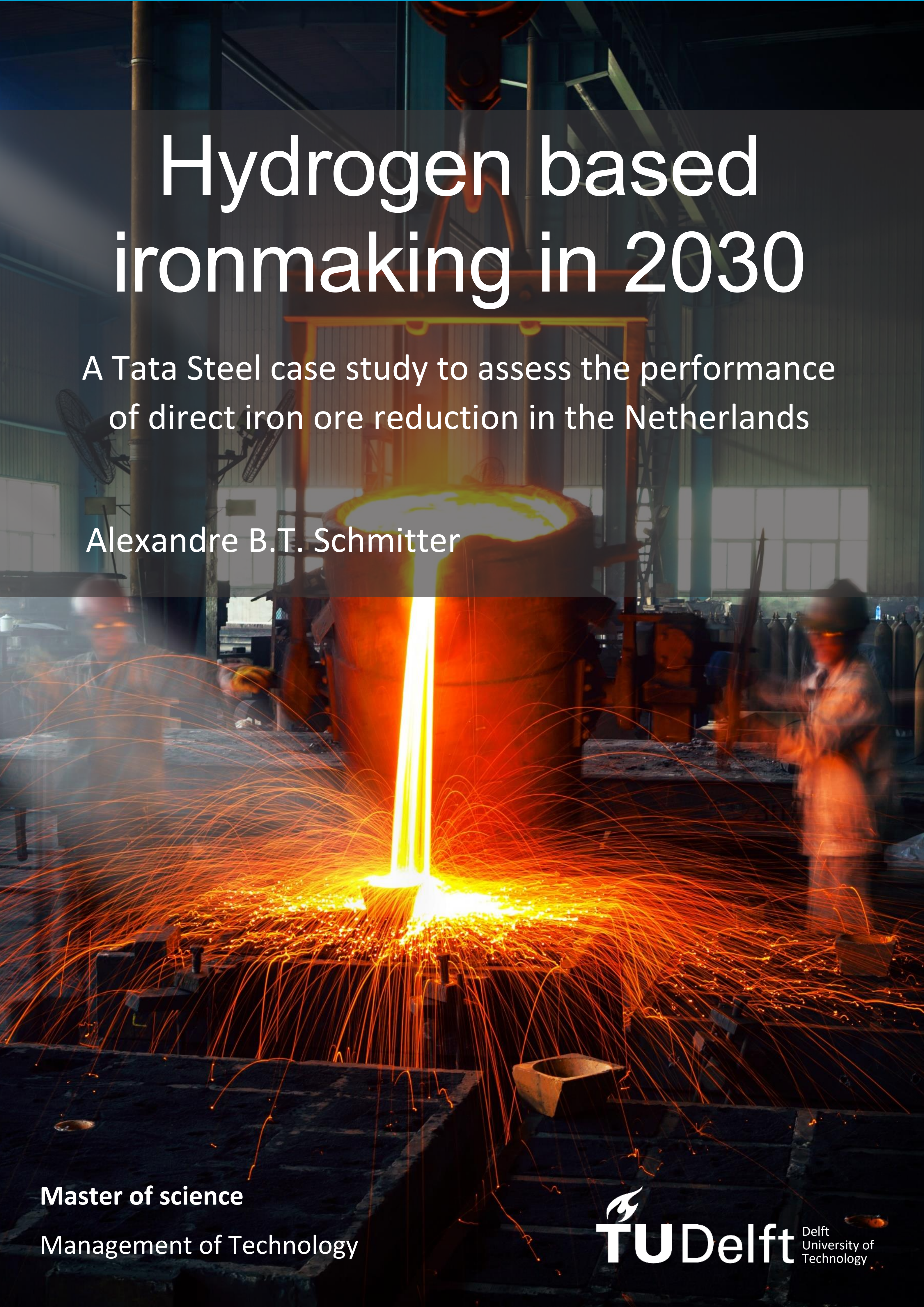

Hydrogen based ironmaking in 2030

A Tata Steel case study to assess the performance of direct iron ore reduction in the Netherlands

Alexandre B.T. Schmitter

Master of science

Management of Technology

TU Delft Delft University of Technology

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by

A.B.T. Schmitter

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Thesis committee:	Prof.ir. R.A (Rudi) Hakvoort,	TU Delft, chair
	Prof.ir. R.A (Rudi) Hakvoort	TU Delft, Supervisor
	Dr.ir. (Zenlin) Roosenboom-Kwee	TU Delft, supervisor
	Dr. P. (Peter) van den Broeke	Tata Steel, Company supervisor

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Enjoy the read!

Alexandre (Sacha) Schmitter
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Abstract

The Iron and Steel (I&S) industry is the largest contributor to man-made greenhouse gas emissions. The products of the I&S industry are a constant necessity, e.g. for civil infrastructure. In addition, their processes are interwoven with coal and natural gas properties, which classifies this industry as a 'hard-to-abate' sector. Furthermore, fundamental technology changes in process and energy utilisation practices are required to fully decarbonise the I&S industry before 2050. Steel processes are divided into two major production routes, the blast furnace and the direct reducing plant. Focusing on the carbon avoidance route, the hydrogen-based direct reduction process is the most promising to decarbonise the I&S industry in Europe due to its ability to use natural gas as an intermediate energy source. Several techno-economic assessments have explored the energy, emissions, and economic potential of such conceptual systems, concluding that carbon emissions are highly sensitive to the CO_2 intensity of consumed electricity. However, none have used the electricity mix to estimate the electricity price and associated CO_2 emissions on an hourly basis to investigate the performance of such systems. Therefore, a case study is proposed of Tata Steel Netherland (TSN), which has recently announced its intention to switch towards hydrogen-based steel through the DRI-REF route. The modelling and simulation research method is used to assess this case-specific process's technical, environmental, and economic performance in 2030. A conceptual model is developed employing the findings of the literature review. Hourly data from the national electricity mix are acquired from the EMF v7.0 model from the company Blueterra, and TSN provides specific process characteristics. From this approach, several simulations could be made for different hydrogen volumes to evaluate the performance of the DRI-REF system in the Dutch context. The simulations showed a significant shift in energy sources for increasing hydrogen volumes, which leads to a reduction of 70.1% in direct CO_2 emissions under the 2030 energy market conditions. However, if the indirect electrical emissions are considered, this reduction potential is only 2.2% CO_2 reduction. Although this demonstrates that in 2030 the CO_2 intensity of the electricity mix is approximately the breakeven point between NG and H2 production, this development also shows a major shift from CO_2 emissions towards the electricity producers. Additionally, the electricity price breakeven point is a factor 3 lower than is currently estimated by using the IPKA0 electricity generation capacity scenario of Tennet. As a result, the levelised cost of production increases by 34.9% for the maximum Htextsubscript2 volume compared to NG-based production, with electricity and capital investments as the largest increasers. Furthermore, the hourly electricity price and associated CO_2 emissions data enabled to determine the variability over time. A significant increase in the interquartile spread in emissions and cost calculations is observed for increasing hydrogen volumes. This implies that in the future when electricity is predominantly produced by volatile renewable energy sources such as wind or solar energy, the production uncertainty will increase significantly if this industry shifts towards hydrogen. However, this also increases the potential of flexibility technologies. Industries with flexible production processes can thrive in the Dutch environment as they could provide load-balancing services.

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Acronyms

1. Introduction

Today, one of society's most significant challenges is anthropogenic climate change. Decarbonising all sectors is essential to mitigate climate change to slow down this crisis. In the last few decades, we have seen an increase in the development and adoption of sustainable solutions in all sectors and industries to move away from Green House Gas (GHG) emitting resources. However, the industries classified as 'hard-to-abate sectors' stand before a crucial transition phase as they must transform their processes to match the international agreements [25]. However, the transition of these sectors is not nearly so straightforward because of a lack in technological development and of prohibitive costs [1]. Of course, these sectors are hard-to-abate because they have a significant relative contribution to global emissions and are neither desirable nor realistically able to phase out.

The heavy manufacturing industry, including the Iron and Steel (I&S) industry is the single largest contributor to anthropogenic GHG emissions, accounting for 2.7 Gt CO_2 or 7%-9% of the direct global emissions and is classified as a 'hard-to-abate' sector [33; 69]. The products of the iron and steel industry are necessities in buildings and civil infrastructure, transportation, mechanical and electrical equipment, and energy systems like renewable energy systems [69]. In addition, they have processes that are interwoven with the properties of coal and Natural Gas (NG), as well as employing extremely high-temperature processes that can, as of today, only be achieved cost-effectively by burning fossil fuels. The consecutive industrial processes are also highly integrated and complex, making the challenges of finding carbon-free alternatives just as complicated. Many of these companies are reluctant to pursue change because large amounts of funds have already been sunk into refining these processes [55].

Meanwhile, the required demand for sustainable energy sources for the I&S industry is so high that a complete transition towards these carbon-free high-density energy sources is not feasible yet with our current energy system. Incremental changes in current industrial production technologies would not reach the emission reduction goals [2]. However, recent research suggests that it is technically and economically possible to decarbonise the I&S industry within the time frame specified by the Paris Agreement, that is, to go for zero emissions by 2050. Fundamental changes in technology, process, and energy/feedstock utilisation practices are required [4].

1.1. Transition of the iron and steel industry

Nowadays, crude steel production in Europe is almost entirely divided between steel produced via the Blast furnace - Basic Oxygen Furnace (BF-BOF) route and the mainly scrap-based Electric Arc Furnace (EAF) route. They represent respectively 58.5% and 41.5% of the

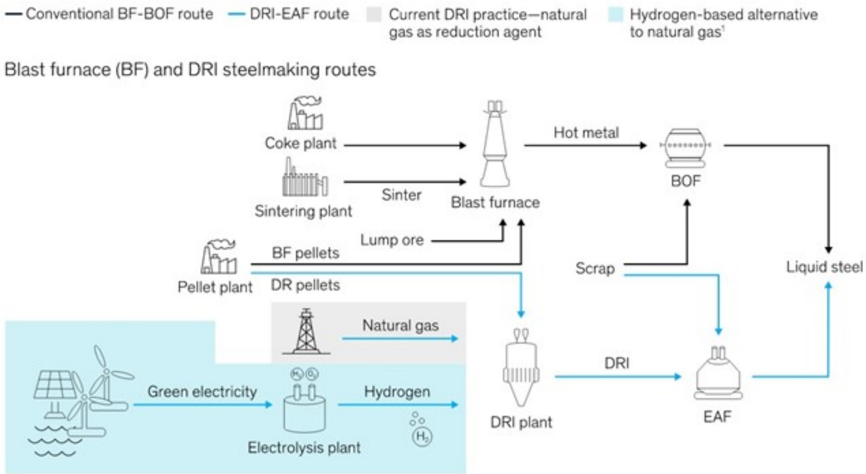


Figure 1.1.: Most common steel production routes in Europe can be divided into two groups, namely the Basic Oxygen Furnace and Electric Arc Furnace route. Picture adopted from Doyle and Voet[19]

EU28 steel production [WorldSteel]. For illustrative purposes, Figure 1.1 demonstrates the major steel production route.

The current European emission intensity of the dominant BF-BOF route is reported in the range of 1,650-1,920 kg CO_2/$ton_{Crude\ Steel}$(t_{CS}) depending on process configurations, system boundaries and geographical location [12; 49; 44]. The majority of the emissions are released from the blast furnace (61%) and coke-making plant (27%) [9]. Furthermore, due to constant optimisation of these processes, the technology is approaching the technical minimum of 1518 kgCO_2/t_{Steel} due to non-zero mass and energy conversion losses) [28]. The primary carbon emissions from the blast furnace are process-related emissions, where CO, from the gasification of the cokes, reacts with the oxygen from the iron ore to produce CO_2 and liquid iron. It is recognised that process energy efficiency improvements, including using the Best Available Technologies (BAT) and carbon capture systems, will not suffice to abate emissions required to reach the climate change mitigation goals [3].

Focusing on carbon avoidance routes, two trends can be anticipated. First, an increase in secondary steelmaking (i.e., scrap-based) via electrical arc furnaces EAF is expected, representing 23% of annual steel production. However, the secondary route is constrained by limited scrap availability and steel quality requirements and is expected to be at most 45% of steel production by 2050 [26]. Second, various alternative steel production processes are being researched and tested to reduce carbon footprint significantly. These methods are gas based Direct reduced Iron (DRI) using Natural gas-based DRI production (DR(CH_4)), Carbon Capture and Storage (CCS), Electro winning (EW) (electrolysis of iron ore) and Hydrogen-based DRI production (DR(H_2)) production. The most promising steelmaking technology to significantly reduce carbon emissions is the direct reduction of iron ore with hydrogen (DR(H_2)) as coke (coal) is no longer necessary [67]. Hydrogen-based steelmaking is known as Electrical Power to Hydrogen (PtH_2) steelmaking as the hydrogen is produced via electrolysis with the electricity from low-carbon emitting sources, as illustrated in figure 1.1.

