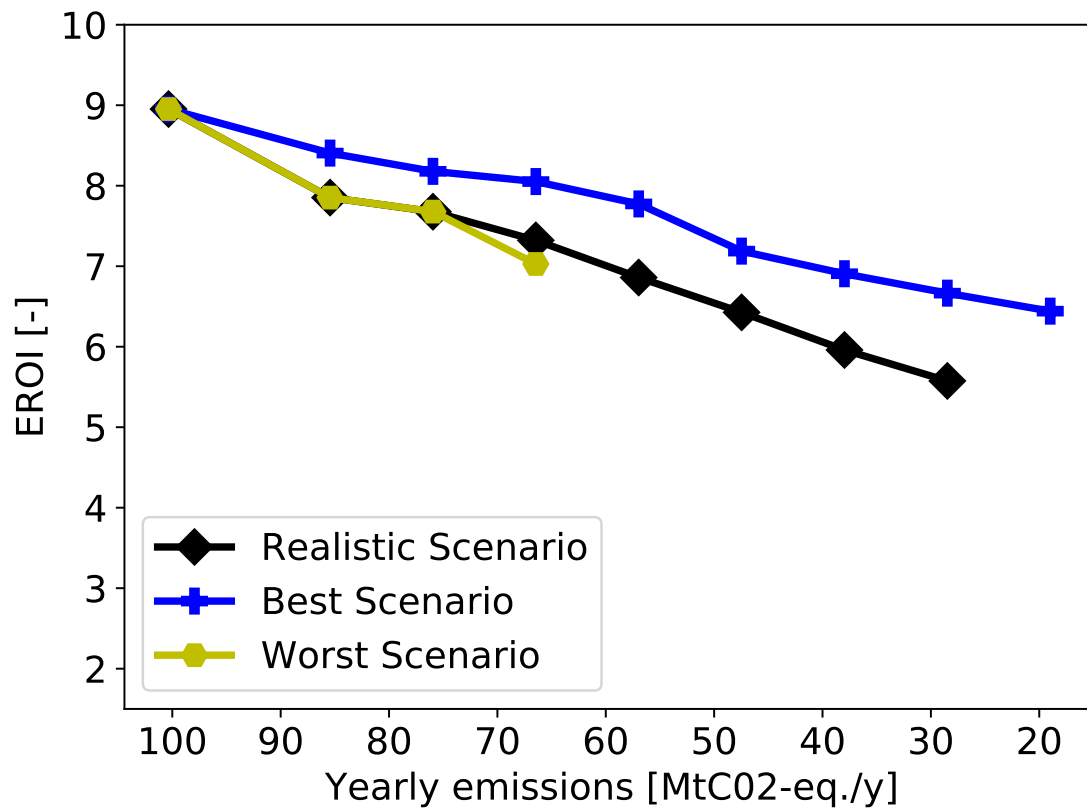
In Figure 4.14, the model can converge to a reduction of 70% of  $CO_2$  emissions in comparison with 2015 emissions. In the beginning, the EROI of the system is the same as in the 2015 scenario. It reaches an EROI of 5.5 at a reduction of 40%. After that, the  $CO_2$  emissions are too high for the model to converge to a solution. To see how the model adapts to reach those values can be seen in the appendix A.6.

In Figure A.13, it can be seen that the system is based on hydrogen at almost 20% of the all energy input. The model installs solar panels and wind turbines and imports electricity. The models use all the biomass available mainly for heat and electricity production, not for the transformation of biofuels. The model still imports some conventional natural gas. It is essential to highlight that hydrogen is used as fuel for freight, and the public mobility, hydrogen and electricity are used in the same proportion. Therefore, this scenario is quite a good trade-off between the use of biomass, wind, solar, and hydrogen.

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### Comparison between the scenario

To compare the different scenarios, the change in EROI is analysed in the following figure:



**Figure 4.15.** EROI comparison between the different scenarios for 2035

As shown in Figure 4.15, all the scenarios start from the same EROI value. The pessimist and realistic scenarios follow the same curve. When synthetic fuels are required, the pessimist scenario does not converge to lower  $CO_2$  emission levels. The difference between the optimist and realistic scenarios is due to the use of hydrogen. In the first scenario, hydrogen is used directly due to its high EROI, and in the realistic scenario, hydrogen is not the priority due to a lower EROI. This graph shows that there is a disparity between the different scenarios. There is a difference of 1.5 in EROI at 60% reduction of  $CO_2$  emission. In terms of cost, it is not relevant to analyse it precisely since the cost has not been changed accordingly with the change of the invested energy. It is still interesting to analyse the cost optimisation to see how the model reacts.



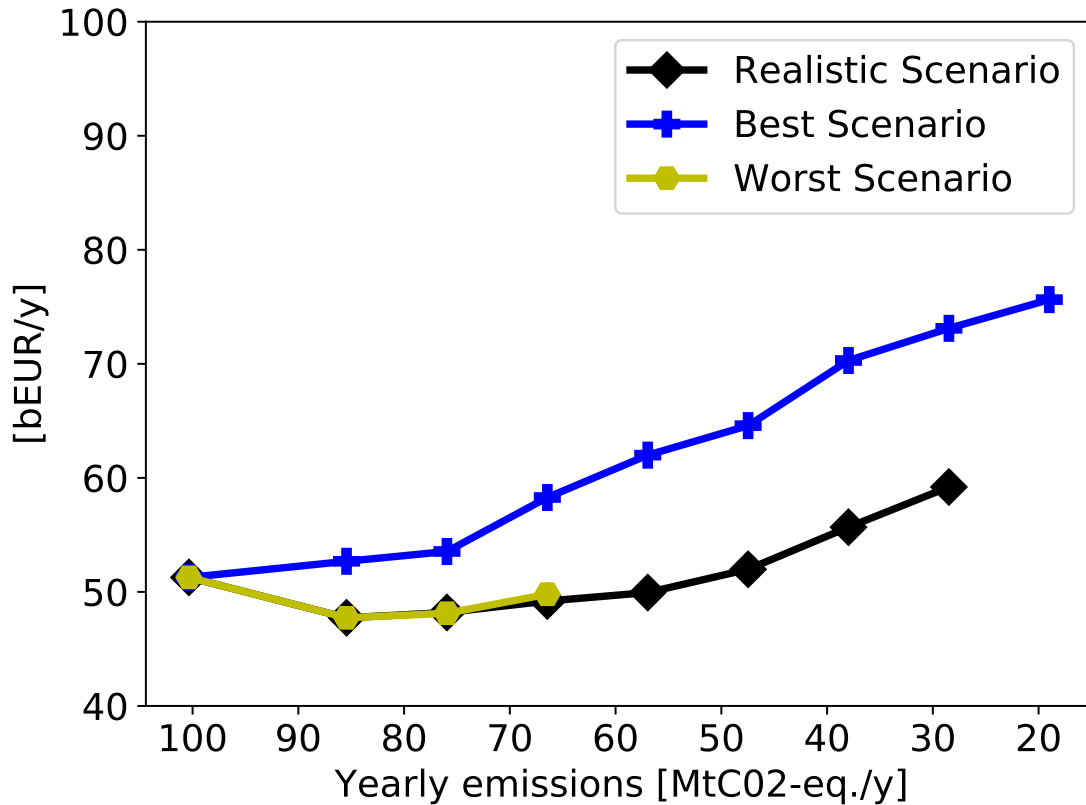


Figure 4.16. Cost comparison between the different scenarios

It is interesting to see that the cost curves follow the trend presented for the EROI. Since the optimist scenario uses hydrogen rapidly, the cost rises as it is the most expensive resource. The costs are the same at the beginning for the realistic and pessimist scenarios. In the end, if the trends of the realistic scenario continue, the price of the system may reach the price of the optimist scenario. So from both the curve 4.15 and 4.16, the realistic and pessimist scenarios follow the same path at the beginning of emission reduction. Therefore, it is not necessary to go for the best scenario directly, but after half of emissions reduction, it is recommended to aim for the best one.

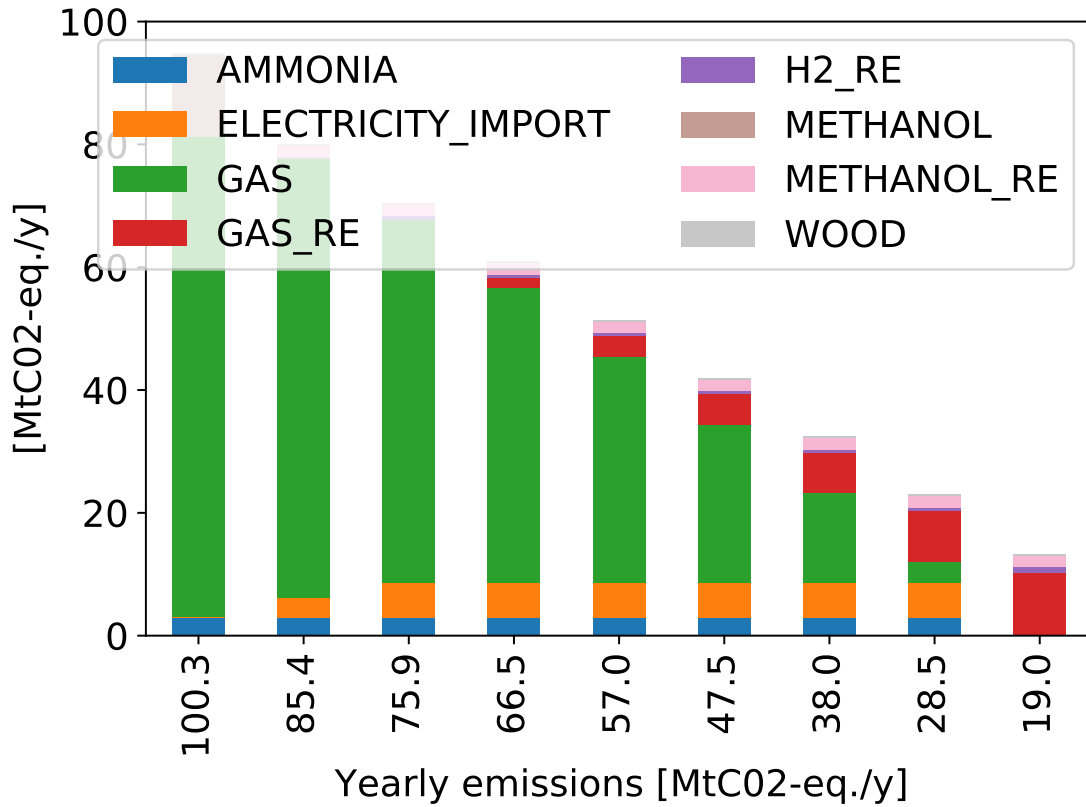
### 4.2.3 case 2050

In this subsection, the model is used with the data developed for 2050 to see if the energy system can be even more  $CO_2$  efficient and to verify that the trajectory proposed by the 2035 case scenario goes accordingly. Then a comparison between the different scenarios is made to see how the model changes.