Several recent techno-economic assessments explore the energy, emissions and economic potential of conceptual DR(H_2) systems [7; 36; 44; 48; 49; 65]. These techno-economic assessments all conclude that carbon emission from steelmaking is highly sensitive to the carbon intensity of the electricity used to produce the hydrogen for the reduction process. However, these assessments do not consider carbon intensity swings of electricity production on a national level and its effect on operational emissions of DR(H_2) steelmaking. Due to geographical disparities in the electricity decarbonisation pace, certain regional grid emission factors would remain prohibitively high for grid-driven DR(H_2) deployment beyond the current decade [49]. Therefore, it is crucial to determine under which circumstances hydrogen can be used to replace fossil fuels (i.e., coal, natural gas) in the DRI process to achieve emission reduction first and, secondly, to achieve the emission targets. The literature mentioned above and additional literature will be further reviewed in chapter 3.

Strategies to shift towards hydrogen-based steelmaking should need to pursue various aspects, including being economically feasible, achieving a carbon-neutral production process, and having the security of energy supply through renewable electricity and green hydrogen. To contribute to the growing body of literature on hydrogen-based steelmaking and its environmental impact, a case study of Tata steel Ijmuiden in the Netherlands is presented.

1.2. Tata Steel Ijmuiden case

TSN is a major steel producer in the Netherlands . Due to its location, it has excellent access to harbour infrastructure and maritime trade routes. This has led to steady operations since its foundation in 1918. In the last fiscal year, 2019/2020, Tata Steel Ijmuiden produced 6.78 million tonnes of liquid steel with a carbon intensity of 1.86. tonnes of CO_2 per tonne of crude steel. The audited European Union Trade System (EU ETS) direct emissions amounted to 6.35 million tonnes of CO_2, and the scope 1-3 emissions totalled 12.31 million tonnes of CO_2 [57]. Placing these numbers in perspective, the Dutch economy emitted 189.5 million tonnes of CO_2 in 2019. This means that Tata Steel Ijmuiden contributes to approximately 6.5% of total Dutch CO_2 emissions.

In 2021 Tata Steel decided to shift from its future business strategy. The Carbon Capture and Storage CCS route is replaced by the DR(H_2) route with hydrogen as a reduction agent. Their ambitious goal is to replace one of the two blast furnaces in Ijmuiden with a DRI plant by 2030 that runs on hydrogen and natural gas as the primary feedstock for the iron ore reduction process in the DRI Plant (see figure 1.1). In the coming decades, the DRI technology will still need to develop further to accommodate an increasing percentage of hydrogen. The anticipated use of hydrogen as a feedstock in the area of TSN leads to a doubling of electricity demand due to the shutdown of the BF-BOF off-gas powered electricity station and the placement of electrolyser capacity [45]

One of the critical aspects of the gas-based DRI process is hydrogen production. Based on the electric power demand and supply mechanism, the CO_2 intensity of the electricity generation sources fluctuates over time as different types of assets are being used, ranging from offshore wind, solar to natural gas-fired power plants. Therefore, not only the price but also the carbon intensity of the electricity generation varies hourly. Today's Dutch electricity generation capacity is a mixture of fossil and renewable capacity with an average of 328 kg CO_2e/MWh (2020) [20]. This means that the Dutch electricity mix is not an ideal source for providing the required electricity for the electrolysis due to the greenhouse gases released.

However, is it still the case in 2030 when large quantities of renewable electricity generation are installed? As renewable energies increase their penetration in the energy mix, so does the possibility of directly using grid-sourced electricity to produce nearly carbon-free hydrogen for the steel industry. Due to the shift towards hydrogen use in the steel production process, TSN is becoming increasingly dependent on the electricity market behaviour. TSN has indicated that it lacks a thorough understanding of future energy market behaviour and how this could affect the iron production process.

The coupling of the future energy market behaviour with the ironmaking process has yet to be researched for the Dutch situation. Therefore, there is no technical and economic assessment of the relative amount of hydrogen and natural gas requirements for the specific technology that TSN will apply. The specific ironmaking process will be further elaborated in section 5.1. However, it can be seen as a deviation from the most common steelmaking process explained in figure 1.1, where the DRI is typically further processed in an EAF. The practical knowledge gap comes from the missing data on the specific ironmaking technology applied in this research. However, this thesis uses new data acquired from TSN based on their applied ironmaking process in 2030 and is the first academic project to do so. Furthermore, new data from an EMF model enables the detailed performance analysis of hydrogen-based ironmaking. The academic knowledge gap comes from the fact that there is no thorough understanding of the effect of varying the hydrogen fractions on the economic and technical performance of the DR(H_2) process with an Reducing Electric Furnace (REF) in the Netherlands under given electricity grid settings in 2030 and what the optimising conditions are. From this knowledge gap, the main research question derives:

How do various hydrogen volumes affect the technical, economic and decarbonisation performance of a DRI-REF process in the Netherlands in 2030?

This thesis project focuses on understanding how varying hydrogen content in the feed gas of the DRI process affects the technical and economic performance of the DRI-REF process in the Dutch context in 2030. Additionally, this thesis uses hourly data from the EMF model coupled with a specific ironmaking process which can provide additional insights into the environmental performance of the system. This information can be of significant help when planning for long-term strategies towards to low-emission industrial sector.

1.3. Research decisions and boundaries

Several research decisions are made to define and limit the scope of this research project and are presented below.

- The chosen DRI process technology is the 'Energiron' technology, elaborate in chapter 2 and 5. TSN applies this specific ironmaking technology in the future.
- The decarbonisation transition of TSN is divided into three steps. Only the first transition step is considered in this research, as further explained in section 2.2.
- The availability of data for the near future scenarios is a constraint which limits this research to the year 2030. For the assumed Dutch electricity generation capacity in 2030,

the TenneT 2030 IPKA0 scenario is considered. This scenario is used for calculating the input dataset, further elaborated in section 2.3.

- The potential change in the energy procurement method leads to various opportunities and challenges. This thesis will model the system of interest on an hourly basis to provide insights into the effects of this temporal scope, further elaborated in section 2.3.2

1.4. Thesis outline

This thesis is structured into multiple chapters. These chapters guide the audience through a sequence of steps from the problem definition towards the results and conclusions. A short explanation of these chapters is provided.

Chapter 1: Introduction
The thesis subject is introduced and the case study is presented.

Chapter 2: Contextual information
Contextual information is provided on the aim of TSN, the energy market developments and the hydrogen production plans in the Netherlands are explained.

Chapter 3: Literature review
The literature review analyses existing literature on steel manufacturing with hydrogen and natural gas. In specific, the literature concerning the DRI process is reviewed. Lastly, a research gap is identified that provides a basis for this research.

Chapter 5: Conceptual model
The conceptual modelling chapter presented the primary methodology of this thesis project. The problem situation is laid out as well as the inputs, outputs, simplifications, and assumptions.

Chapter 6: Data
The data chapter elaborates and analyses the data used in this research project. The parameters and data sets are based on the literature review or from TSN and serve as inputs for the conceptual model documented in the previous chapter.

Chapter 7: Technical model implementation
The implementation of the conceptual model is done in this chapter. Firstly, the base model with the Key Performance Indicator (KPI)s is elaborated, and the hydrogen implementation is subsequently presented.

Chapter 8: Economic evaluation
The economic evaluation is presented in a separate chapter. First, the levelized cost of production is calculated, which sets the basis for the economic performance evaluation. Furthermore, the last KPIs are presented.

Chapter 9: Results
The results of the use of technical modelling and economic evaluation are presented in this chapter. The simulations are explained, and the results are presented in separate subsections.

Chapter 10: Discussion
The results and findings are discussed and compared with the literature findings of chapter three. Furthermore, the limitations of the methodology used in the research are discussed.

Chapter 11: Conclusion
The last chapter of this thesis concludes the research. First, the answers to the sub-research questions are provided, supporting the main research question. Lastly, a reflection is provided on both academic and practical viewpoints.

2. Contextual information

This chapter provides contextual information on the case study, technological transition, hydrogen developments around Tata Steel Ijmuiden and detailed information on the Dutch electricity system. This chapter and the next chapter, the literature review, provide essential knowledge in this thesis project to better understand the decision-making process, methodology and analyses.

2.1. Tata Steels ambition

As introduced in the case study, on September 15, 2021, TSN announced that it wants to transition towards green steel-making with hydrogen-based DRI technology to meet climate targets. This decision was made with the Federation of Dutch Trade Unions (Dutch: Federatie Nederlandse Vakbeweging, FNV), which had previously expressed its preference for this direction. On Augustus 30, 2022, TSN chose their technology pathway for this route [66]. The company Danieli will be responsible for the engineering design for the plant and technology that delivers the (Energiron) DRI, the 1st step in the iron-making process. Hatch is a technology licensor of the REF that melt the DRI and help to reduce the oxygen content further, thereby improving the final steel quality. The REF and DRI plants are closely coupled to form an integrated production system.

Currently, the employed blast furnaces at TSN are one of the most carbon-efficient in the world, but at the same time, they are the most significant industrial emitter of CO_2 in the Netherlands. In the National Climate Agreement, the Dutch industry has made commitments to reduce its emissions in a stepwise manner [43]. To this end, TSN has a CO_2 reduction target of 30% by 2030 (3.8 Mton per year) and, based on its ambition, increased this target towards 40% (5Mton per year), which is presented in an Expression of Principles with the Ministry of Economic Affairs and Climate Policy [57]. In addition, TSN is also investing € 300 million in 'Roadmap Plus' to reduce other emissions in the current decade. However, the Roadmap Plus developments are outside this thesis research's scope. Finally, through several transition steps, the ultimate goal is a carbon-neutral steel production process, further elaborated in the next section.

The leading factors for the decision to switch towards the hydrogen-based DRI route:

1. **The time is now:** Novel economic and technological developments have created the opportunity and utilisation of hydrogen and DRI technology to decarbonise steel production.
2. **Local emissions can be reduced:** In combination with Roadmap Plus, the DRI technology offers the opportunity to accelerate a reduction in local emissions and public problems. The National Institute for Public Health and the Environment (RIVM) once again accentuated the importance in a report published on September 2, 2021 [41].

3. **Hold onto a leading position as a steel company:** The transition towards the hydrogen route offers TSN the chance to retain its leading position by enabling high-quality and green steel production. The added quality to the steel products is done in the BOFs. TSN is keeping these facilities to retain the desired steel quality output. Only the blast furnaces, that operate on coal, will be changed for DRI and REF facilities. This transition is further elaborated in the problem situation in chapter 5.1.

2.2. The transition from the blast furnace to DRI and hydrogen

In the transition towards full hydrogen-based DRI, the site of TSN will undergo a complete transformation. The new facilities are planned to run on sustainable power sources like green- hydrogen or electricity instead of coal. The green electricity needed for this endeavour is planned to be generated in the offshore wind farms in the North Sea and elsewhere. This makes it possible for a share of green hydrogen to be produced on-site, further elaborated in section 2.3.1. However, due to the vast quantities of hydrogen needed, the hydrogen will also need to be imported [57].

2.2.1. DRI technology as a replacement for blast furnaces

TSN will transform its site in three steps to become a greener steel company. The steps contain the replacement of the two blast furnaces and finally operating entirely on hydrogen. To start, the first Blast furnace (BF) (BF6 or BF7) is envisioned to be replaced before 2030 with the first DRI plant and a REF to help reduce the oxygen content further, thereby improving the final steel quality. This replacement will be coupled with the closure of the coke and gas plant. At first, the DRI will mainly operate on natural gas because insufficient (and cost-effective) green hydrogen may not be available to TSN. The DR(CH_4) route is termed as a bridging technology between the carbon-intensive and dominating BF-BOF steelmaking route and the radically new DR(H_2) steelmaking route. This is because the DR(CH_4) technology is based on the same production principles as the DR(H_2) technology, and there is no need for prohibitive equipment modification [39]. One characteristic of this process is that it can increase its share of hydrogen without much difficulty [49]. So, as soon as the hydrogen becomes available (green or otherwise) in sufficient quantities, the DRI process can run on an increased share of hydrogen. The change in the facilities in the first step can yield a net CO_2 reduction of 3.1 or 4.4 Mton per year (depending on the closed BF) when operated entirely on natural gas. The CO_2 reduction potential nears or meets the targets in the Climate Agreement (see section 2.1) but is not enough for the 40% reduction ambition that TSN has announced in the Expression of Principles [17]. This ambition will be realised in the second step.

The developments of the second and third steps will be outside the scope of this thesis project. However, for background information purposes, a summary is provided. The second step will include replacing the second and last blast furnace with the DRI plant and REF facilities. This is also paired with closing the last coke and gas plants and the sinter lines. In the third step, TSN will further bring its CO_2 emission to zero by increasing the hydrogen share to the maximum as technically possible. The speed at which this transition will take place strongly depends on the availability of sufficient hydrogen at the right price, which is dependent on the infrastructure for transport and storage facilities. These developments will strongly indicate the transition from natural gas to hydrogen. Finally, specific innovation measures will have to be taken to become fully climate-neutral, which measures remain unknown and are dependent on future technological development. This applies to the whole steel industry [17].