This case scenario proposes a realistic scenario with the values of 2050 to see by using EnergyScope which reduction of  $CO_2$  can be reached. Therefore, after trying to constrain the system as much as possible, the reduction of 83% of  $CO_2$  emission has been reached. The Sankey diagram can be seen in the appendix A.6

In Figure A.14 while constraining the system, the model starts to use synthetic natural gas (SNG) rather than hydrogen. At first, it uses only SNG. Then it starts using hydrogen

when the system is constrained a lot. If the technology is going to be even more efficient, using SNG is the trend that the model is following. The freight is almost totally using hydrogen. On the other hand, public mobility uses half hydrogen and half electricity. In the following figure, the decomposition of GWP due to the operation of the system is shown:

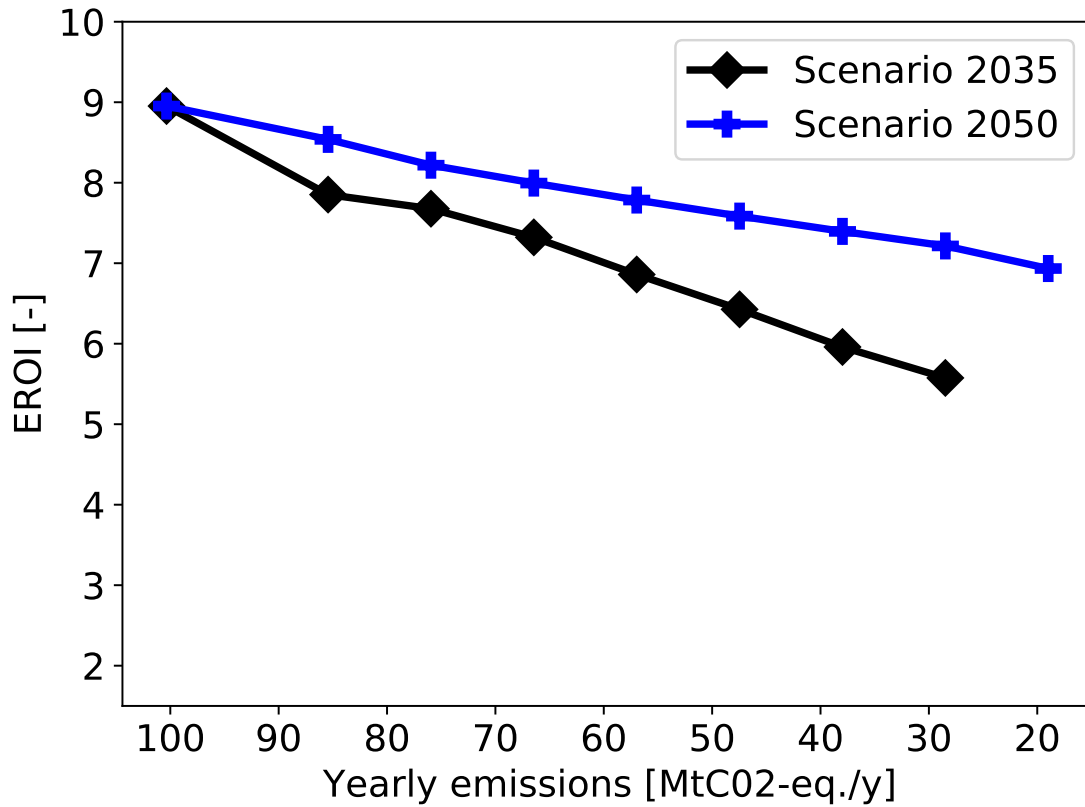


**Figure 4.17.** Decomposition of the operation GWP emission for the scenario 2050. The RE stands for the renewable equivalent of the standard fuel on the label.

In Figure 4.17, the residual emissions for the lowest emissions are due to only synthetic fuels. Those emissions due to these fuels are 10 MtCO<sub>2</sub> per year which is a reduction of 90% from the 2015 emissions. Moreover, natural gas is replaced slowly by renewable gas. The graph also shows that the system prefers electricity imports from the beginning. In the end, the electricity imports are not used anymore.

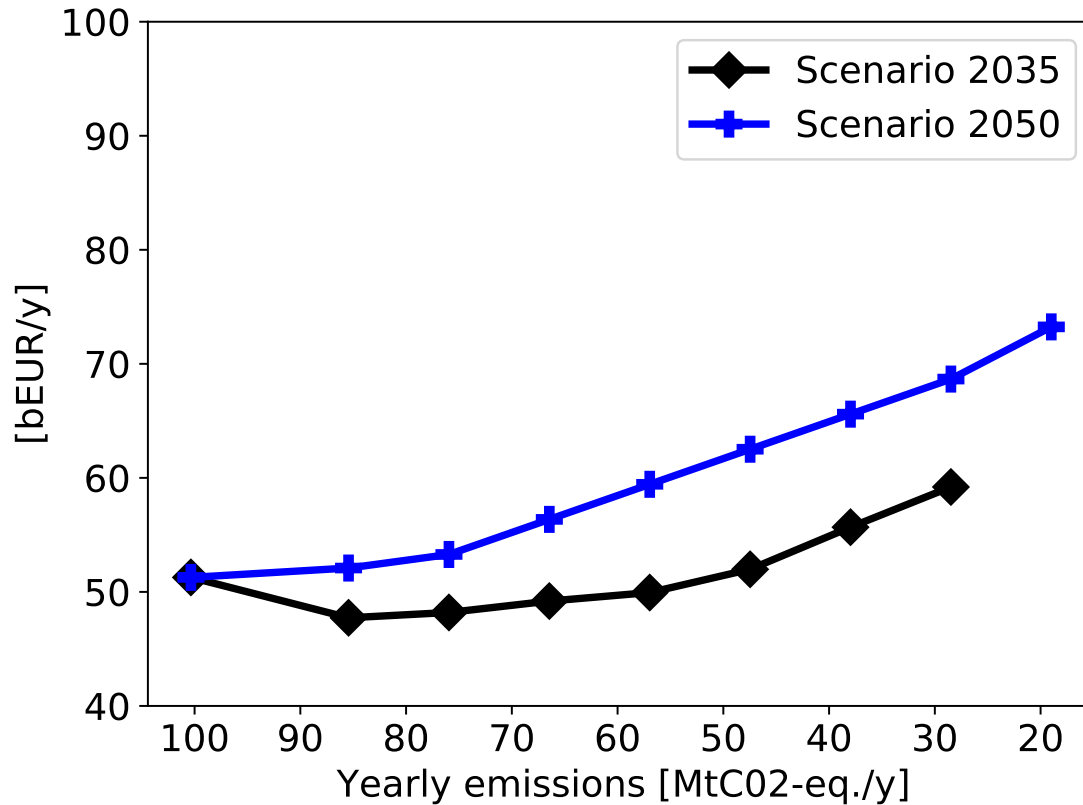
### Comparison between the different scenarios

The comparison between the different scenarios for 2035 and 2050 can be seen in the following figure:



**Figure 4.18.** EROI of different scenarios as a function of the yearly emission

In Figure 4.18, the first few reductions in  $CO_2$  do not show a big difference between the two first scenarios. The model does not use synthetic fuels at the beginning of the transition. Therefore, the change is insignificant. At 70% of the actual emission, synthetic fuels start to be used by the model. Therefore, the slopes of the curves start to change more importantly between 2050 and the realistic case scenario. In the end, there is almost a difference of EROI of 2 between the scenario 2035 and the one of 2050. The value of EROI at 75Mt $CO_2$  for scenario 2035 is the same at 45Mt $CO_2$ . Therefore, if the technology continues to improve, it could lead to a potential stabilisation of the EROI of the system. A cost comparison can be shown even if it is not relevant since the price of the different fuels has not been changed accordingly with the GWP and  $E_{inv}$ .



**Figure 4.19.** Cost of system as function of  $CO_2$  emission per year

In figure 4.19, the system is cheaper in 2035 and much more expensive in 2050 since the use of SNG. SNG is the most expensive resource of EnergyScope. Therefore, the system's price rises significantly, and the system is 10 billion per year, more expensive than in 2035.

#### 4.2.4 Resume of the scenarios

To conclude this section, the different optimisations of each scenario are summarised in the following table:

| Name of the scenario    | GWP Reduction compared to 2015 emissions | Base fueled used                           |
|-------------------------|--|--|
| Realistic case scenario | -76%                                     | Hydrogen + Biomass                         |
| Worst case scenario     | -35%                                     | Biomass + Waste                            |
| Best case scenario      | -87%                                     | Hydrogen                                   |
| 2050 scenario           | -83%                                     | Hydrogen + Biomass + Synthetic natural gas |

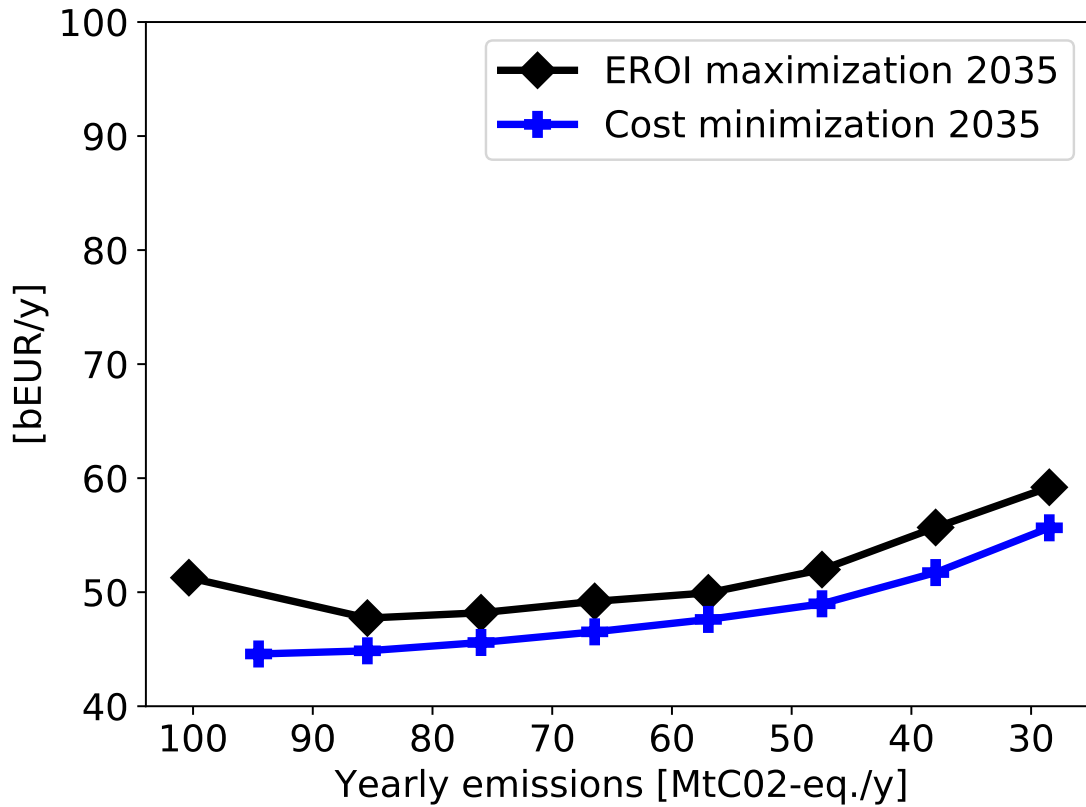
**Table 4.28.** Different scenarios with the value reach the most constrained point. The main fuel at the end used by the model is stated

The table 4.28 shows that for 2035 a huge part of the  $CO_2$  reduction can already be achieved. It also shows the difference between the two base models for 2035 and 2050. In 2050, the system is using synthetic natural gas. It raises the question of which fuel should be prioritised for development.