These benefits can make the DR(H_2)-EAF economically and environmentally the most attractive route and contribute to stabilising the grid and storing excess energy in a 100% renewable energy system. There are many initiatives to develop and prepare the hydrogen market for large-scale diffusion, like the European Hydrogen Backbone [63], consisting of 31 infrastructure operators.

2.3. Energy market developments

In the following sections, several topics relevant to the case study will be discussed and provide information for decisions made later in the thesis. The information presented in this section is used in the Data chapter and serves as a basis for the input formulation. This will be further elaborated in Chapters 5 and 6.

2.3.1. Hydrogen and electricity capacity developments up to 2030

As stated earlier, the hydrogen-based steelmaking route TSN has chosen cannot be realised without sufficient hydrogen (green or otherwise). Other industrial sectors will also need large quantities of hydrogen for their decarbonisation pathways. Generation of this green hydrogen requires immense quantities of (renewable) electricity generation capacity to provide enough renewable electricity. Also, the electrification of other processes throughout the Netherlands will demand an increase in electricity. Due to its geographical location, the Netherlands will generate most of this renewable electricity from offshore wind, which requires the construction of external infrastructure for energy generation and transport. This section will elaborate on the current and planned developments around renewable electricity, green hydrogen, and phasing out of existing electricity generation capacity. The future electricity generation capacities are summarised in Table 2.1.

To fulfil its national responsibility to limit GHG emissions by 55% in 2030, which is presented in the national frameworks like the Climate Act and the Climate Agreement, the Dutch government has planned a capacity of 21 GW of offshore wind energy by 2030 [43, p.161] . To this day, only 2.5 GW (2020) of offshore wind capacity has been installed, with the total wind capacity (on land and sea) nearing 6.6 GW.

The planned installed offshore wind capacity in 2030 will contribute to green hydrogen generation in the Netherlands. The published Government Strategy on Hydrogen aims to realise 3-4 GW of electrolyser capacity by 2030, whereby the development must be in line with the additional growth in the share of renewable electricity [43, p.173]. Gasunie, a Dutch natural gas infrastructure and transportation company, is also part of developing what is called 'the hydrogen backbone', which aims at defining the critical role of hydrogen infrastructure and realised before 2030 [63].

Scenario and sensitivities		2020	2022		2025		2030 (planned to be realised)				
		-	KA0	KA1	KA0	KA1	KA0 KA2	KA1	IPKA0	IPND0 IPND2	IPND1
Nuclear	[GW]	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Coal	[GW]	4.0	4.0	4.0	4.0	4.0	0.0	0.0	0.0	0.0	0.0
Gas (methane)	[GW]		17.6	16.0	15.9	14.3	14.3	12.7	14.5	12.7	12.7
Hydrogen	[GW]	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.4	1.4
Biomass	[GW]	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	2.2	2.2
Waste incineration	[GW]	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8
Renewable energies											
Solar	[GW]	10.7	14.9	14.9	21.0	21.0	25.2	25.2	30.8	46.2	30.8
On-shore wind	[GW]	4.1	5.3	5.3	6.4	6.4	7.2	7.2	8.8	11.6	8.8
Off-shore wind	[GW]	2.5	3.1	3.1	6.8	6.8	11.6	11.6	11.5	16.6	11.5
Electricity demand	[TWh]						132	132	149	180	180

Table 2.1.: Electricity generation capacity scenarios [58]

The number of green hydrogen projects in the Netherlands is increasing. On the TSN site, the H2ermes project aims to realise a 100MW electrolyser [45]. Elsewhere in the Netherlands, the NorthH2 project aims to add 4GW of hydrogen production capacity by 2030 [46]. Additional to local hydrogen production, several parties are investigating the possibility if hydrogen can be imported from countries like Southern Europe or the Middle East, which have high concentrations of solar and wind. Although the construction of these large-scale electrolysers is promising for the ambitions set for 2030, the final large-scale rollout of hydrogen production and infrastructure is still awaiting. This is mainly due to the lack of off-takers willing to pay the required price to make these projects economically viable [17]. Meanwhile, energy-intensive companies are delaying hydrogen uptake due to the lack of competitive prices. The difference in price between supply and demand depends partly on the electricity, gas, and carbon emission taxes.

The quantity of hydrogen needed for the DRI process that runs (partly) on hydrogen could break this deadlock, according to a Roland Berger report [17]. TSN can act as a catalyst for Dutch hydrogen projects. In 2050 when both DRI plants will run entirely on green hydrogen, approximately 380kton of hydrogen is needed per year, which would require 4 GW of green electrolysis capacity [17]. Following the realisation of the DRI system, TSN could provide a stable (or even flexible) hydrogen demand for large quantities of green hydrogen, allowing economics of scale.

Table 2.1 provides an overview of the planned electricity generation capacity in the Netherlands for the coming years. The values are based on the scenarios that TenneT, a transmission system operator, has published in the security of supply report [58]. The IPKA0 scenario will be used as a reference for the electricity input dataset, further explained in section 6.1. The scenarios are based on diverse generation options that remain uncertain in the future. The KA scenarios are mainly based on the recent climate and energy reconnaissance. On the other hand, the IPKA scenarios are based on the investment plans from the years 2022-2031. Furthermore, throughout these scenarios, several changes in assumptions are made. The TenneT report provides a complete description and explanation of the content of these scenarios.

2.3.2. Energy procurement method

This subsection will elaborate on the recent developments in European energy procurement methods. These changes will significantly change how we contract renewable energies in the future, affecting business cases and strategies of energy-intensive players. First the current situation is explained, then the developments are discussed.

Current situation
The demand for renewable energy is growing at all times of the day. Since 2001 in the Netherlands, there has been a digital certification program based on the Guarantees of Origin (GoO) and Certificate of Origin (CvO) [10]. A GoO can verify that the electricity supplied to a company has been generated in a renewable way, such as wind, water, sun, biomass, solar thermal and geothermal. Based on the same principle, a CvO proves that electricity has been generated from fossil sources. A GoO is created by measuring renewable energy production monthly and issuing a certificate valid over a 12-month period. These certificates can be traded on the European market. The benefits of this method are apparent when only small quantities of renewables are part of the energy mix. Corporate electricity consumers can use GoOs to cover their electricity consumption and thus declare using "100% renewable energy" on the final annual disclosure. However, as renewable generation capacity increases, this method significantly overestimates the carbon-saving potential [70]. This means that electricity consumers following today's criteria for using fully renewable electricity are still constantly relying on carbon-emitting electricity from the electricity grid. To accurately capture the carbon emissions of the electricity used and determine required flexibility options for load-following behaviour, carbon metrics must shift towards hourly data [16].

Proposed developments
On the institutional level, developments are accommodating this change towards a more realistic energy procurement method. The European Commission has proposed revising the renewable energy directive in July 2021 [24] as part of the package "Delivering on the European Green Deal" to reduce GHG emissions by 55% by 2030 and increase the uptake of renewables in the EU. There are additional elements for facilitating Power Purchase Agreements (PPA) with the time-related and geographical correlation between the electricity production unit and the fuels of non-biological origin (e.g., hydrogen) production. This means that renewable electricity generated will get a time bounded GoO and can only be traded within a limited area. There are several initiatives for the labelling of such time-bound GoO [35]. An example is the EnergyTag initiative that strives to define and build a market for granular certificates that enables energy users to verify the source of their electricity and carbon emissions in real-time (hourly based) [23]. These hourly certifications can give customers and companies additional transparency into the sustainability of their electricity consumption. Furthermore, companies can make their sustainability ambition more explicit, enabling participants to contribute better to the decarbonisation of the grid.

2.4. Chapter summary

The key findings of the contextual information chapter are summarised to conclude the contextual information chapter. First, TSN's ambition results in its desire to retain its high-quality steelmaking position. The steel quality must remain constant during the technological transition to achieve this goal—especially the carbon content of the products. Second, the reference used for the generation capacity scenario to simulate the electricity system is based on the Tennet IPKA0 scenario, as documented in table 2.1. The most notable difference between the Tennet scenario and the nationally planned electricity generation capacity is the difference in offshore wind capacity. Where the IPKA0 scenario utilises 11.5 GW, the Dutch government has the ambition to establish 21 GW by 2030. This difference could influence the results in this thesis and is discussed in chapter 10. Lastly, a change is expected in the electricity procurement methods, resulting in a more granular and time-sensitive market. This development has motivated the usage of hourly data and the usage of electricity originating from the Dutch electricity mix.

3. Literature Review

A literature review is conducted to establish common ground regarding the research topic, explore the core concepts and identify a possible knowledge gap. The main research field of interest is the steelmaking employing the DRI process technology using either natural gas or hydrogen as the reducing gas. This literature review aims to provide an overview of the research related to the gas-based direction reduction technology and the primary technology characteristics of the DRI process. Furthermore, this review identifies relevant input parameters and KPIs for the technological and economic performance evaluation.

The literature review is divided into three parts. First, the literature review starts with the methodology and presents an overview of the variations in results of the direct reduction of iron and steelmaking technology. Second, selected papers are examined, and the properties of the various studies are compared. Finally, a knowledge gap based on the findings and the reasoning for the main research question is presented to conclude this literature research.

3.1. Search methodology

The thesis's most fitting literature review approach is a semi-structured or narrative approach. This approach is designed for topics that have been conceptualised differently and studied by various groups of researchers within diverse disciplines. This method can be used to understand complex areas and detect themes, theoretical perspectives or common issues [56].

To commence the literature review, the SCOPUS database was consulted in June 2022. The main body of the literature is found through a structured search with different search strings as documented in table 3.1. Additional relevant articles and papers were found through snowballing from this literature base. To compose a fitting search string in the SCOPUS database, keywords relevant to the field of interest were used. Direct reduction iron/steelmaking is an extensive topic consisting of several levels of technology depth (from the molecular scale to the system level), different feedstock compositions and several other research categories. As stated in the introduction, the goal is to explore the methods and assumptions used for determining the (indirect) emissions of the ironmaking process that uses hydrogen and natural gas as reducing agents. It is therefore desirable to explore the literature that focuses explicitly on the high-level process modelling of the DRI process and use (electricity) carbon emissions or equivalent as parameters.

The development of the search strings required several iterations. It became clear that different words were used for the same principle. For example, the terminology used to describe the DRI process consisted of: DRP, DR, DRI, HDRI, and Direct reduced/reduction Iron/Ironmaking. Other terms are used to describe a sustainable ironmaking process, such as: Green/clean iron/steel, decarbonised iron/steel, hydrogen-based/-reduction iron/metallurgy, fossil-free steelmaking, green-energy steel, and low carbon steel/steelworks. In order to include as many scientific papers appearing in journals, books, and conference proceedings, different distinct search strings are used. In the following table, the entire search strings can be found, and the amount of screened and included scientific literature.

Search String	**N =**	**Screened abstract**	**Screened full text**	**Included**
Model AND clean OR green AND steel AND production AND hydrogen OR renewable	59	14	7	5
Emission AND reduct* AND dri	120	17	8	3
Assessment AND hydrogen AND steelmaking	58	18	9	7

Table 3.1.: Search strings and the included papers in the literature review

Furthermore, the following articles were found through snowballing on the included literature: [12; 13; 48]

3.2. Literature findings

The reviewed articles can be categorised based on their research methodology and analysis methods. The articles can have a technical or economic focus or both. Furthermore, some articles perform scenario analyses to determine the economic performance of the model. We can see that most papers have sensitivity analyses either on economic or emission parameters. Finally, optimisation developments are seen in the latest papers, albeit only on cost minimisation.

Reference	Method/Data base	Analysis		Scenarios (economic parameter)	Sensitivity analysis		Optimisation (economic parameters)
	Modelling and Simulation	Technical	Economic		Economic	Emissions	
[2]		X		X			
[5]	X	X	X	X	X		X
[6]	X	X					
[7]	X	X	X	X	X	X	
[13]	X	X				X	
[18]	X	X				X	X
[22]	X	X	X	X	X		X
[27]		X	X	X	X	X	
[29]	X	X	X	X	X		X
[34]	X	X	X	X	X		
[36]	X	X	X		X	X	
[44]	X	X					
[48]	X	X	X	X	X		X
[49]	X	X				X	
[52]	X	X				X	X
[59]	X		X	X	X		X
[65]	X	X	X		X		

Table 3.2.: Overview of the reviewed literature

3.3. Specific energy consumption

Detailed process-level-focused research has initially been done in the R&D area of low-carbon DRI. These efforts used modelling and pilot demonstrations[12; 22; 49]. More recent techno-economic analyses and modelling studies have been undertaken at the facility level [6; 7; 36; 44; 48; 49; 52; 59; 65] and regime level [2; 27]. These studies evaluate carbon emissions, energy consumption, and the economic performance of conceptual hydrogen-based DRI plants. A similar level of modelling detail, process boundaries and configuration are observed. The differences in modelling detail originate mainly in the EAF process (energy-based [65], mass/energy-based with EAF reactions [7], multi-physics based [44]. Qualitatively, the energy, emission and economic trends agree on the development of the DR(H_2)-EAF route [31] but vary significantly in the quantitative field. Emission-related findings can be highly influenced by assumptions and parameters, particularly the Specific Energy Consumption (SEC), the carbon intensity of the electricity, energy/material losses and hydrogen DRI reactive requirements. Based on the aforementioned studies, the SEC for steel production through the DR(H_2)-EAF process is mainly influenced by the EAF scrap fraction, H_2 consumption for the iron reduction, electrolyser efficiency and type, and degree of DRI metallisation. The determined SEC ranges from 3.48 MWh/t_{CS} [36; 65] with 0% scrap use, 3.96 MWh/t_{CS} [7; 22; 36], and up to 4.25 MWh/t_{CS} [5]. In terms of energy consumption per ton of steel, it even requires slightly more than the conventional BF-BOF route.

The identified parameters are used in the conceptual model and are further discussed in section 5.5. Furthermore, the results of the literature mentioned above are used to validate the technical implementation of the model, documented in section 7.4.

3.3.1. Emissions

Regarding the quantification of emissions in the DR(H_2)-EAF route, the primary source is the indirect emissions originating from electricity input for hydrogen production [13; 18]. However, at near-zero electricity emission factors, the indirect and direct emissions are comparable [7; 13]. The study from Vogl et al. [65] has identified a break-even electricity emission factor of 532 kgCO_2/MWh at zero EAF scrap rate to reduce the DR(H_2)-EAF emissions below of typical BF-BOF process (i.e., 1870 kgCO_2/t_{CS}). Bhaskar et al. assume an electricity emission factor of 412 kgCO_2/MWh (EU 28 average) and estimates that total DR(H_2)-EAF emissions would reach 1930 kgCO_2/t_{CS} [7], which exceeds DR(CH_4)-EAF emissions (980 kgCO_2/t_{CS}). Increasing the scrap rate in the EAF will shift the upper boundary of the electricity emission factor (i.e., 661 kgCO_2/MWh at 25% scrap [65]), which most European countries can meet constantly.

Comparable findings are found in research published from the research and innovation programme of Hydrogen Europe and N.ERGHY . [13] demonstrates the impact of different electricity CO_2 intensities in the BF-BOF, DR(CH_4)-EAF and DR(H_2)-EAF routes in a detailed static process model. The overall CO_2 load of the DR(H_2)-EAF route is in the range from 280 to 2000 kgCO_2/t_{CS}, with the upper bound having an electricity emission intensity of 500 kgCO_2/MWh. To put this into perspective, the Dutch energy grid had an average emission intensity of 328 kgCO_2/MWh in 2020 [20]; meaning that the DR(CH_4)-EAF process would produce significantly less GHG emissions in today's environment. Figure 3.1 illustrates the direct and indirect emissions under different carbon intensities per KWh.

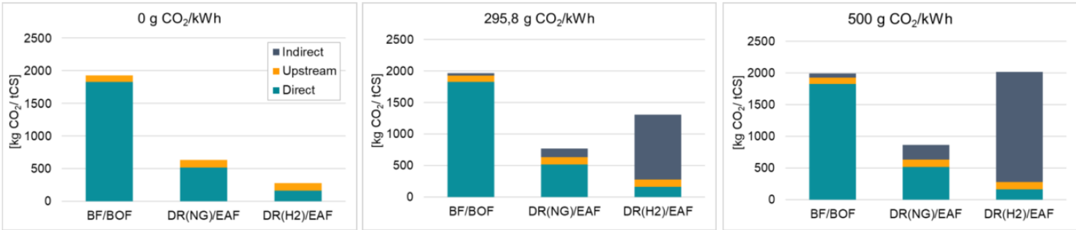


Figure 3.1.: Influence of the indirect emissions on the total amount of CO_2 emitted [13]

Different studies have investigated, using sensitivity analyses [7; 36; 49], the effect of changing the electricity supply's emission intensity factor on the emission per ton of crude steel. Most of these analyses are done statically, meaning they use fixed parameter assumptions over a period of time. This can lead to operational inadequacy and failure to meet long-term decarbonisation objectives, according to [48; 71]. Higher time resolution data for fluctuations in renewable electricity could increase storage requirements [48] and enable optimisation strategies similar to cost minimalisation [59].

3.3.2. Flexibility and optimisation efforts

Several efforts have been made to accommodate for the variability of renewable electricity prices and/or generation in several case studies for the conditions in the UK, Scotland, Germany and Spain [22; 29; 48; 59]. Using the DR(H_2)-EAF process model coupled with a time-series analysis of Vogl et al.[65], Pimm et al.[48] investigated with a minimum production cost optimisation the energy system requirements and storage mix of the UK . They indicate that DR(H_2)-EAF could become cost-competitive with the BF-BOF within 5-10 years. [59] demonstrated that the cost-optimal design of the hydrogen-based steelmaking process depends on the electricity system mix. They show that production following the hourly electricity price that the steelmaking leads to savings in running costs but increases capital cost due to investments in the overcapacity of steel production units and storage units for hydrogen and hot-briquetted iron pellets. A techno-economic energy planning model from [29] investigated the adoption of flexibility options, namely H_2 storage, DRI material storage, and the use of natural gas, from an annual total cost-minimisation perspective while considering fluctuating H_2 and NG prices and increasing H_2 shares. They indicate that in the short term (2030), DRI produced with NG tends to be cheaper than H_2 and that flexible operation with gas and material storage initially has small saving potential. However, with higher shares of H_2 in the DRI process in the long run, electricity price spikes could substantially increase the total cost if buffers are not used.

In the papers mentioned above and the following publications, averages [52] or estimations [2] based on external sources are used to determine parameters such as electricity price [€/MWh] or GHG emission intensity [gCO_2/kWh]. Efforts have been made to optimise the DR-EAF ironmaking process, either with estimations or fluctuating electricity prices. However, none have used the fluctuating electricity emission factor as an input parameter. Additionally, the technological pathways chosen in all the analysed literature are based on the DRI-EAF processes. No paper identified uses the DRI-REF processes as the technological basis for the iron or steelmaking process. This problem situation is further explained and visualised in the Conceptual Model chapter in section 5.1 in figure 5.1.

3.4. Research gap

The exploration of the literature in this thesis, coupled with the contextual information provided in chapter 2, reveals an academic and practical knowledge gap. The literature provides valuable information on DR(H_2)-EAF and DR(CH_4)-EAF process, energy consumption, emissions abatement potential and costs. However, in most instances, the results are driven by assumptions on hypothetical steady electricity sources and low carbon intensities of this electricity source. Furthermore, although several studies have optimised with different flexibility options on costs based on future variable electricity prices, they have yet to use a variable electricity emission factor coupled with the corresponding electricity price. This exclusion can lead to deviating results and produce a mismatch between the envisioned emissions targets and actual emissions. Furthermore, it is seen that the DR(H_2)-EAF process is only emitting less CO_2 in specific circumstances compared to the DR(CH_4)-EAF process.

The analysed literature on the model-based assessment of the low-carbon DRI-EAF route is mainly limited to the DR(H_2) route or, in some cases, the DR(CH_4) route. Furthermore, there is a lack of studies investigating the use of varying feed gasses. In this thesis, only hydrogen and natural gas are considered. As laid out in the contextual information, TSN will employ both natural gas and hydrogen as inputs to their production process in the near future. Due to these aspects, there remains a knowledge gap on several aspects that will be addressed in this thesis :

- The technical and economic performance of the DRI-REF process.
- The effects of varying hydrogen content/volume in the feed gas in the DRI process.
- The performance of the DRI-REF process under the Dutch context for 2030.

Besides this academic knowledge gap, there is a practical knowledge gap in the modelling and evaluation of the method used in this thesis. Adequate data granularity matters immensely in properly assessing direct and indirect emissions at small intervals. Current assessments where short time intervals are considered are solely on costs in the context where renewable energies are a large portion of the energy mix. Throughout the analysed literature, no paper has used the hourly emission intensity factor of the electricity mix, let alone a futuristic evaluation. Therefore, the following practical knowledge gap is identified:

- The effects of using hourly electricity price and corresponding emission factor to determine the performance of the system of interest.

For this project, a data set will be available with future energy market data estimations in the Dutch context, further described in section 5.5.2. In order to attempt to close the presented knowledge gap, the main research question emerges:

How do various hydrogen volumes affect the technical, economic and decarbonisation performance of a DRI-REF process in the Netherlands in 2030?

4. Research approach

The research approach depends on the nature of the research project. The proposed main research question can be dissected into three components that need to be understood. First, to understand how costs and emissions are created in the system of interest with variating volumes of hydrogen as a reducing agent. This can be challenging as various DRI ironmaking production techniques have different configurations [12; 49]. Second, to understand how the Dutch electricity price and associated emissions can be determined in the (near) future. Estimating these parameters is challenging, as predicting the future always has uncertainties. Third, to understand and explore how the highly detailed data can improve decarbonisation strategies technically and economically.

This work aims to evaluate a grid-driven low-carbon ironmaking by introducing hydrogen in the direct reduction process. In this context, specific technologies are considered and elaborated on in chapters 2.1 and 5. Natural gas-based direct reduction is an established ironmaking process, and the substitution of natural gas with hydrogen was successfully demonstrated [47]. Therefore, various configuration stages are assessed, starting from an exclusive NG operation for base care reference towards a co-feed with 80% hydrogen volume. The chosen co-feed boundary is based on the maximum operating condition in the (near) future given by TSN. Based on the work of Müller et al. it becomes clear that additional carbon atoms need to be provided from 65vol% hydrogen in the EAF and REF in order to ensure sufficient carbon content in the crude steel.

Furthermore, a top-down approach is applied to determine the material and energy demand of the system. To elaborate, the output quantity of the system of interest (ton hot metal per year) is determined beforehand and sets the basis for material and energy demands. The material and energy balances in each process step must be met at each time interval which can be aggregated over an entire year. This results in a final material and energy demand.

4.1. Type of research problem

The DRI-REF process is a complex system with many different components and facilities. Additionally, this process is interconnected with the energy system, increasing its complexity. However, it is feasible to analyse the influence of specific parameters by restricting the number of variables and explicitly choosing a particular setup. Thus, the research must limit itself to one specific setting within the dynamics present. Since this research restricts itself to the Dutch electricity mix and Tata Steels Ijmuiden ironmaking production values, the case study approach fits best. As Crowe et al. puts it: "The case study approach allows in-depth, multi-faceted explorations of complex issues in their real-life settings", which applies to certain parts of this research project. Based on the preliminary literature review, we already see that hydrogen in the DR Ironmaking process is not desirable due to high electricity emissions intensity. Therefore, it is not 'very' interesting to restrict the research only to the current situation as the answer can already be determined. Investigating the emissions and economic performance of DR(H_2)-REF in 2030 with high precision is appealing because it can generate valuable insight for the players involved. To determine the suitable research approach for this thesis, the type of research problem has to be considered. The problem focuses on understanding the effects of variating hydrogen volume on technical, economic and environmental performance. Addtionally, this problem explores how insights based on high data granularity can improve decarbonisation strategies. Therefore, the primary research approach must be suitable to solve this problem. The specific research problem is a case study of TSN, but it is also a more general ironmaking system problem and thus needs a suitable research approach.

4.1.1. Modelling approach

The research problem described above has two components: an exploratory and an evaluative research question. First, it explores the performance of the DRI-REF process but also gathers insights into variating hydrogen volumes. Second, it evaluates the effect of various hydrogen volumes on techno, economic and environmental performance. The primary research approach needs to measure this system's behaviour and characteristics and explore its performance under different settings. For this reason, the main research approach is a modelling and simulation approach. Modelling and simulation approach can be considered both a method and a tool and has attracted tremendous interest among researchers [54].

There are several reasons why this method is suitable for this type of problem. Based on the research problem, it becomes clear that analytical mathematical methods are not optimal for solving this complex problem. Especially if uncertainties, such as future developments of hydrogen (-ironmaking) technology, energy market dynamics and stochastic influences, are part of the problem and solution of the thesis project. Furthermore, interaction with the energy market is a complex problem that demands specific methods and tools. Complex systems with dependencies on internal and external factors are best solved with modelling and simulation approaches [54]. The DR(H_2)-REF process will be modelled, and emissions and costs will be simulated based on specific demand requirements and input data. Furthermore, for this project and its audience, exact numbers and numerical results are not the most essential outcomes but rather the insight into different hydrogen volumes affecting the techno-economic parameters. Also, this project can show how precise data can provide a stepping stone for future optimisation, thus improving long-term decarbonisation strategies. To effectively model the system of interest, several aspects of the research problem have to be researched. Therefore, several sub-research questions are formulated to help answer the main research question.