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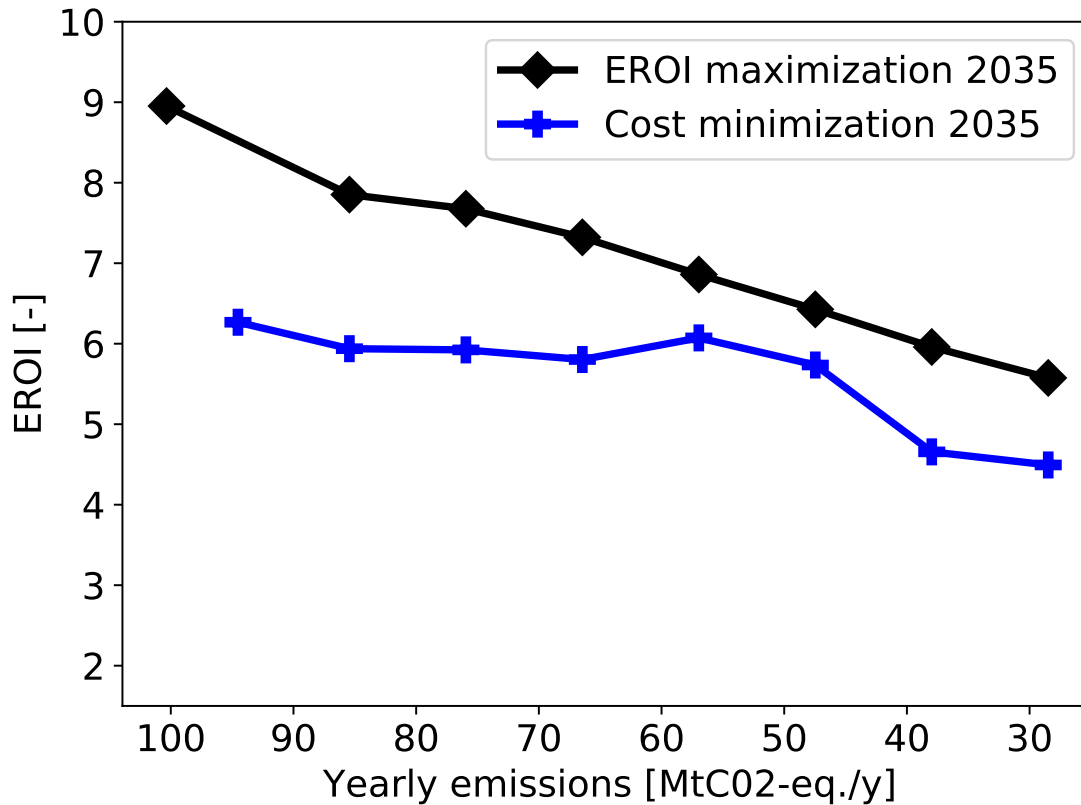
### 4.2.5 Cost optimization

In this short subsection, the cost optimisation of the system is done to see how much it changes from both the base scenario and the optimisation of the GWP. Therefore, since the price for synthetic fuels has not been changed in the data set. The data for EnergyScope is for 2035. It is to show what the advantages are to optimise the EROI.



**Figure 4.20.** Comparison of the cost between cost and EROI optimisation for the base scenario as a function of the yearly emissions

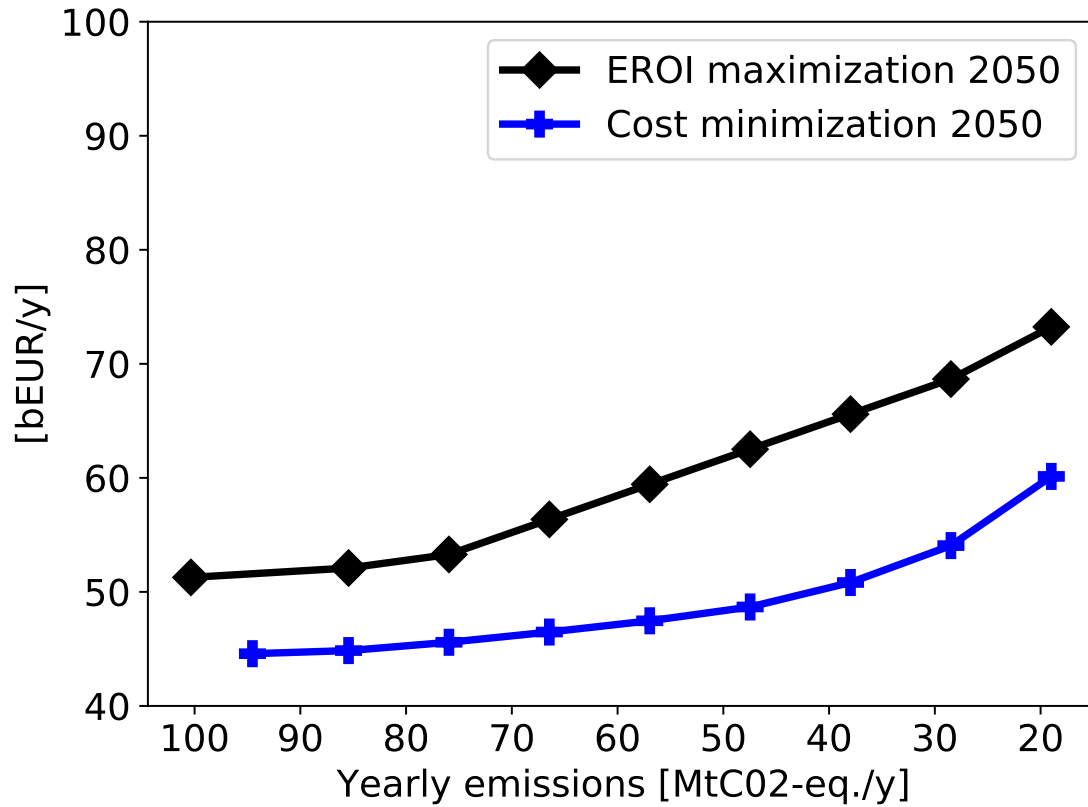
In Figure 4.20, it can be seen that optimisation on the EROI does not lead to a more expensive system than the optimisation on cost. It is leading to 4 billion more in terms of expense. The snapshots created from the different optimisations show almost the same system. The system optimised on the EROI is using little more synthetic fuels. It is relevant to look at the comparison between the EROI of the system depending on cost optimisation or EROI optimisation. The comparison is as follows:



**Figure 4.21.** Comparison of the EROI between cost and EROI optimisation for the base scenario as a function of the yearly emissions

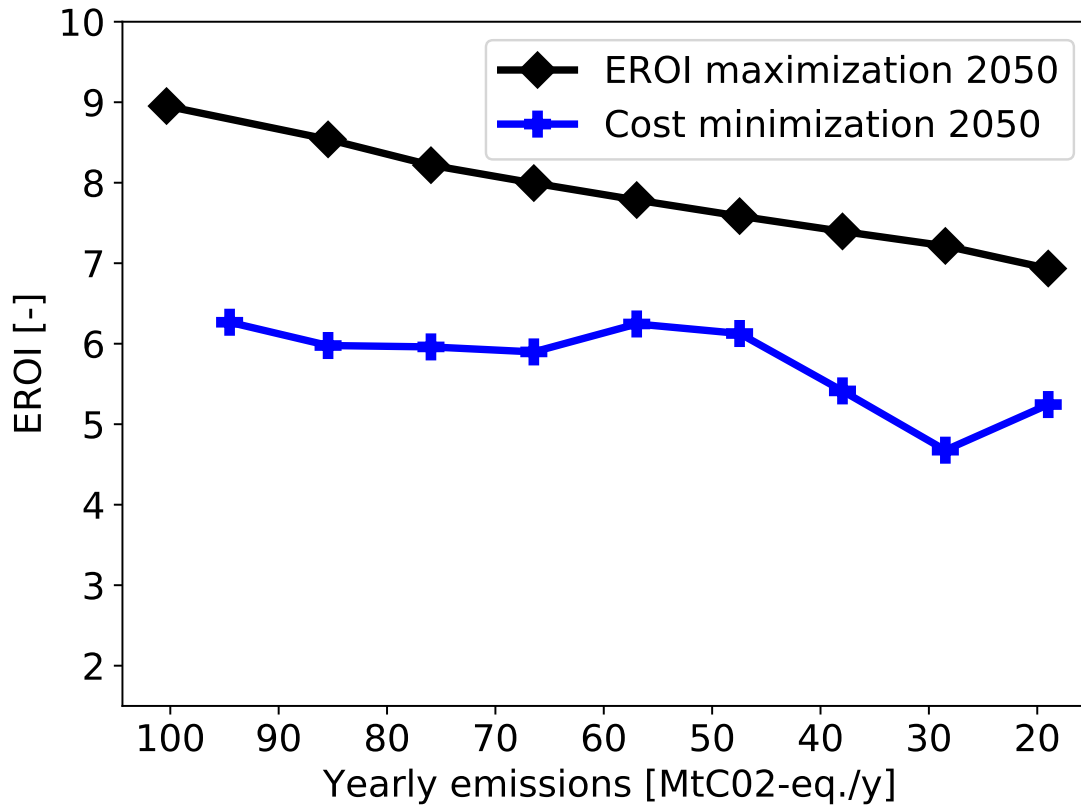
In Figure 4.21, it can be seen that the EROI of the scenario optimised on the cost is more or less constant until 50% of emission reduction. After that, when the emissions are constrained, EROI decreases rapidly fast. On the other hand, the decrease of EROI when optimised on EROI is decreasing almost linearly. The main difference between those optimisations is that renewable ammonia is used in cost optimisation instead of hydrogen. Moreover, in the cost optimisation, less CHP and more heat pumps are installed than in EROI optimisation. Apart from that, the model uses the same technologies and the same resources. Therefore, as the actual energy system in Belgium is normally optimised on the cost <sup>1</sup> Concerning the scenario 2050, the comparison between the different optimisation can be seen in the following figure:

<sup>1</sup>The Sankey of the optimisation on the cost for the actual emissions can be found in the Appendix A.6



**Figure 4.22.** Comparison of the cost between cost and EROI optimisation for the scenario 2050 as a function of the yearly emissions

Contrary to the previous example, the cost difference is way more important. The figure 4.22 shows a difference of 15 billion between these two optimisations at the most constrained point. It is explained by using renewable ammonia in the system, which is cheaper than the other synthetic fuels, especially since the scenario 2050 uses synthetic natural gas. In terms of EROI, the two simulations show the following trend:



**Figure 4.23.** Comparison of the EROI between cost and EROI optimisation for the scenario 2050 as a function of the yearly emissions

On the other hand, it can be seen that in Figure 4.23, if the last point on the right is not taken into account, the difference between EROI is 2.5 and 2 for the lowest emissions snapshot. The system EROI rises in the end because the simulation is forced to use synthetic natural gas instead of renewable ammonia. So as stated previously, the model uses renewable ammonia since it is the cheapest synthetic fuel. To reduce the emissions, it uses SNG since the emissions are the lowest of the synthetic fuel, but it is the most expensive. It is why the EROI is rising. Therefore, it leads to a common final EROI point when the GWP is constrained to its maximum. The value reached is an EROI of 6 for a system cost of 82 billion. This point is common to both scenarios since it is the same simulation. Finally, optimisations show that the system's prices rise when the system is constrained the most. Moreover, the optimisation of EROI shows that the reduction of GWP leads to an increase in the system's price. Therefore, it is more relevant to have a system where the prices rise gradually since the learning rate could have been put on the prices of synthetic fuels. Unfortunately, predictions are complicated to find. In addition, the system is using ammonia while optimising the cost because it is the cheapest fuel for 2035, but that could change in 2050.

Moreover, for a higher price, the system can have one more point of EROI. Following Lambert et al. [48], the HDI index increases significantly for EROI values between 0 and 10. Therefore, if EROI can be increased by 1, the policy-makers should take it. To conclude, the synthetic fuel on which society is based has to be taken thoroughly, and



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optimisation of EROI is relevant to keep the quality of life as it is now.

# Discussion 5

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The discussion can be performed into three parts linked to the questions that need to be answered by the research gaps. To remind those questions are the following: (1) What are the different processes for synthetic fuel production? (2) What are those synthetic fuels' CO<sub>2</sub> emissions and EROI values following different scenarios? (3) How do those values affect the future Belgian energy system proposed by Limpens [50] and how does the model change as a function of the different scenarios? The discussion is divided into three parts the methodology, the processes and the models.

## 5.1 Methodology

In the methodology, the LCA is used to assess the global warming potential. It is widely spread and used in the industry sector. The main issue in this work is the coherence between the studies. All the studies used in this work have different hypotheses. Therefore, the version defined is not used thoroughly during the analysis. Nevertheless, LCA was the method to use in this study.

The EROI is another indicator of the cost. The EROI considers more elements than the cost, such as technology improvement, quality of life and actual cost. Therefore, it encompasses all technology's social, technical and economic aspects. As seen in 2022, the price for electricity and other resources rose drastically and does not represent the reality of the energy system. In this report, the study on EROI has shown that the difference between cost and EROI optimisation is insignificant. Therefore, if society needs a high EROI to be more efficient, the model should follow the EROI scenario and not the cost one since estimating the cost of a resource seems impossible.