4.1.2. Sub research questions

A modelling and simulation research approach will approach the main research question. The sub-research questions that support solving the main research question can have their approaches. The proposed sub-questions are:

1. What are the energy market and hydrogen capacity developments in the Netherlands up to 2030?
2. How can the DRI-REF process be modelled to assess the technical and environmental performance under various hydrogen volumes?

3. What is the levelized cost of the DRI-REF process in the NL under given energy market conditions?

4. How does purely grid-driven DRI(H_2)-REF compare with the conventional DRI(CH_4)-REF process technically and economically?

In the following section, the individual approach, activities, methods and tools used for each sub-research question are described in detail.

4.2. Project overview

As mentioned in the research approach, the primary thesis approach is a modelling and simulation approach. The specific content will be to perform a case study for the combined DRI and REF process. The research project will be carried out by creating a conceptual model that describes the energy and material balances of the system of interest with various hydrogen volumes. Technical data from TSN are being used as a basis for the modelling. To start, the model is used to calculate the hourly and annual energy consumption, emissions, and material requirements in terms of a given output capacity for DRI and hot metal production. Subsequently, the technical and economic performance evaluation will use the model in combination with energy market data. These datasets for the energy market originate from the EMF v.7.0 model, acquired from Blueterra B.V. The levelized cost of hot metal production is calculated for the conventional NG-based production and grid-based DR(H_2)-REF production using a discounted cash-flow analysis. In the last step, key performance indicators are used to compare the different process configurations, which can provide insights into the long-term decarbonisation strategies of steel manufacturers. The results of this thesis will mainly serve the steel manufacturing players and energy market players. The EMF v7.0 model is temporarily provided by the company BlueTerra for energy market analysis with high data granularity, further elaborated in the Data chapter. A research flow diagram, illustrated in figure 4.1, provides the research outline and summarises the deliverables, theories and methods. The sub-research questions are listed in their respective research phase. This section further elucidates the research phases with their limitations, and to conclude, the thesis outline is presented.

4.2.1. Research phases

The sub-research questions are presented to support the primary research approach in this thesis. These sub-research questions can be seen as a sequence towards a working model that can compare different hydrogen volumes in the system of interest and determine its technical or economic performance. Different research phases are used to create an outline of the model that will be used to answer the main research question. Each phase builds onto the next one. In this section, the research phases are shortly elaborate and how they contribute towards solving the main research question.

Phase 1: Information & definition
The first research phase sets the foundation for the research project and introduces contextual information on the iron and steel production in the Netherlands. The first sub-research question explores the energy market and hydrogen capacity developments until 2030. The

generation capacity of renewable energies is expected to increase, but to what extent? This information is used later to substantiate the model inputs and simulation results.

Phase 2: Model conceptualisation
The second research phase tries to answer the second research question. This research sub-research question has a few components which make this a complex sub-research question. The first step is based on a literature review which explores the current states of NG and hydrogen-based steelmaking using the DRI process. The literature review will define and evaluate the modelling methodology and determine suitable key performance indicators for the performance evaluation in the subsequent research phases. Then, based on the modelling requirements determined in the literature review, the second step of the sub-research question can be initiated. The second step is to define and elaborate on the input parameters for the conceptual model.

Phase 3: Model formulation
The third phase will start formulating the actual model based on the first and second phases. The modelling methodology is conceptualised in phase 2 and then implemented in a programming language. Finally, the economic evaluation and the respective key performance indicators are formulated. The deliverable of this phase is a working model that can simulate the economic and technological performance of the system of interest under set market and geographical conditions.

Phase 4: Model simulations
This phase will simulate the various hydrogen volumes of the modelled system. The input data and data sets gathered and defined in the previous phases are used to generate the precision needed in the simulation runs. The output of this phase are the complete simulation runs over an entire year on an hourly basis for the different key performance indicators defined in the previous phases.

Phase 5: Analysis & Conclusion
The last phase of this research project analyses the results of the simulations and the KPIs. In addition, a sensitivity analysis is performed on specific parameters, which can substantiate the discussion part of this thesis. Finally, the results and analysis are visually presented as well as numerically.

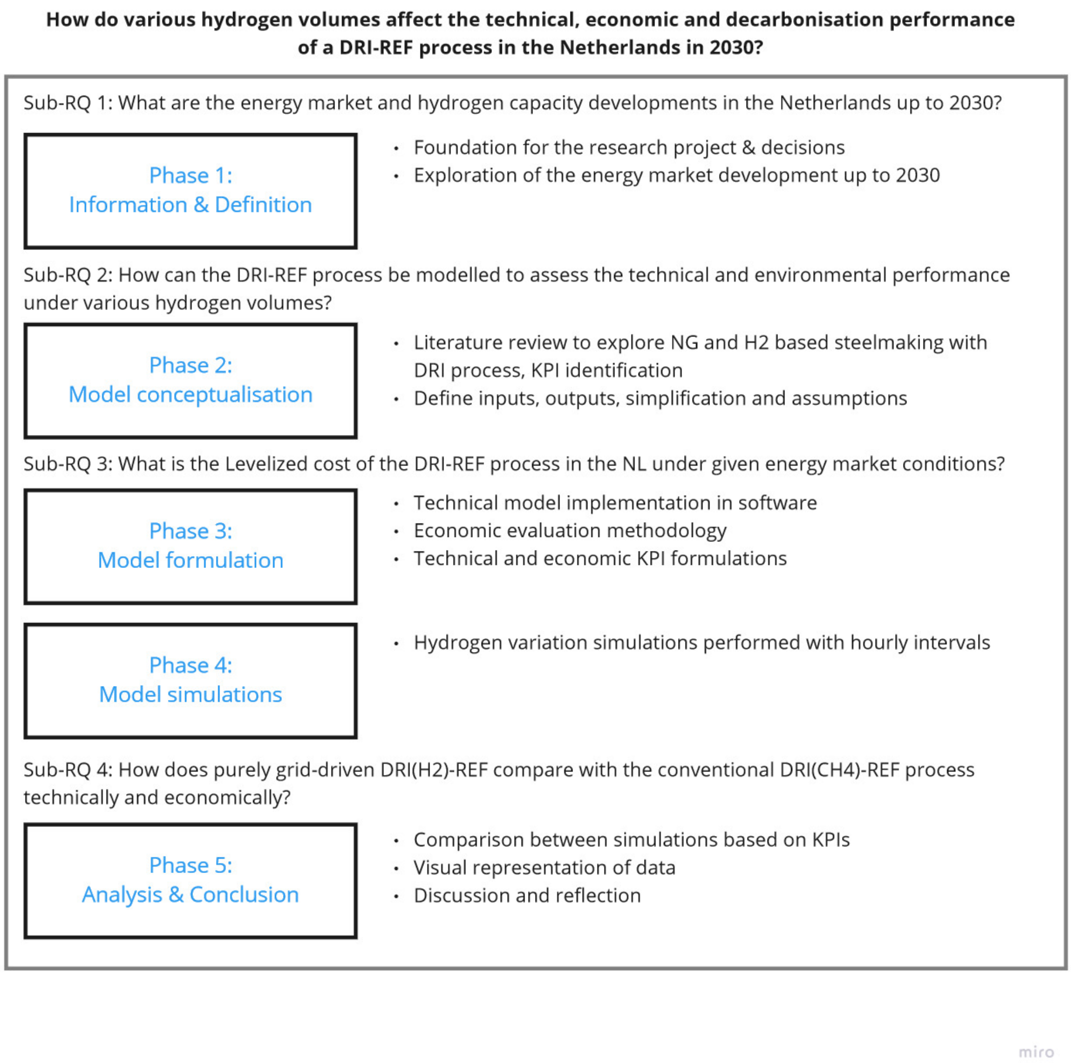


Figure 4.1.: The research flow diagram. The diagrams provides an overview of the phases with the methods and theories to produce the outputs.

5. Conceptual model

This chapter will describe the conceptual model used to gather insights into the technical and economic performance of variable hydrogen fractions of the DRI-REF process. First, the conceptual model is created for the system of interest, and then simulations are conducted to research the effects of different parameters and scenarios. During the development of the simulation model, decisions are made about what to include and exclude from the model. This process of selection and abstraction is widely known as conceptual modelling [51, p.vii] . The book of Robinson et al. provides a comprehensive view of conceptual modelling, stating that there is no fixed way to perform the abstraction needed in conceptual modelling [51, p.8]. Even more recently, there are quite different views and opinions on the definition, purpose and benefits of conceptual modelling [50].

Because of these differences in views and opinions, it is essential to clearly define the research problem to properly formulate the conceptual model based on one of the definitions. From the literature review, it is clear that the conceptual models are based on hypothetical assumptions with processes that have yet to be technically achieved. Nevertheless, the conceptual model in this project is not different. Thus, identification and description of the system's characteristics and properties, such as inputs, outputs, assumptions and simplification, must be defined appropriately. The purpose of the conceptual model is for communications purposes and sets the bases for the simulation model, which is an implementation of the conceptual model in a programming language. Furthermore, the most crucial part of the conceptual model is to communicate all assumptions and simplifications that are part of the system of interest and its processes. As seen from the literature papers that use the modelling and simulation approach, providing this information makes it possible to reflect on the outputs and results and how these are formed based on the assumptions.

One of the most practical perspectives on conceptual modelling is that of Robinson [50, P.13], where a framework is presented based on their extensive experience with developing and using simulation models of mainly manufacturing and service systems [50, p.74]. The system of interest in this research project is an iron manufacturing system which can be viewed as an operations system and thus fits within the framework application. The framework is based on a sequence of activities required to develop a conceptual model. The order of these activities is not fixed because the formulation of the conceptual model is subjected to iterations and is also part of the simulation study [50, p.75-76]:

1. "Understanding the problem situation"
2. "Determining the modelling and general project objectives"
3. "Identifying the model outputs (responses)"
4. "Identifying the model inputs (experimental factors)"
5. "Determining the model content (scope and level of detail), identifying any assumptions and simplifications."

The framework for developing a conceptual model starts with understanding the problem situation, presented in section 5.1. Afterwards, the modelling objectives are formed in section 5.2. Contrary to the sequence presented above, section 5.3 and 5.4 presents the modelling content before the modelling inputs and outputs. The objectives provide the basis for the derivation of the conceptual model, first by defining the outputs (responses) of the model, then the inputs (experimental factors), as seen in section 5.5. Throughout the steps mentioned above, assumptions and simplifications are identified and are documented in the final sections 5.6 and 5.7. As already explained, the main research question will be answered through a series of sub-research questions. The conceptual model and the model implementation chapter will try to answer sub-research question two in chapter 4.1.2.

Sub-RQ 2: *How can the DRI-REF process be modelled to assess the technical and economic performance under various hydrogen volumes?*

This question is answered using the technical model, contributing to solving the research problem and, thus, the main research question. However, the problem situation must be understood and adequately defined first.

5.1. Problem situation

To define the problem situation, the system of interest must be understood. Therefore, the earlier mentioned framework will serve as a stepwise approach towards a structured conceptual model.

The formulated conceptual model in this chapter is a simplified version of the system of interest; the iron-making process based on the DRI-REF method with natural gas and hydrogen as a reducing agents. The envisioned transition defines the boundaries of the system of interest explained in sections 2.1 and 2.2. The overall content and scope of the conceptual model will be further elaborated in section 5.4. The building blocks of the envisioned system can be seen in figure 5.1. As laid out in the research gap, one crucial aspect to note is that the system of interest in this thesis is slightly different from the analysed literature. The system of interest in the analysed papers consists of either the conventional BF-BOF routes and/or the DRI-EAF routes. Both these routes have steel as outputs.

In this thesis, the system of interest will consist of the electrolyser, DRI plant and REF plant. Contrary to the analysed literature, where mainly an EAF is used to produce hot metal for TSN, the output of the REF plant will be fed back to the BOF. Other parts of the steel process are outside the system boundaries and unaffected. The analysis considers the hybrid operation of the DRI process with mixtures of H_2 and NG as the reducing gases to be fed to the DRI plant and gas heater. The NG is obtained from the gas grid, and the H_2 is directly obtained from the electrolyser. No gas or material storage is considered in this system of interest.

The problem situation can now be situated within the system of interest. The problem that the conceptual model will address is motivated by the research gap documented in chapter 3.4. The problem situation is that it is not known how the actual hydrogen volumes affect the technical and economic performance of the system of interest in the Ijmuiden region with specific energy market characteristics. The conceptual model is developed to provide the first insights into the performance of the DRI-REF process under these unknown circumstances.