## 5.2 Processes

As seen in the different processes, electricity production (Wind turbines and PV panels) accounts for 60% of the emissions of synthetic fuels. Therefore, there is a need to create PV panels and wind turbines with the most efficient technologies. The goal is to reduce the greenhouse gas emissions of the production of those technologies. It has to be also correlated with the efficient placement of the wind turbines and the PV panel. As seen in the Energy Production, capacity factors of those technologies impact electricity emissions can be twice more significant for a low CF than a high CF. Those two elements have to be taken into account for the future development of renewable energies. In addition to this, wind turbines with high capacity factors are the technology to look up since this is the technology that produces less CO<sub>2</sub> emissions as low as 7g per kWh.

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Concerning the different processes for producing synthetic fuels, some different processes are more likely to be used than others in terms of feasibility. From the  $CO_2$  emissions and EROI, the biomass is likely to be used for other purposes than synthetic fuels. Even if this statement has to be carefully taken, biofuels are less efficient than electrofuels, and there is a question of biomass availability for the Belgian energy system. It is a limitation of this study. It is discussed further away.

From this study, using ammonia as an energy carrier for hydrogen looks like an unfeasible idea since the liquefaction of hydrogen and its transports do not emit as much as creating hydrogen to form green ammonia transport it, and transform it back to hydrogen. The succession of the processes to produce first green hydrogen and then ammonia to transport to produce hydrogen is not efficient.

Moreover, producing ammonia, methane, and methanol from hydrogen are efficient processes. Therefore, using a synthetic fuel or another seems to be quite a function of the application and the possibility of transportation. The model uses synthetic fuels (mostly SNG and hydrogen) for what renewable technologies cannot produce for electricity production. Therefore, it can be interesting to study the comparison between hydrogen and electricity imports by looking at both EROI and  $CO_2$  emissions. For the moment, electricity imports are more attractive.

Concerning the transport of the synthetic fuels, the liquefaction of hydrogen is 20% less efficient than the other fuels but still in terms of emissions as it is equivalent to transforming this hydrogen into another fuel. The liquefaction of hydrogen seems to be something to develop further.

Moreover, transport has not been studied extensively. The losses due to storage have not been estimated, considering synthetic fuels are used directly for production.

Finally, future scenarios have their data changed for 2050, but more could be done like assessing change in synthetic fuels transportation. Moreover, those values are based on estimations. They will be false, but they show the trend that the GWP of synthetic fuels is going down.

### 5.2.1 Future scenarios

In the different scenarios, it can be seen that in the energy system, when the global warming potential is constrained, hydrogen starts to be the main base of the energy system. For the best scenario, the system is defined by almost 60% of hydrogen. In reality, hydrogen will be indispensable since the electricity imports and renewable technologies for Belgium are limited, and the possibility of electricity imports for all systems is almost impossible. On the other hand, in the pessimist scenario, the model prefers biomass resources (wood, wet biomass, and waste) rather than synthetic fuels. It is due to lower emissions of greenhouse gases emissions of the biomass and the need for heat by the energy system. Actually, in terms of EROI, it is more relevant to use biomass since biomass has one of

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the highest EROI in the model, around 20. An interesting trend for all the scenarios is that freight and private mobility use hydrogen and electricity. The freight uses hydrogen almost all the time until 2050, and private mobility primarily uses electricity.

Concerning the scenarios for 2050, the EROI of the system is 1 point higher than the one with the data for 2035. There is a scenario in 2050 that is considered to be a possible scenario for the future. This scenario must be taken with much precaution since many hypotheses have been taken. Those are explained throughout the report. Those hypotheses can be summarised as follows: (1) The transportation of synthetic fuels has not been changed. (2) Only the efficiency of the processes has been changed. (3) The energy of construction of the power plant has not been changed. (4) The EROI has been changed following learning rates.

With the technologies available in 2035, the minimum emissions are -35%, -76% and -87% for the worst, realistic and best case scenarios compared to the 2015 emissions. It shows that if inefficient development is made for synthetic fuel and the policymakers do not try to invest in synthetic fuels, the  $CO_2$  reduction for Belgium is meagre. On the other hand, if synthetic fuel development is performed, the difference between the realistic scenario and the best case is not enormous. It shows that the energy system relies on synthetic fuels for the future (Belgium can only create 30% of its energy). In 2050, the reduction reaches 84%, which is lower than the best-case scenario of 2035.

Therefore, this minimum of  $CO_2$  emissions is a proposition, but practically this value could be lower. The decomposition of the  $CO_2$  emissions is relevant to investigate. As explained in the Methods, the global warming potential is divided into two parts the construction and the operation. The GWP due to construction is almost constant, around 8.5 MtCO<sub>2</sub>-eq/y which mobility represents 60% of the emissions. The GWP op, due to the operation of the energy system, represents the most significant part of the global GWP emission. In figure 4.17, for 19 MtCO<sub>2</sub>-eq/y, the emission due to the operation is only composed of imported electricity, renewable methanol, and renewable hydrogen. There is still a bit of wood and biomass, but this is not very important. That emission represents 14 MtCO<sub>2</sub>-eq/y for the operation, which is still a reduction of 85% of compared to the actual situation. These emissions rely only upon the value of  $CO_2$  of the synthetic fuels. Due to the different hypotheses, those emissions could be 5-10% lower if the change in transportation is taken into account. On the other hand, the main emissions factors are electricity production which has been changed using learning rates. Therefore, the best way to assess the change in emissions in the future is to see how those technologies will improve  $CO_2$  emissions-wise year by year and see how the trend will evolve.

### 5.3 Limitations and future works

This study has several limitations from all the hypotheses taken throughout the study. The limitations are as follows:

1. The transportation is assumed to be liquefied due to the high distance between the place of production and Belgium. The storage of those synthetic fuels also has been

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neglected. A complete analysis can be done only on this subject to make the data more accurate. Assessing other transport technologies such as pipeline, truck, and maritime transport could be interesting.

2. The biomass has been avoided in the data creation due to the difficulty of defining the potential capacities available for Belgium. Moreover, the validation of the data about biomass is not straightforward. Therefore, performing an extensive analysis on biomass adapted to the Belgian energy system could be relevant.
3. The prediction of different future scenarios is difficult to estimate. The different technologies have their efficiencies risen, but the evolution of EROI is estimated, but more could be done.
4. This study looks into the model EnergyScope and only for the Belgian case. Since the Belgian potential for renewable energy is shallow, there is a critical need for synthetic fuels. Therefore, analysing other countries or even the European region could be relevant.
5. The model can import as many synthetic fuels as it wants; therefore, the results are not limited by the availability of the different fuels. Therefore, estimating the different capacities available for the Belgian/European region can be relevant to making the model more robust for the result. To estimate those capacities, the potential for wind turbines and PV panels has to be estimated for several regions to see which percentage is possible for synthetic fuel production.
6. The costs have not been updated in phase with the EROI change. Therefore, it can be relevant to see if the costs changed for 2050 affect the simulations differently.

# Conclusion 6

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## 6.1 Conclusion

To conclude this work, several points have to be highlighted. First, this study is creating data for a list of different processes. The data created for the production of synthetic fuels are both  $CO_2$  emissions and EROI. These new data for synthetic fuels fill the literature gap and give better data to be used in the EnergyScope model. The data is made for technologies in 2035. In the following years, these values are estimated to evolve according to projections of the IPCC and technology improvement. All those values are available in the database and can be used/changed/updated for further use.

Secondly, the data created for this work proposes a wide range of values for EROI and  $CO_2$  emissions, showing the different possible paths for producing synthetic fuels. An optimist and pessimist scenario is generated to have a range of possible scenarios. The proposition for the realistic scenario with 80% PV panels and 20% wind turbines is an assumption, and it is impossible to know if this scenario is future development. From this process, study hydrogen is the fuel that is more suitable in terms of  $CO_2$  and EROI.

From the different scenarios, for the beginning of the reduction of GWP, the system is using only technologies/resources already existing, such as PV panels, wind turbines, heat pumps and biomass. Therefore, the first 40% reduction of the  $CO_2$  emissions is easily possible and can be implemented rapidly.

It allows some time to reach technology maturity for synthetic fuels. As can be seen in the report, the two primary synthetic fuels used by the model are hydrogen and synthetic natural gas. The main factor impacting the choice of fuel is liquefaction. The fuel used by society mainly depends on the ability to transport the different fuels properly.

Moreover, the EROI of the society taken from different scenarios ranges from 4 to 7, confirming the significant value disparity that the literature proposes. The link between EROI and HDI has been proved by Lambert et al. [48], it is more dependent on values of 0 to 10. The decision-makers should follow the scenario that proposes an EROI of 7.

Lastly, the scenario proposed for 2050 showed that the world will be based mainly on synthetic natural gas. However, the reduction of 83% of  $CO_2$  emissions in comparison to 2015 values is the scenario proposed for 2050. It represents the proposition for the lowest emissions possible for 2050 with the data created. The emissions from the system's operation ( $GWP_{op}$ ) are 10 Mt of  $CO_2$  per year. For a world based on synthetic fuels,

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reaching 0%  $CO_2$  emissions is unfeasible since most of the remaining emissions are due to the production of synthetic fuels.

To conclude, different scenarios show that synthetic fuels are used in every case. The most important thing is to choose between hydrogen and synthetic natural gas as base gas for the future. For the assumptions in this report, the world is based on synthetic natural gas for 2050.

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# Appendices A

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## A.1 Altered values of the resources files of EnergyScope

Here are the values that are used for the different scenarios used in the simulation. Thus, there are 3 scenarios for the situation in 2035 and 2050. If the resources file of Energyscope is looked into the file has much more resources but only those that has been changed are displayed.

| Category  | parameter name | gwp_op_2035                  | gwp_op_2050                  | gwp_op_max                   | gwp_op_min                   |
|-----------|----------------|------------------------------|------------------------------|------------------------------|------------------------------|
|           | units          | [ktCO <sub>2</sub> -eq./GWh] | [ktCO <sub>2</sub> -eq./GWh] | [ktCO <sub>2</sub> -eq./GWh] | [ktCO <sub>2</sub> -eq./GWh] |
| Renewable | BIOETHANOL     | 0.245                        | 0.245                        | 0.245                        | 0.245                        |
| Renewable | BIODIESEL      | 0.22                         | 0.22                         | 0.22                         | 0.22                         |
| Renewable | GAS_RE         | 0.078091                     | 0.039542                     | 0.018936                     | 0.38304                      |
| Renewable | H2_RE          | 0.051066                     | 0.026634                     | 0.01053                      | 0.2484                       |
| Renewable | AMMONIA_RE     | 0.063108                     | 0.045324                     | 0.03834                      | 0.1872                       |
| Renewable | METHANOL_RE    | 0.074484                     | 0.047412                     | 0.03042                      | 0.2916                       |

**Table A.1.** Global warming potential values of different synthetic fuels as function of scenarios

| Category  | parameter name | einv_op_2035 | einv_op_2050 | einv_op_max | einv_op_min |
|-----------|----------------|--------------|--------------|-------------|-------------|
|           | units          | [GWh/y]      | [GWh/y]      | [GWh/y]     | [GWh/y]     |
| Renewable | BIOETHANOL     | 0.1          | 0.1          | 0.1         | 0.1         |
| Renewable | BIODIESEL      | 0.1          | 0.1          | 0.1         | 0.1         |
| Renewable | GAS_RE         | 0.147465     | 0.090807     | 0.10954     | 0.643037    |
| Renewable | H2_RE          | 0.134318     | 0.094722     | 0.086118    | 0.5372      |
| Renewable | AMMONIA_RE     | 0.295284     | 0.25112      | 0.268278    | 0.53854     |
| Renewable | METHANOL_RE    | 0.145875     | 0.10934      | 0.120825    | 0.489782    |

**Table A.2.** Invested energy values of different synthetic fuels as function of scenarios

## A.2 LCA

This appendix is showing how to conduct a LCA in Simapro. The first thing to do in Simapro is either load a database or create a new one. In this case, a database has been created and can be found here <https://zenodo.org/record/7014677>.