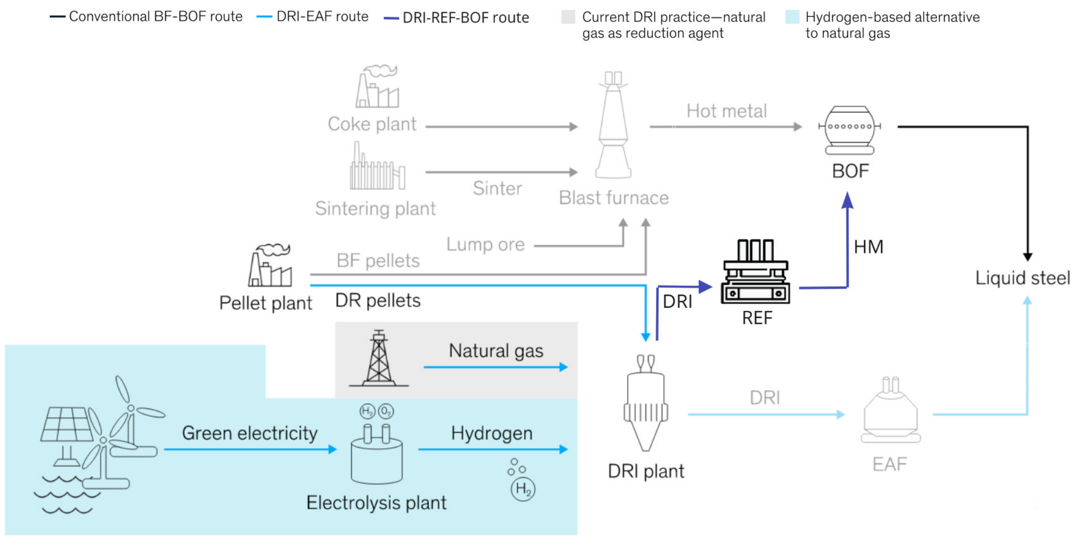


Figure 5.1.: System of interest consisting of energy source (electricity, hydrogen and natural gas), DRI plant and REF plant. Picture adapted from [19]

5.2. Modelling objectives and constrains

The second step in the framework of Robinson is to determine the objectives based on the system description and the problem the model aims to solve. The objectives of the conceptual model can be formulated irrespective of its content. Robinson et al., clearly states that developing these objectives are essential for an appropriate model and can be expressed in three components: achievements, performance, and constraints [51, p.78-79]. Achievements are what one hopes to achieve with the model. Performance is the measurement of change in KPI, and finally, constraints are boundaries with which the modeller must work.

Before proceeding with the modelling objectives, it is helpful to identify the aims of TSN on this subject. TSN wants to reduce its carbon emissions by transitioning towards a new steel production process while keeping the same production capacities and quality. It also wants to stay competitive in the steel market by upholding the current quality standards. Therefore, the overall goal of the conceptual model and the technical model by the end of this study is to determine the emissions and costs of the system of interest with different settings based on the future Dutch electricity generation composition, observe the system behaviour under various hydrogen volumes, and generate insights into the technical and economic performance. These results will answer the related research questions, and the acquired insights could contribute to the long-term decarbonisation strategy.

Now that the overall goal of the conceptual model is presented, we can place this model in a broader context to determine the system's nature and identify the objectives and constraints. The system has physical boundaries regarding plant and process capacity but is also a market where energy demand and supply must always match during operations. To specify, the system of interest is a production process where materials and energy interact with each other to create liquid steel.

5.2.1. Objectives

The main objectives and constraints can be formulated with the explanation of the system of interest (section 5.1). One aspect to consider is an overall objective: the modelling should be on an hourly basis and over an entire year. Modelling on an hourly basis is an objective since, according to the literature findings and identified knowledge gap, modelling with long time intervals can lead to operational inadequacy and failure to meet long-term decarbonisation objectives [48; 71]. This is because more detailed data can improve estimations, increase storage requirements and enable optimisation strategies [48; 59]. On the other hand, modelling with more extended time intervals might not showcase the system's actual behaviour. The modelling objectives are presented and explained in more detail in the list below.

1. To determine the necessary material and energy balance for the DRI-REF process over an entire year
2. To determine changes and limits in material and energy balance under different hydrogen penetrations
3. To calculate the specific energy consumption and CO_2 emissions under different hydrogen penetrations on an hourly basis
4. To calculate the Levelized Cost Of Production (LCOP) for different hydrogen feed gas compositions

The objectives of the modelling need to be clarified to further structure the conceptual model. Furthermore, the modelling objectives are also reflected in the main research question of this thesis, which has two components. The first component is understanding how adding hydrogen as a feedstock impacts the DRI-REF process. The second component is to analyse the system's performance when electricity price and carbon intensity characteristics with high resolutions are used. Objectives 1 and 2 aim to solve the first component of the question. First, the material and energy balance specific to TSN must be determined when the process is fully operational on natural gas. The limits and constraints of objectives 1 and 2 are based on the facility characteristics of TSN and its technology choices. Based on the literature analysis, it becomes clear that the technological starting points and process characteristics need to be identified and explained. The technological model in Chapter 6 will elaborate on the technological choices and the relevant process characteristics used in this thesis.

Objective 1 enables to model the base configuration of the DRI-REF process and subsequent configurations where increasing amounts of hydrogen percentage are used. It is crucial to determine the influence hydrogen has on the material and the energy balance, as this can affect further calculations. This explanation needs some additional clarification. As described in the problem situation, the quality of the hot metal output of the system must remain constant irrespective of its feedstock inputs. Among others, one of the characteristics of hydrogen is that it decreases the carbon content of the DRI. To compensate for this development, additional feedstock material with high carbon content must be added in the following processing step, which results in additional CO_2 emissions. The aim of objective

2 is to determine the changes in material and energy balance that can influence the performance of this system under different hydrogen penetrations. Achieving this objective is essential for the following modelling objectives 3 and 4, as well as establishing metrics to answer the sub-research questions that the conceptual and technical models attempt to answer.

Objectives 3 and 4 set the basis for the performance analysis in technical modelling, which is determining and quantifying under which circumstances hydrogen has a positive contribution towards the company's aims. The available inputs for determining the CO_2 emissions and energy-related process costs are on an hourly basis. Therefore, there are several necessary inputs to calculate these two objectives. One set of inputs is exogenously provided to the model, and the second set is based on the outcomes of the first two objectives. The inputs for the conceptual model will be discussed in more detail further.

5.2.2. Constraints

Several constraints can be identified based on the objectives mentioned above and the problem situation. Similar to the objective's subsection, the constraints will be listed and explained in more detail. The following constraints have been identified:

External modelling constraints

1. The model must run over a full calendar year using a 1-h resolution
2. The electricity input dataset comes from an external model and is based on the scenario year 2030
3. Steel quality must remain constant and need to be checked to enable comparison of key findings with related work

Design modelling constraints

4. Process (chemical and thermal) and facility properties must always be followed.
5. The total output of hot metal must be equal in every configuration
6. Electricity, hydrogen and the material balance must match at each time interval

The constraints can be arranged into two categories: external modelling constraints and design modelling constraints. The external modelling constraints apply to the scope, inputs and other external factors influencing the conceptual model. As mentioned in the objectives, the model must run over an entire year with a resolution of one hour. This is to demonstrate the effects of daily and seasonal variability in CO_2 emissions and hot metal production costs, which will provide insight into the performance of using hydrogen as a future feedstock under the set conditions. Additionally, the higher modelling resolution improves potential insights into energy storage capacities and requirements, as mentioned earlier. The input data to calculate the performance of hydrogen in this system of interest comes from an external model with specific settings. This data and model will be further elaborated in section 6.1. The characteristic of this data is crucial for the result of the research. Variability in electricity price and corresponding CO_2 emissions of the electricity mix over an entire year is shaped by interactions between diverse parameters. Therefore, one cannot simply use randomised numbers as this is detrimental to the actual behaviour of the system of interest.

Another external constraint is the quality of the hot metal. This modelling output will be discussed in detail in section 5.4. The steel quality must remain the same under different process conditions, meaning that a change in hydrogen penetration must be compensated elsewhere in the system of interest. Also, keeping the hot metal quality constant in this study decreases the number of modelling variables and enables the comparison of key findings with related work. These external constraints are necessary to attempt to close the knowledge gap and make it possible to solve the problem situation.

Constraints 4 to 6 provide boundary conditions for the design of the process model. First of all, constraint 4 states that the properties of the process facilities to manufacture hot metal must be derived from the actual plant size provided by TSN. This allows analysis with parameters based on realistic values, increasing the value of the results. Also, these values must remain constant throughout the different analyses with variating hydrogen penetrations to allow comparison. The second modelling design constraint, no.5, could be seen as a simplification and a constraint. The annual steel/hot metal output cannot be decreased to reduce costs or emissions and is set at 3672 Mton/year. In practice, iron and steel are made through batch production; thus, energy and feedstock demand vary over time. Furthermore, if prices are too high, the production process will be delayed or even terminated. Because the operation schedule is not known for this new DRI-REF plant, a simplification is made. The required production capacity is equally divided over the hours of a whole year, which in turn requires a constant input of materials and energy. Finally, constraint 6 states that the material, hydrogen, and electricity demands calculated using the process model outlined in section 4.3 are met in each time interval.

5.3. Model content

The model content and scope are provided to understand better the inputs and outputs and, subsequently, the simplification and assumptions. The order of the activities of the applied framework is not fixed due to the iteration of the conceptual model development. At this point, the model content and scope must be explained. The conceptual model formulation is visualised in figure 5.2, where a flowchart is used to illustrate the formulation steps. The inputs, outputs and simplifications will be elaborated on in the subsequent sections.

In this section, the motivation behind the choosing of the included system components is explained as well as their conceptualisation in the model. To assess hydrogen-based ironmaking, a time-series process model is developed. This approach is chosen to identify and quantify possible barriers for the hydrogen use in the DRI-REF process under certain energy market conditions and thus improve process understanding. In this context, specific technologies are considered and elaborated below. The conceptual model is designed to enable variation of crucial input parameters and analyse their effect on energy consumption, production costs and associated CO_2 emissions. The parameters to be varied include electricity costs, the associated CO_2 intensity of the electricity and the amount of hydrogen fed into the system. To determine the energy demand for the indicated base case (see explanation below), material and energy balances need to be set up for the system, which will also serve as a foundation for further calculations on production costs. Furthermore, as already explained, determining the material and energy balances under different hydrogen

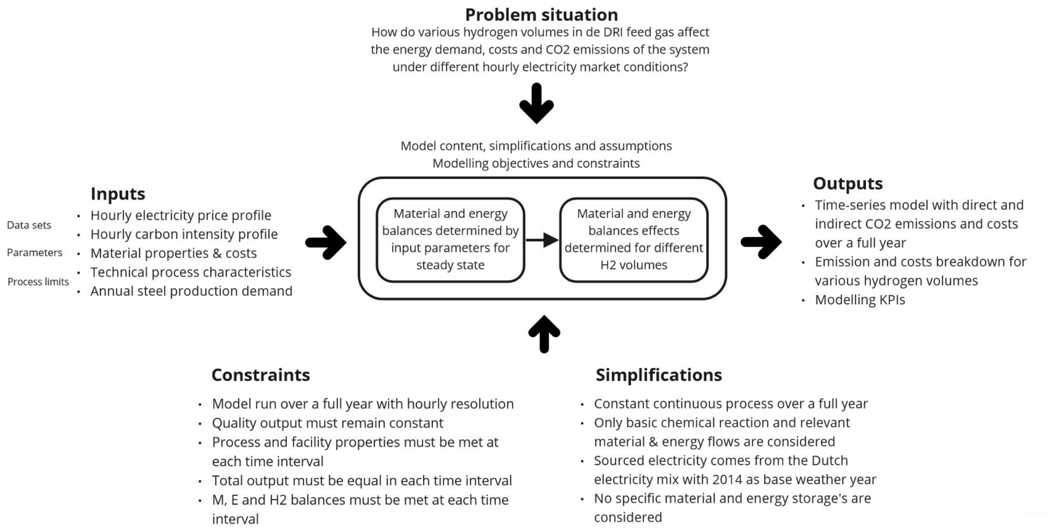


Figure 5.2.: Conceptual model visualisation

volumes is an objective. However, it should be noted that the conceptual model is not a full thermodynamic model.

The mentioned 'base case' in the conceptual model visualisation is a complete DR(CH_4) process (Base case: 100vol% NG, 0vol% H_2). This process technology is an established production process, as elaborated in the introduction of this thesis. The substitution of natural gas with hydrogen is successfully demonstrated in earlier work [47]. Based on the literature review and acquired values from TSN, the maximum considered co-feed composition is 80vol% hydrogen (Max H_2 case: 20vol% NG, 80vol% H_2). The chosen hydrogen volume results in a slight decrease in carbon content in the DRI [44]. This decrease needs to be accounted for in the REF process as additional carbon needs to be introduced to ensure sufficient quality in the hot metal.

5.4. DR(H2)-REF model content

This section presents a detailed system description. A simplified flowsheet specifying the different flows of the modelled process and the system boundary is depicted in figure 5.3.