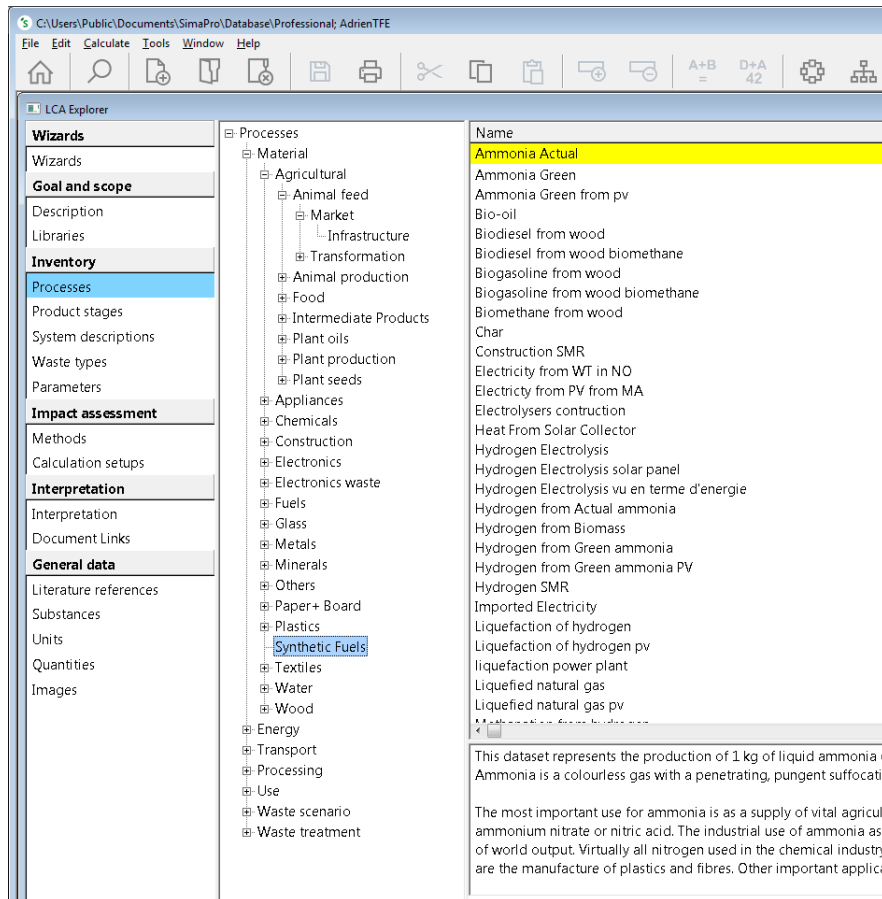
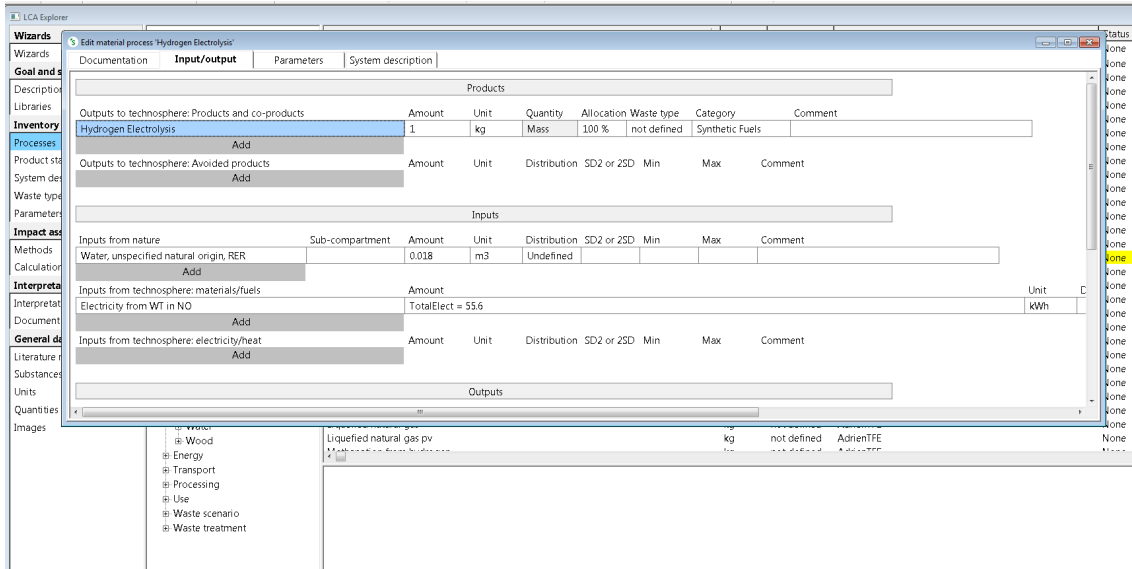


Figure A.1. Simapro software with the Processes open on the synthetic fuels tab open

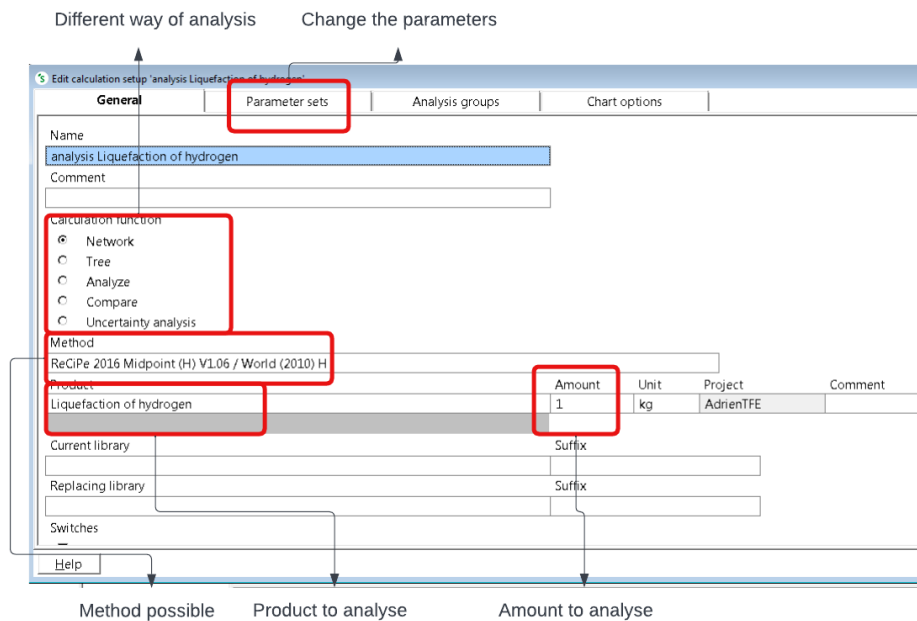
In this Figure A.1, the main tab is called the LCA explorer and on the right side the main four stages of a LCA. Those stages are important to decide which database to use as explained in the Simapro section. Those can be chosen in the **libraries** tab. All the processes are defined using the *ecoinvent 3 -allocation cut-off by classification* data base. All the created processes can be found under the name **synthetic fuels**. In the following figure, a processes is presented:





**Figure A.2.** Example of the process for hydrogen production through electrolysis, the different part of the window are highlighted in the picture

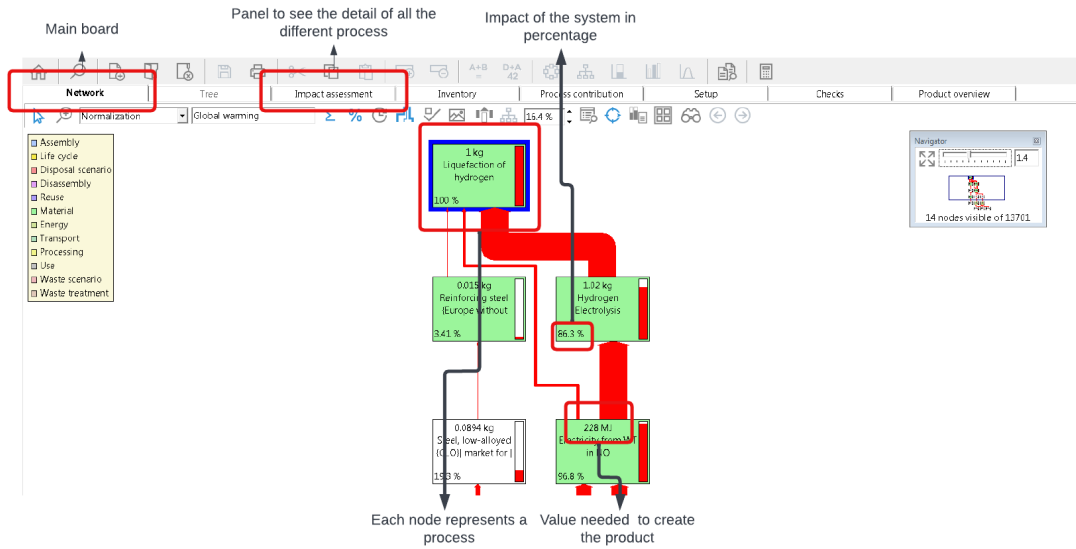
The most important part missing is that in figure A.2 is the output. Actually, it follows the same idea that the inputs, a process or a pollutant/waste has to be chosen from the database. If this product does not exist, it has to be created. The parameters are a useful tool to use the methods. In the following figure:



**Figure A.3.** Calculation setup of a LCA

In the calculation setup window, several object can be changed as seen in figure A.3. The most important thing is to choose the right method to work with. There are two mains types of analysis: impact to the environment and the energy analysis (CED). Finally, the

treatment of the results after the calculation is quite straight forward since SimaPro is giving you all the answers in the results tab as following:



**Figure A.4.** Result window of a study analysis of a process. All the different panel are shown in red

In this figure A.4, the panel of results is a mine of information and it is almost impossible to explain it all. Therefore, the most important two tabs are the network and impact assessment. Both of them represent the same thing, the network tab show the results very graphically where on the other hand the impact assessment tab shows the result more number wise.

### A.3 CED

The Cumulative Energy Demand (CED) of a product represents the direct and indirect energy used throughout the life cycle, including the energy consumed during the extraction, manufacturing, and disposal of the raw and auxiliary materials [80]. From this definition, CED could be considered directly as the energy invested necessary for EROI calculation. Therefore, the EROI is calculated after analyzing the different technologies to determine the energy invested in the different resources. For the technologies (e.g. nuclear, hydropower plant and renewable technologies), the calculation of the EROI is defined as the energy total produced by the technologies divided by the Cumulative Energy Demand [81]. For the resources (e.g. natural gas, oil and coal), the analysis proposed by Valente, Iribarren, and Dufour [77] considers only the non-renewable part of the CED to compare the different resources as a function of their technologies. Unfortunately, this is only interesting GWP-wise since this value correlates quite well with the  $CO_2$  emission of the considered fuel. Therefore, the CED is defined as follows by Modahl et al. [56]:

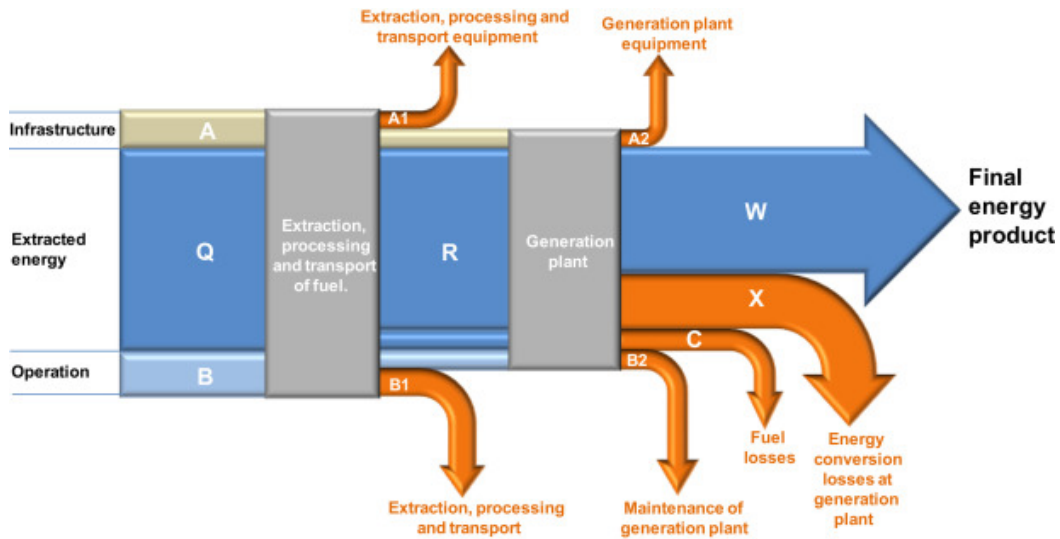
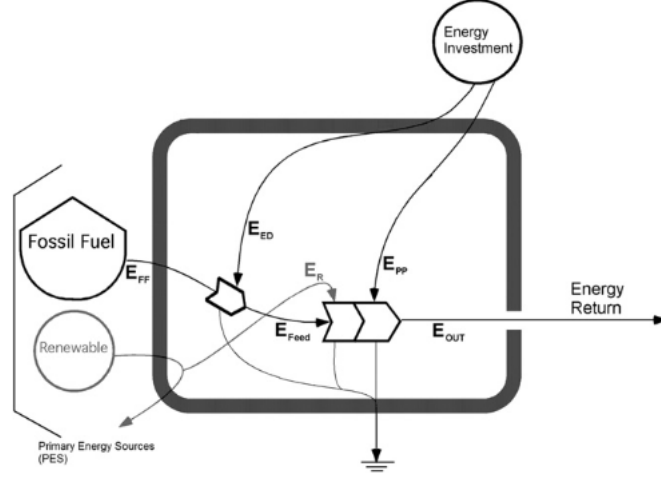


Figure A.5. Energy Balance of a Process [56]

The CED is therefore defined in Figure A.5 as follows:

$$CED = \frac{A + Q + B}{W} \quad (A.1)$$

From the article [63], the EROI can be evaluated as the energy invested in the fuel, as can be seen in the picture :



**Figure A.6.** Definition of the energy flux of a process to highlight the energy invested from [63].  $E_{ff}$  is the energy from the fossil fuels,  $E_{Feed}$  is the direct energy input for electricity production.,  $E_{ED}$  is the energy for extracting and delivering fossil fuel.  $E_{PP}$  is the energy necessary for the power plant's construction, maintenance and end of life.  $E_{out}$  is the energy output.  $E_R$  is the energy produced by renewable energy.

From Figure A.6, the energy invested is equal to  $E_{ED}$  which is defined as  $E_{ED} = \frac{E_{feed}}{E_{EROI_{fuel}}}$ . So, the EROI of the fuel fueling the process is considered in the invested energy. The  $E_{PP}$  is the energy for constructing the power plant and its end of life. Therefore, [63] defines the EROI as follows:

$$EROI = \frac{E_{out}}{E_{ED} + E_{PP}} \quad (A.2)$$

In addition to this, another method is studied to determine the EROI. Then, the method proposed by Muyldermans and Neve [59] is to since the LHV of the fuels is known, the EROI can be calculated as follow:

$$EROI = \frac{LHV}{CED - LHV} \quad (A.3)$$

Therefore, the invested energy for 1 TWh can be easily computed as it is the reverse of the EROI. Oliveira, Gasi, and Lourenço [61] proposes to look into the CED as follows:

$$EROI = \frac{LHV}{CED - (LHV + E_l)} \quad (A.4)$$

With  $E_l$  is the energy losses of the process. Therefore, it takes into account the energy used only by the process more precisely since it can be considered that the losses can be used for another purpose. The equation A.4 will be used to calculate the EROI of the different natural resources (e.g. natural gas, biomass and coal) since it is the most relevant for the system. The EROI of the technologies is calculated as the ratio of the energy output divided by the energy of construction, maintenance and end of life. It is the base necessary for all the different processes studied in this work.

From all the different definitions of CED, EROI calculation for a more complex process such as synthetic fuels is challenging since many different elements have to be considered.

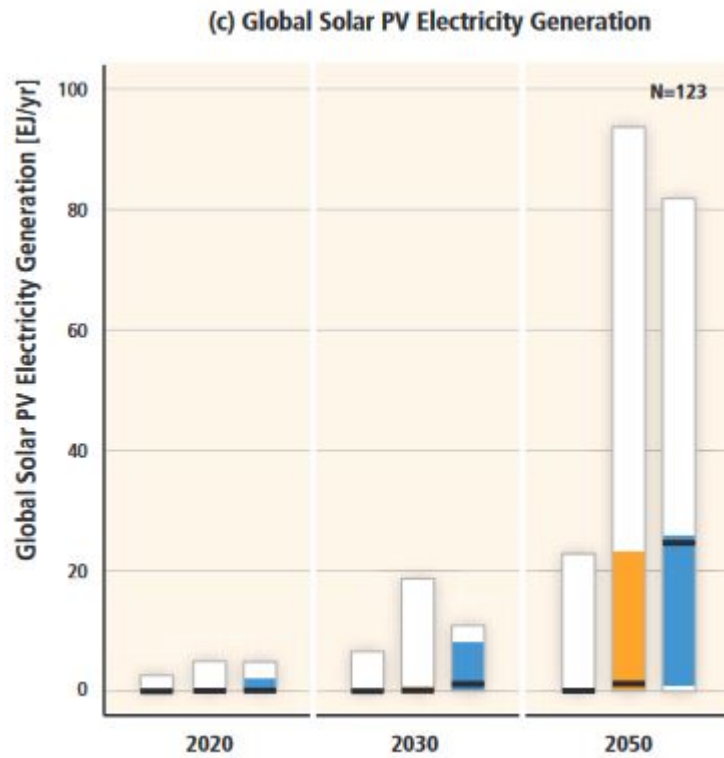
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Therefore, the EROI of a process is calculated by multiplying the energy output of resources by the efficiency of the process studied. The energy invested is taken from the resources necessary for the process and the energy necessary for constructing the power plant. For example:

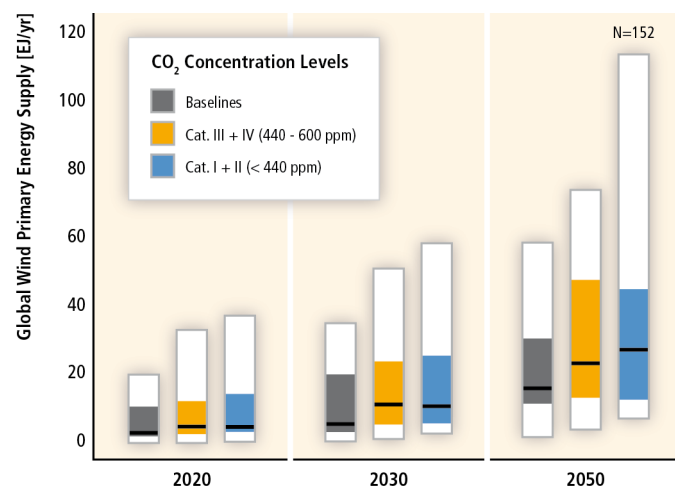
1. For hydrogen electrolysis, electricity is used for hydrogen production. The electricity comes from wind turbines. Therefore, the energy output is the electricity produced times the efficiency of the process. The energy invested is the energy invested necessary for the wind turbines and the energy for constructing the electrolyser.
2. For hydrogen from biomass, the main resource is biomass and heat. Therefore, the energy output is the sum of the energy output of the biomass and heat times the efficiency of the process. The energy invested is the sum of the energy invested of the resources and the energy for constructing the power plant.

## A.4 IPCC

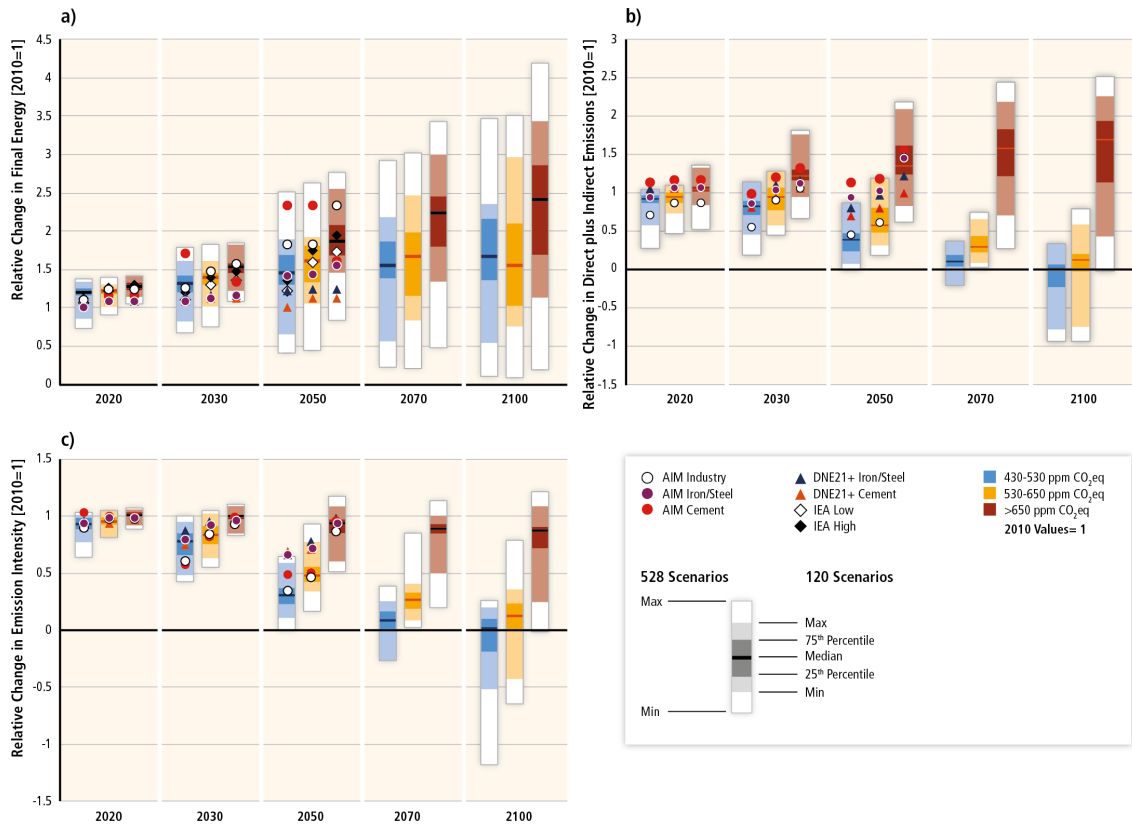
In this Appendix, all the figure used for the description of how the future scenarios are used for the determination of the future trends for industry and renewable technologies. The trends for the renewable development can be seen in Figure A.7 and A.8. The reduction of  $CO_2$  can be seen in Figure A.9



**Figure A.7.** Global Solar Energy Generation for different scenario for 2030-2050. The different bars are for the median 25th and 75th percentile range of different long term scenarios [65]



**Figure A.8.** Global wind turbine Energy Generation for different scenario for 2030-2050. The different bars are for the median 25th and 75th percentile range of different long term scenarios [65]



**Figure A.9.** Industry sector scenarios over the 21st century that lead to low (430 – 530 ppm CO<sub>2</sub> eq), medium (530 – 650 ppm CO<sub>2</sub> eq) and high (> 650 ppm CO<sub>2</sub>eq) atmospheric CO<sub>2</sub>eq concentrations in 2100. All results are indexed relative to 2010 values for each scenario. Panels show: (a) final energy demand; (b) direct plus indirect CO<sub>2</sub>eq emissions; (c) emission intensity (emissions from (b) divided by energy from (a)). Indirect emissions are emissions from industrial electricity demand [2]