The system of interest can be divided into three main process steps; Hydrogen production, DRI production and hot metal production. The hot metal is subsequently sent to the steel production plant. This work evaluates only the processing of iron ore to hot metal. Additional up- and downstream operations and processes related to the full steelmaking are not considered. In depicting the modelled process's flowsheet, only flows that contribute to a change in energy usage or affect the emissions of the system of interest. Solid black lines represent the relevant material flows. The energy flows are composed of solid blue lines (electricity) and red lines (heat), respectively. The process properties will be further elaborated in section 6.2 of the Data chapter.

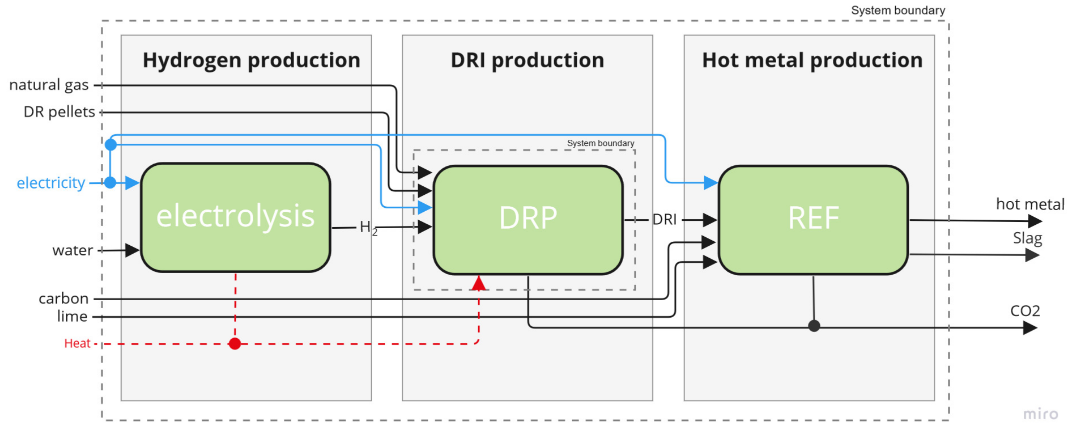


Figure 5.3.: Simplified flowsheet of the power to hydrogen DRI-REF model. The system boundaries are indicated for the DRP (direct reduction plant) and for the entire system of interest.

The material inputs of the modelled system are iron pellets, carbon, water, and natural gas, whereas hot metal and slag represent the outputs. No water flows across the system boundaries in a continuous system where hydrogen losses are neglected. The iron DR pellets contain 95% hematite (Fe2O3) and 5% inert substances. The possible scrap charged to the REF is not included in this thesis, as it would add another variable. The hot metal contains only iron, whereas all other elements leave the REF through the slag.

Electrolyser
Hydrogen generation by electrolysis is included in the system boundaries for several reasons. First of all, by including the electrolysis in the system boundaries, a better image can be created of the energy demand of hot metal, assuming that the reduction process uses hydrogen. Secondly, the characteristics of the produced hydrogen can be better understood. Ultimately, TSN wants green steel production that requires green hydrogen. Therefore, it is essential to know the carbon intensity of the hydrogen given the electricity input. Incorporating the electrolyser in the DRI-REF system enables analysis between the electricity market and hot metal production. Thus, it is assumed that the hydrogen is generated onsite; thus, the CO_2 emissions from the used electricity become part of scope 2 emissions, otherwise known as indirect emissions. Even more important, due to the change in the PPA regulations, elaborated in section 2.3.2, TSN would ultimately require some control over the sources and properties of the electricity used in the electrolysis plant.

In the electrolyser, hydrogen is produced and used further as the reducing agent in the DRI process. Water is the main feed stream of the electrolysis step. The water molecules are split with electricity to form hydrogen and oxygen based on the reaction 5.1:

$$H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2 \qquad \Delta h_0 = +285.8kJ/mol \tag{5.1}$$

The different electrolyser technologies have different process properties that could be integrated into the steel manufacturing process. In the case of high-temperature electrolysis, Solid Oxide Electrolyser (SOEL), the low-temperature waste heat of the DRI process and REF can be reused to evaporate the feed water in the electrolyser. This would reduce the thermal energy demand. An in-depth discussion of waste heat management is presented in the work of [44]. The low-temperature electrolysis can be represented by polymer electrolyte membrane electrolysis (PEMEL) and proton exchange membrane (PEM) electrolysers. Both technologies already have high commercial maturity [source], unlike the SOEL technology. Chapters 6 and 7 will elaborate on the electrolyser implementation and the process parameters applied in the modelling.

Hydrogen produced from the electrolyser can be directly fed to the direct reduction process or temporarily stored for later use. This thesis will not evaluate storage options and different utilisation degrees to optimise hydrogen production and usage. At this stage of the technological transition, there are too many unknowns about the hydrogen infrastructure. Based on the aim of this thesis, it is chosen to exclude any energy storage options for either hydrogen or electricity.

DRI process, Energiron technology

The second step, visualised in figure 5.3, is the DRI production process. The selected technology for the DRI process is the Energiron direct reduction process. The Energiron process applied in this thesis will be based on the ZR (zero reformer) scheme, which means that the reducing gases are generated by "in-situ" reforming of hydrocarbons in the reduction reactor, which is illustrated in figure 5.4. These hydrocarbons can be natural gas or other reducing gases such as syngas and coke oven gas. However, this thesis will exclusively focus on natural gas. The DRI process can be operated with different input compositions of H_2 and NG, which allows flexible operation and facilitates the transition process towards full decarbonisation. The assumed natural composition is presented in appendix C. How exactly the process scheme is implemented in the technical model is further elaborated in chapter 7.

As can be seen in figure 5.4, the feedstock (hydrogen/natural gas) entering the reactor is mixed with the recycled reduction gas from the shaft furnace. The feed gas is conditioned via wetting, heating and partial oxidation and fed to the shaft furnace from the bottom part. Iron ore pellets are fed at the top of the shaft furnace, and both streams are routed in a counter-current manner. The hot DRI (HDRI) is obtained from the bottom of the furnace and routed to the REF. The H_2 and CO-rich top gas is cooled, filtered, dried and subsequently fed to an amine scrubbing unit to separate CO_2. The remaining CO and H_2 are mixed with the fresh feed gas stream to be again fed to the shaft furnace. Depending on the technological choices, the gas supplying the pre-heater can comprise natural gas, hydrogen or DRP tail gas.

Two relevant characteristics should be noted in this process. First, the required energy [GJ] decreases in the reduction process as the hydrogen volume increases. This is due to the nature of the chemical reactions happening in the shaft furnace. In short, it requires approximately 10 GJ/t_{DRI} to reform hydrocarbons (natural gas) in the shaft furnace for the reduction process, which is essentially happening with CO and H_2. Supplying H_2 directly to the shaft furnace thus decreases the total required energy [GJ]. The molecular reactions are further elaborated in appendix A as they are not part of the main calculation performed in this thesis.

On the other hand, metallic iron (Fe), a product of the reduction process, reacts with natural gas. This results in the carburisation of the direct reduced iron (Fe_3C). Increasing the amount of hydrogen relative to natural gas decreases the number of available carbons for

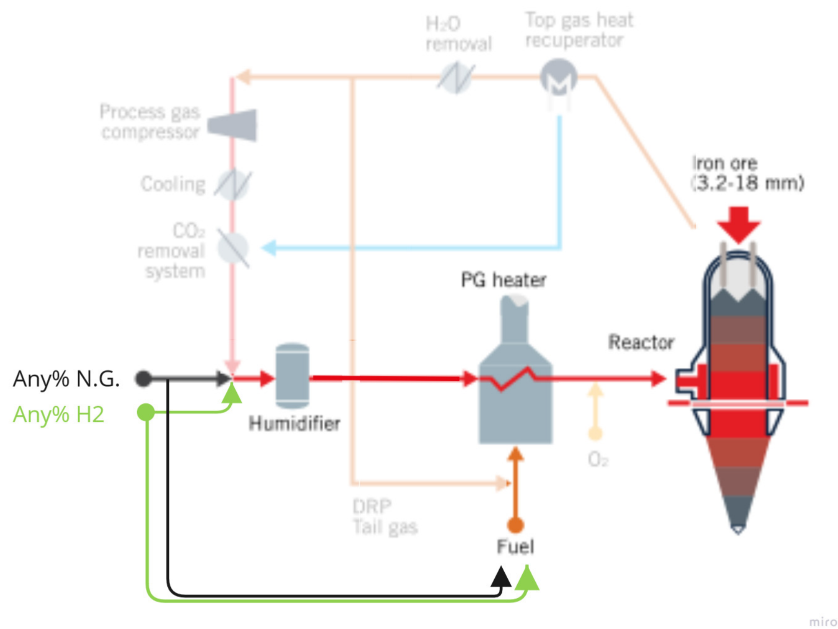


Figure 5.4.: Process scheme of the 'Energiron ZR' DRI process used in this thesis. Picture adapted from [15]

this reaction in the shaft furnace. For quality reasons, TSN wants to keep the same material composition. The hot DRI is then transferred to the REF, where different materials are added to produce consistent hot metal for steel production.

REF Process
In the REF, several materials are added to produce the necessary quality. Only the relevant materials affecting the outputs are considered. As already explained, increasing the hydrogen volume in the reduction process reduces the carbon percentage in the DRI output. In the REF this is compensated by adding the Anthracite (coal) material which results in additional CO_2 emissions due to efficiency losses. The REF process is new to TSN, which leads to many unknowns. The REF process will operate fully on internally made hot DRI, and no scrap material will be added. The first estimates in process characteristics are provided by TSN and are used in this thesis. Furthermore, only relevant data is incorporated that can affect the KPIs presented in chapter 7. By choosing these three processes and incorporating them in the conceptual model and the subsequently in the technical model, the effects of variating hydrogen volume on the CO_2 and production costs per ton of hot metal can be explored.

5.5. Inputs and outputs

The inputs and outputs of the conceptual model can be determined based on the modelling objectives and the overall scope. The model's outputs dictate the required inputs, with one of the input parameters that the model will run over an entire year on an hourly basis. This makes the conceptual model a time-series model. In the simulated period, time-dependent inputs such as electricity price and corresponding CO_2 intensity are used to model the technical and economic performance of hydrogen in a DRI-REF process.

5.5.1. Outputs

The conceptual model has two main outputs, specifying the other outputs to determine the performance of the modelled system of interest. The first main output is the specific energy consumption, expressed in [kWh/$t_{\text{hot metal}}$], based on the natural gas and hydrogen consumption expressed in [GJ/$t_{\text{hot metal}}$], for different hydrogen volumes at each time interval. This output will vary with a change in the hydrogen volume in the feed gas. Changes in material and energy balances must be made to ensure adequate hot metal quality. This output results from objectives 1 and 2 and will set the basis for further analyses.

The second main output can be split in two: the CO_2 emissions [$tCO_2/t_{\text{hot metal}}$] and the associated energy costs [€/$t_{\text{hot metal}}$] at each time interval. This output can be calculated using the results outputs from the modelling and is presented in a time-series model. To do this, electricity and natural gas market data are incorporated into the modelling with the hourly resolution, which is an input and will be discussed in the next section. This second output can be classified as modelling KPI, as a result, will be used to compare and quantify the performance of hydrogen under different penetrations. Furthermore, because the electricity market data set is provided on hourly basis, detailed analysis can be made on the conditions where one type of feed gas performs better than the other on a technical and economic basis.

5.5.2. Inputs

The inputs of the model can be sorted into different categories. The modeller determines some inputs based on information or literature findings, whereas other inputs are data sets acquired from other sources. Chapter 6 will explain and analyse the data sets gathered and used for the model inputs. The input identification for the conceptual model will be shortly explained and what role they play. The inputs, as visualised in the overview of the conceptual model in figure 5.2, can be classified into different groups; Input parameters, input data sets and process limits.

Input parameters
The input parameters can be subdivided into the material, process, and economic parameters. The material properties contain the necessary information needed to calculate the model outputs. In the model, two different types of reactions occur, i.e., thermal and chemical. Each type of reaction uses different kinds of material properties. Natural gas properties vary quite significantly depending on their origin [64]. For example, the natural gas from Groningen has a different molecular composition than the natural from the Middle East. This changes the heating values and, thus, the quantity used in the system and further emission calculations. Another type of input parameter are the process parameters. Each distinct process has its own parameter such as efficiency, material usage, energy consumption and conversion factors.

A different kind of input parameter are the economic parameters. To identify the effect of electricity prices on the whole system, natural gas and hydrogen prices need to be assumed or calculated. Additionally, to calculate the production costs, price estimates on carbon emissions in the European Union need to be assumed as well as the Capital Expenditure (CAPEX) and direct and indirect Operational Expenditure (OPEX). These values will be based on (grey) literature findings that estimate these prices for 2030. All the input parameters will be elaborated in full in the following chapter.