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## A.5 Model parameters used for the models

This appendix is to propose a table summarizing all the hypothesis taken for all the simulations. For all the simulations, the capacity of several resources and technologies are limited. For technologies, wind turbines and PV panels that can be installed in Belgium are limited to 16 GW and 60 GW respectively. For the resources, the wood, wet biomass and biomass are limited to 23.4, 38.9 and 33.4 TWh respectively. Moreover, the electricity imports are limited 27.6 TWh.

| Name of the scenario | Data set used              | Hypothesis on the data                                   |
|----------------------|----------------------------|--|
| Base case scenario   | Initial data of ES-TD      | All GWP for synthetic fuels are equal to 0               |
| realistic scenario   | GWP and inv op 2035 column | synthetic fuels produced wit 80% PV and 20% WT           |
| Best case scenario   | GWP and inv op max column  | 100% WT  |
| Worst case scenario  | GWP and inv op min column  | 100% PV  |
| Scenario 2050        | GWP and inv op 2050 column | 80% PV and 20% with $CO_2$ reductions and learning rates |

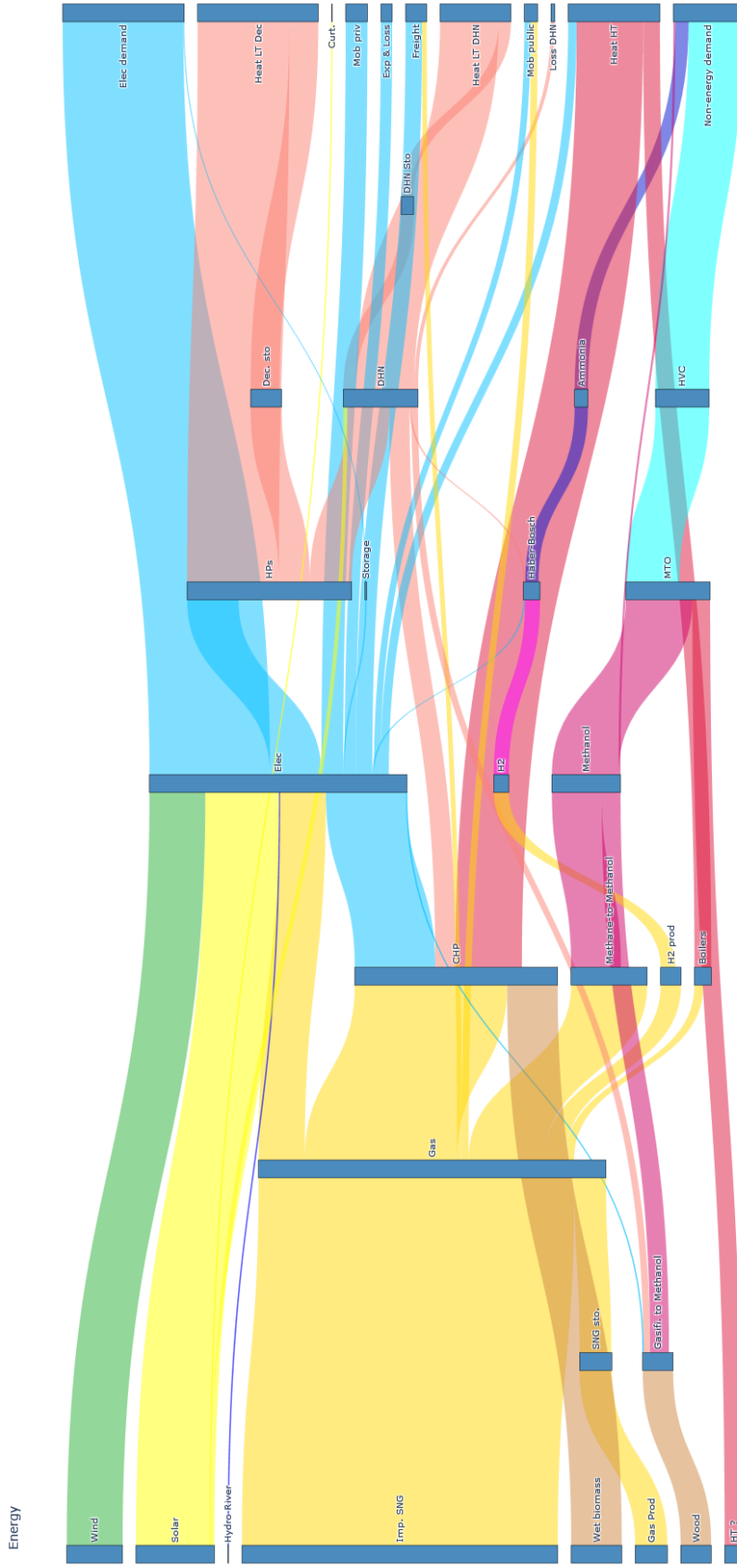
**Table A.3.** Different parameters used for the simulation of the different scenarios



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## A.6 Sankey Diagram of the Different Scenarios

The different Sankey diagrams proposed can be seen in this appendix. There is one for each scenario at their most constrained point. They have been put there to have a better clarity and readability in the report.



**Figure A.10.** Sankey diagram for 90% CO<sub>2</sub> emission reduction for the base case scenario in 2035 (scenario initial before this work)

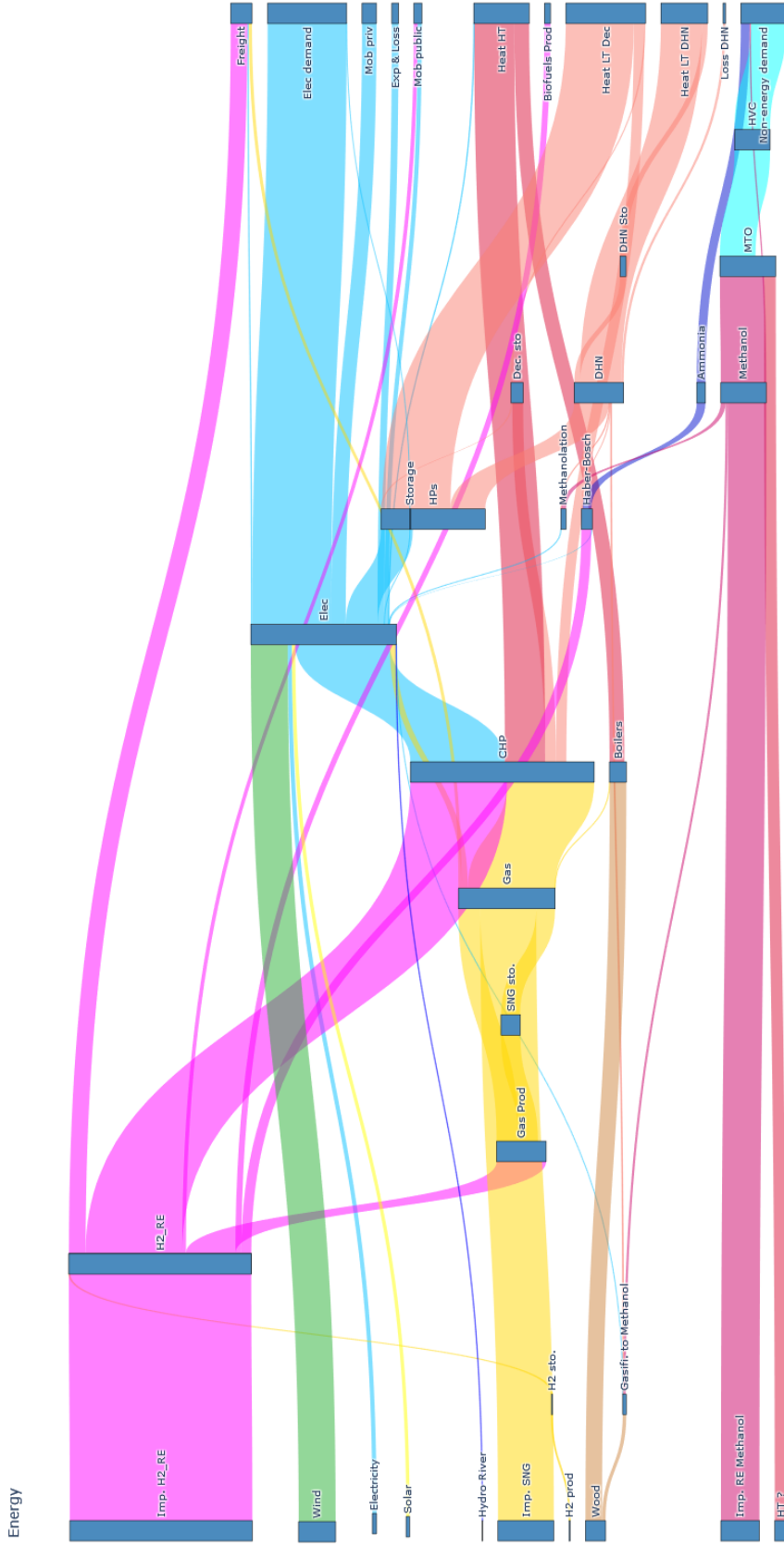


Figure A.11. Sankey diagram for 87% CO<sub>2</sub> emission reduction

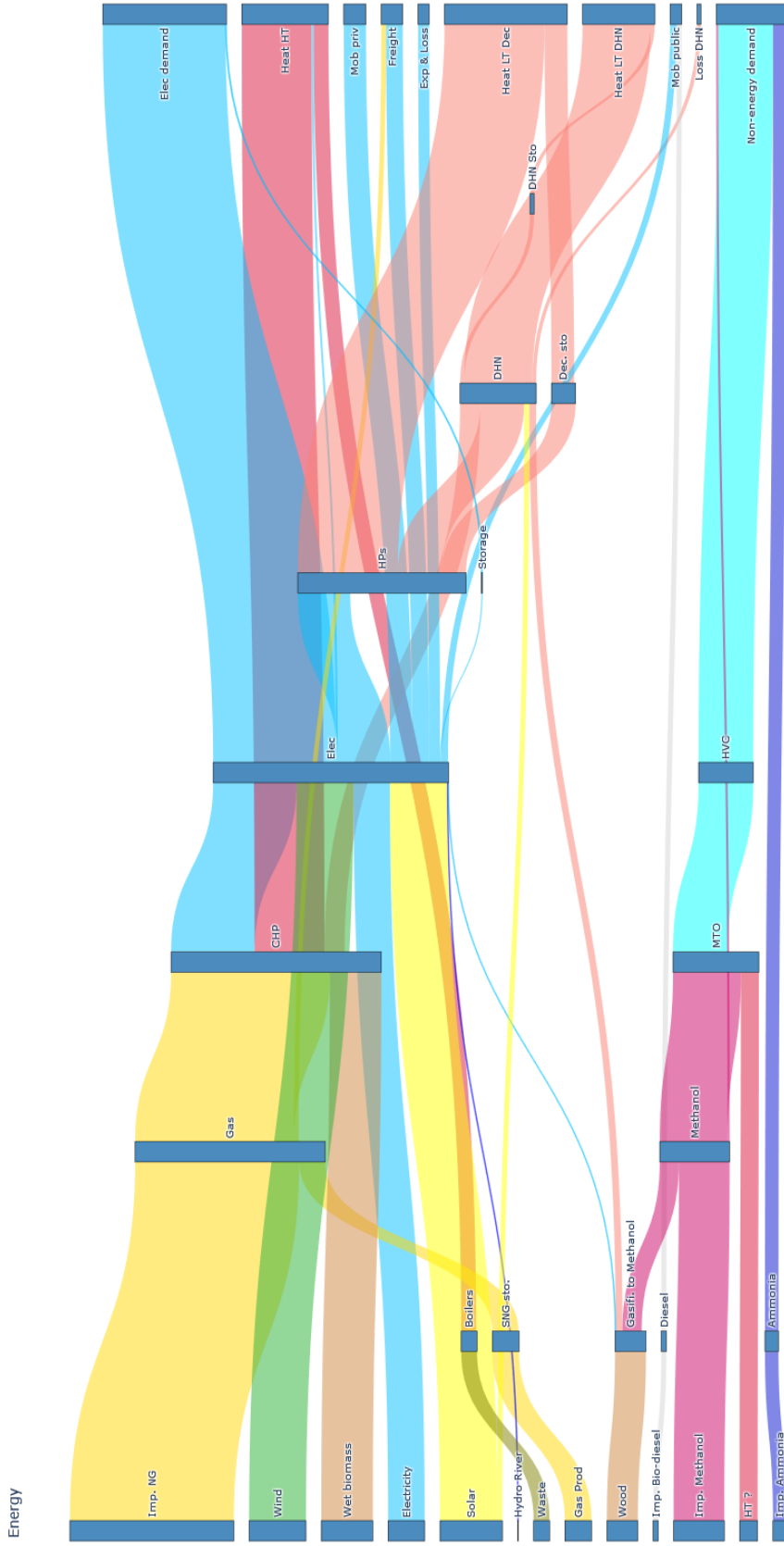


Figure A.12. Sankey diagram for 30% CO<sub>2</sub> emission reduction for the worst case scenario in 2035

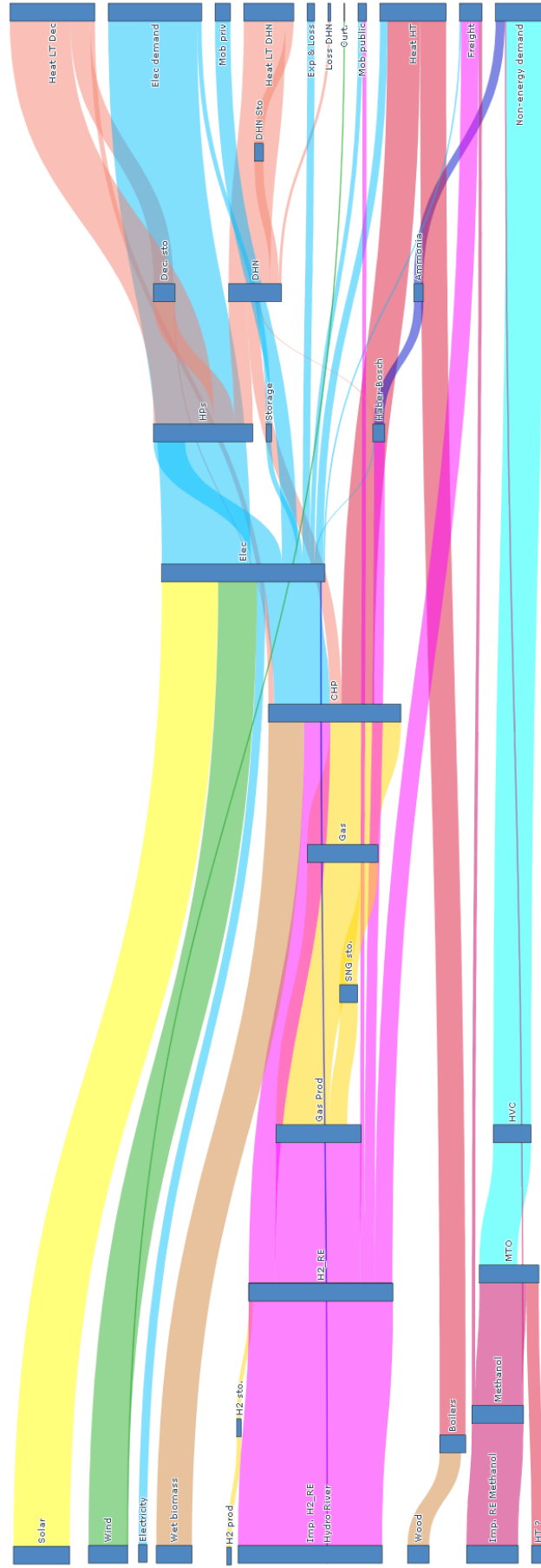


Figure A.13. Sankey diagram for 80% CO<sub>2</sub> emission reduction for the realistic case scenario

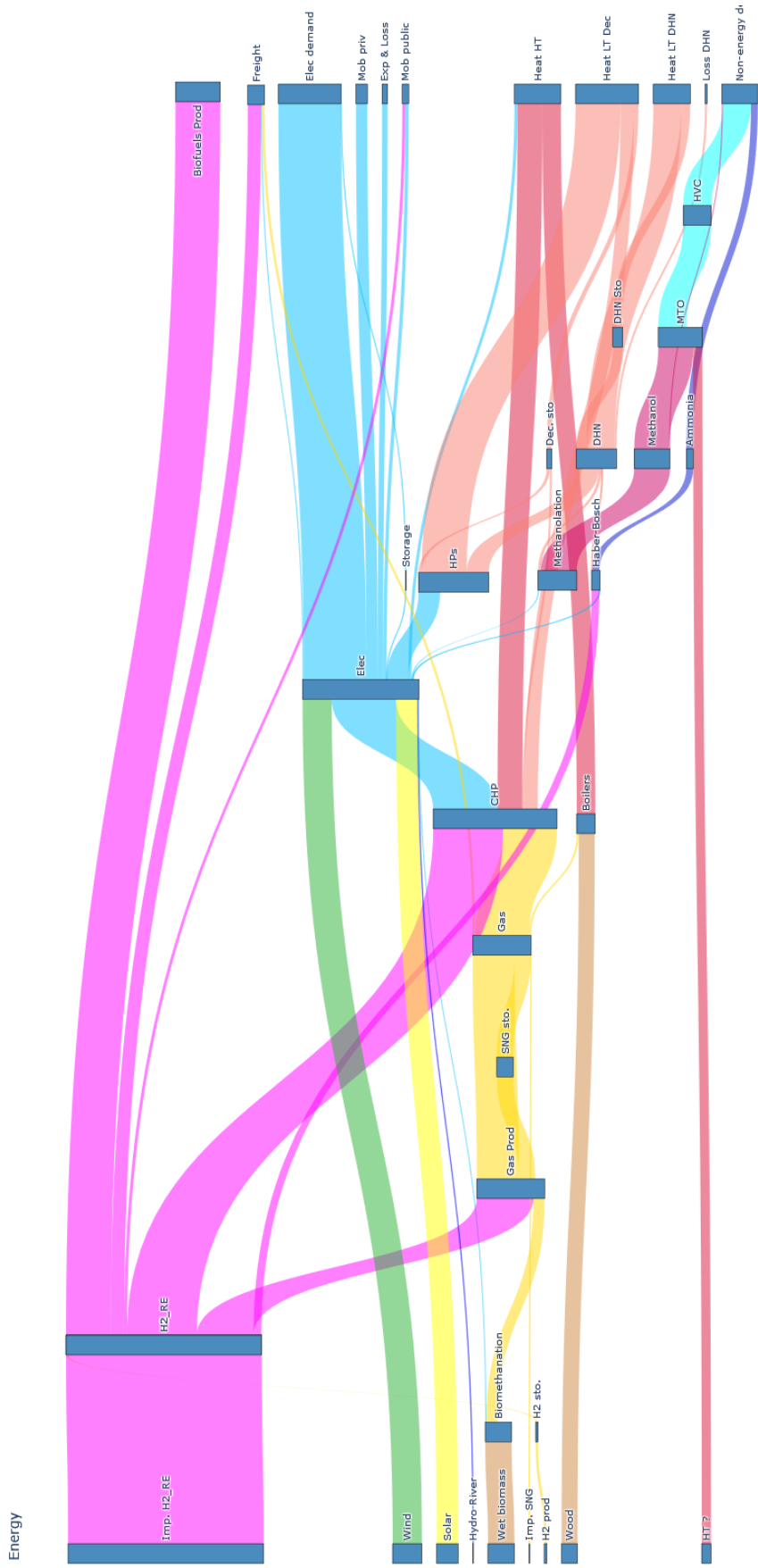


Figure A.14. Sankey diagram for 83% CO<sub>2</sub> reduction for 2050 scenario

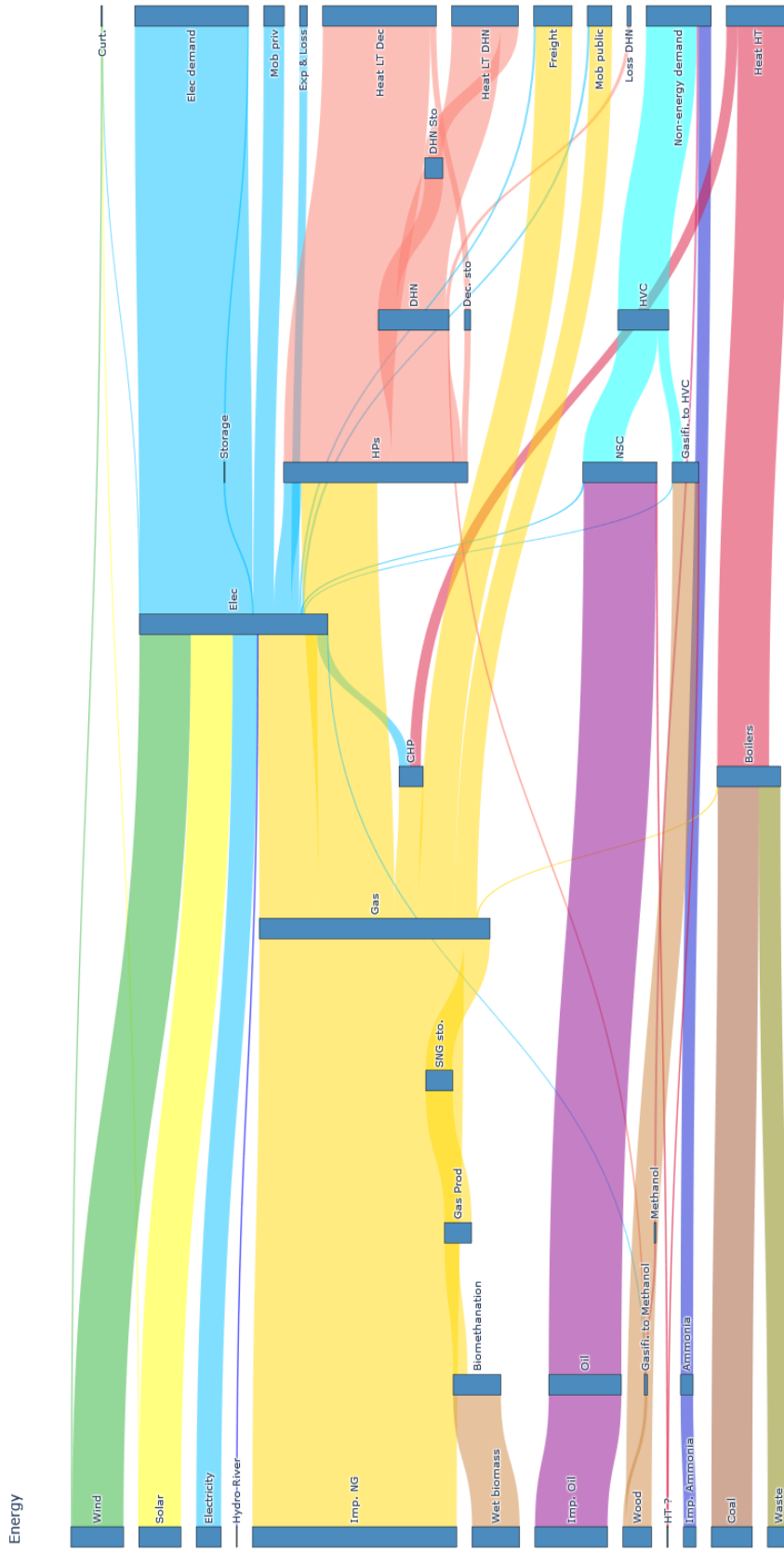


Figure A.15. Sankey diagram for no CO<sub>2</sub> reduction for 2035 scenario. Sankey created with optimisation based on the cost