Input dataset
The input datasets are significant components of the model itself, the electricity market data, divided into electricity price and CO_2 intensity. These two inputs are essential as they define the results and enable the performance of hydrogen based on the formulated KPIs. However, constraints dictate the size of these data sets, as the data set must run over an entire year on an hourly basis and have substantiated claims for the estimations done in the year 2030. The electricity market data set is a fundamental strength of this research, as very few publications use hourly electricity market data [5; 22; 59]. However, these publications are based on systems with on-site renewable generation [22], countries with large shares of renewables [59] or do not take the emission intensity factors or carbon costs into account [59]. Moreover, hourly-based electricity market data sets based on the Dutch context used for the system of interest have not previously been used for academic purposes. The electricity market data set is obtained from the EMF v7.0 model from the company BlueTerra. How this data set is handled to represent the Dutch electricity market is explained in detail in chapter 6.

Process limits
Besides the input parameters and the input data set explained above, the process limits of the system of interest are acquired from TSN. Adopting realistic process limits and capacity levels increases the practical value for TSN and enable future research to be more realistic. However, the technology combination of the system of interest is new to TSN, many process parameters and limits are unknown at this time, and thus assumptions must be made. The substantiation for the assumptions will be based on the analysed literature of chapter 3. This way, the process limits and design constraints can be formulated despite limited input data. This is explained in more detail in section 5.2.

5.6. Simplifications

In the preceding subsections, the conceptual model's components, inputs and outputs have been formulated and explained. Simplifications and assumptions impact the formulation project of the conceptual model. However, they are necessary as they target and focus the conceptual model on the problem situation. The system of interest is based on the modeller's perspective of a future real-world system: the DRI-REF process. The problem situation is identified within the system of interest, and subsequently, the conceptual model is formulated. This is done by simplifying processes and using assumptions to define the implementation of specific steps. This section explains the main simplifications that shape the conceptual model. The simplifications apply to sections or processes within the conceptual model, whereas assumptions are more detailed and focus on specific formulation decisions.

One of the main simplifications in this work is how the material and energy balance is calculated. Throughout the analysed literature, three distinct types of research methods are identified. The first group of papers use the detailed Shomate equations taken from the NIST webbook [11] to calculate the specific heat and enthalpy of different species [5; 22; 65].These papers are characterised by their analytical nature and require solid mathematical and process understanding. The second group of papers uses specific flowsheet modelling software such as Aspen Plus to calculate the flow streams of the system [34; 44]. This requires in-depth knowledge of the software environment and process components. The last group of publications uses the results from the previous two groups and/or uses data from the grey literature. Assumptions on specific energy and material consumption are used to calculate the intended outputs [59]. This thesis will use the last approach for several reasons and is termed as the main simplification. First of all, time and process knowledge constraints dictate the depth level of the technical modelling. The specific DRI-REF process is not represented in the public literature, limiting the available knowledge on this configuration. Because of the lack of knowledge and real-world data concerning the system of interest, it is chosen to perform the modelling on a holistic level to provide general insights into the system's behaviour. Only relevant flows are used that influence the outputs of the conceptual model. Future research can add depth and process components to the modelling, which will be discussed in more detail in chapter 10.

A second major simplification is how the source of electricity is formulated in this research. It is assumed that the electricity source comes from the Dutch electricity mix, which has several implications discussed here. Currently, in the real world, TSN contracts companies to provide (renewable) energy (wind & solar) for a certain price level. However, this renewable energy generation is volatile as the generation is based on weather conditions which influence the generation capacity factors. Therefore, the deficit between renewable energy supply and demand will be provided from the grid and is based on the electricity mix. By assuming that the electricity source is solely coming from the Dutch electricity mix, contracted renewable energies by other companies are partly used by TSN in this simplification. This results in lower practical value as it decreases the realistic component of this research. However, using the electricity mix as an input can provide insights on a national level independent of any contractual agreements.

Furthermore, the choice of analysing a grid-driven DRI-REF process is verified using the paper from Elsheikh and Eveloy [22] . They have formulated a 100% hydrogen-based steel process powered by the Spanish electricity mix and an on-site solar power plant. However, TSN has no plans to produce its own electricity; thus, on-site renewable electricity generation is excluded from this research. Additionally, the feedstocks in the system of interest will almost always be based on a mixture of natural gas and hydrogen, so the influence of the electricity is expected to be lower than in a fully hydrogen-driven system. Furthermore, applying this simplification enables future analysis of which electricity procurement strategy, fixed power purchase agreements or electricity procurement from day-ahead electricity markets, is most cost-efficient [5].

Finally, this thesis will not use any material or energy storage options. Also, scrap metal is excluded from the analyses to reduce the number of variables and parameters. However, based on the literature review conducted in chapter 3, it is clear that these parameters do influence the outputs quite significantly. However, the added complexity would be too time-consuming; thus, these parameters are kept for future research.

5.7. Assumptions

The assumptions made in this work can be seen as detailed design choices of the model and should not be confused with the assumptions made for the input parameters. The assumptions are grouped based on what part of the process they affect. The most crucial assumptions will be discussed, and the motivation behind them will be addressed. Some assumptions can have a significant impact on the model results. These impacts will be discussed and reflected upon in the discussion part of this thesis.

The most critical simplification/ decision, assumption 11, is centred around the energy source. As it is unknown if and how these time bounded PPA's will be traded on the market, let alone determining their price, a simplification is made. The source for the electricity input of the modelling, further explained in the conceptual model chapter, is the Dutch electricity mix. The electricity mix is the average generation of wind, solar, gas, coal, nuclear, etc. and can be estimated based on the scenarios in table 2.1. Thus, this thesis disregards any contractual agreements between TSN and the electricity suppliers. However, by taking the electricity mix as the electricity source, the 'real' effects of switching to hydrogen can be determined [62].

no.	Assumption	Motivations/reasoning
1	No downtime in processes, 8000h to 8760h	Minor influence on results. The plant capacities are taken from 8000h operational process on a yearly basis and spread over 8760hours. Furthermore, it is unknown how long and when the facilities are producing.
2	Facilities are operating on their hypothetical full capacity.	With the realisation of the DRI-REF plant in 2030, full production capacity would not be available. In this work, it is assumed that it is the case.
3	Continuous production, no batch production	Minor influence on results. The DRI process is in fact a continuous operation where downtime in this process is kept to a minimum. The REF production process on the other hand, is a batch process. However, this is neglected in this thesis.
4	No cycling of the DRI process	What is meant by the cycling of the DRI process is the switching of natural gas to hydrogen when circumstances demand it. In this thesis, it is assumed that the predetermined volume of hydrogen is fixed throughout a whole simulation (a full year). Future research could enable this cycling methodology to optimise production on costs and emissions [59].
5	All material and gas flows are used in the same time interval	Minor influence on results. There are some operational delays in the material and energy flows. However, it is not expected to influence the results notably, as the results will be aggregated on a yearly basis.
6	No hydrogen storage	Significant impact on results but add much complexity to the modelling process. Various types of control and optimisation strategies are needed for this implementation. Outside of skill and time scope

no.	Assumption	Motivations/reasoning
7	No choice of electrolyser technology	Minor impact of results. Based on the holistic view of this thesis, choosing a specific technology would not affect the results much. For an effective electrolyser integration, as done in the paper of Müller et al.[44], it is necessary to choose a particular technology. However, this would also require extensive modelling of the electrolyser process in dedicated software. Furthermore, the aim is to go beyond the process level and analyse broader system implications of the system of interest.
8	No DRI to Hot Briquetted Iron (HBI) storage.	Medium impact on results. Comparable to hydrogen storage, a type of control mechanism should be designed. Additionally, the operational characteristics are unknown for the DRI-REF process. Consequently, minor material and energy flows to compact DRI to HBI are thus excluded.
9	System boundaries purposefully do not include downstream processes	Minor impact on results. The bulk of the emissions and energy consumption comes from the iron ore reduction to crude steel. Downstream operations, such as casting and rolling, will not change their production process, so there is no academic or practical contribution. However, the consequence is that not all emissions from the integrated route are considered.
10	All emissions from the NG are released in the system boundaries	Minor impact on results. A few percent of the NG carbons atoms bind with the iron molecules. These carbon atoms are then released in the BOF process, outside the scope of the system of interest. However, this thesis assumes that all NG carbon atoms are emitted within the system boundaries. This results in a minor deviation in the results.
11	Energy market data coming from the EMF V7.0 model BlueTerra B.V.	Large impact on results. This assumption is the most important. Predicting the electricity price and associated carbon emissions has inherently some error margins. Also, predicting the future is not possible. However, an educated 'guess' can be made for future prediction based on developed models with historical data. Each model has its own set of assumptions; thus, no two models are the same. Assumptions concerning the settings of the EMF model are documented in chapter 5

Table 5.1.: Assumptions made in the modelling process

6. Data

The purpose of this chapter is to provide information and explanations on the data used to implement the technical model. The data sets in this chapter are the inputs discussed in the previous chapter, section 5.5. These inputs are sorted based on their characteristics and will be elaborated as such in this chapter. First, in section 6.1, the electricity input data set is discussed, which is used to close a significant part of the identified knowledge gap. Secondly, section 6.2 describes the input parameters and the process limits.

As explained in the research gap, section 3.4, a data set with the key elements of a future electricity market is not commonly used in the analysed literature. The connection between the Dutch electricity market and the system of interest described in this thesis has yet to be published in academic literature. Therefore, acquiring a representative data set for the Dutch electricity market plays a central role in this research. Here we use an Electricity Market Forecast Model (EMF) for the year 2030 that uses the capacity of installed assets in MW in combination with a specified weather scenario to determine the electricity price (in €/MWh) and associated CO_2 emissions of the individual deployed assets (kg/MWhe).

6.1. Electricity input dataset

The economic and emission modelling of the system of interest is based on the hourly electricity price and the associated CO_2 emission intensity data. These datasets originate from the Energy Market Forecast model v7,0, developed by the company BlueTerra, previously known as EnergyMatters. The following sub-sections will explain the central workings of the EMF model, as this is crucial for validating the results. The electricity market is a complex system that makes predicting difficult, let alone predicting the future, which is even more complex and uncertain. The model outputs are summarized in table B.1 in appendix B.

6.1.1. Price of electricity

The EMF model utilises the IPKA0 scenario developed by TenneT as the base case, see section 2.3, to estimate the electricity generation capacities in 2030. Subsequently, electricity price forecasts can be made based on a merit order illustrated in figure 6.1. The merit order curve is conventionally called the supply curve in economics. Hence, the merit order principle can be seen as a supply-demand model. This section will briefly describe the merit order principle and elaborate on how the EMF model estimates an hourly electricity price in future scenarios.

Electricity is produced in the Netherlands by a wide range of techniques such as renewable energies (solar, wind), fossil fuels (coal, gas) or nuclear power plants. As electricity demand varies over time, the total available capacity for electricity production is not always necessary to be deployed. In the context of the merit order, two classes of producers can be distinguished. The first class includes volatile electricity producers such as solar panels and wind turbines which produce electricity irrespective of the demand and the must-run electricity production. The second class consists of dispatchable producers, including coal and natural gas-fired power plants.

In contrast to the volatile producers, the dispatchable producers can react to variations in electricity demand. Therefore, these specific generation sources will only be started or phased out if there is a certain electricity demand. The ranking of which electricity generation capacity is used is mainly based on the short-term variable costs of the electricity produced, which depends on the specifics of each technology, such as fuel costs, CO_2 price, maintenance costs, transmission tariffs, levies, etc.

The cover the electricity demand, the power plants with the lowest operating costs are switched on until the electricity demand is met. The most expensive power plant needed to cover the electricity demand, also known as the marginal power plant, determines the electricity price on the intraday and day-ahead spot market. In most cases, the most expensive power utilities are gas-fired power stations. This is the primary mechanism of the merit order and is visualised in figure 6.1.

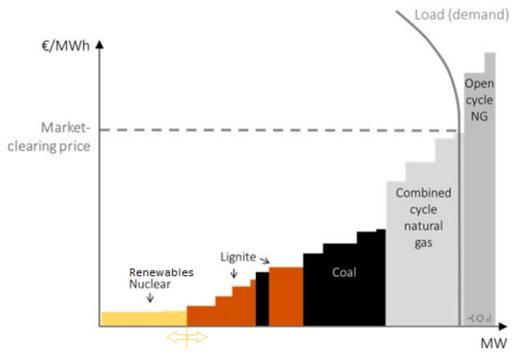


Figure 6.1.: Illustration of the merit order principle, providing the relationship between the available capacity in MW for the different power utilities and the electricity price in euro per MWh. Picture adopted from: [30]

As the penetration of renewable energy increases, so does the demand for flexibility in the electricity supply. Coal-fired power plants cannot technically and economically meet the flexibility demand [37], so the more expensive but flexible natural gas turbines are used to cover the residual load in the future. Additionally, in the 2030 scenario, all the coal power plants will be completely phased out in the Netherlands, as seen in the IPKA0 scenario in section 2.3.1. These developments result in more expensive electricity during certain hours and will generally increase price fluctuations. The electricity price data set of the EMF model for two different scenarios are presented in figure 6.2 as an electricity price duration curve graph. These curves show how often a certain electricity price level is attained throughout the year.

For the year 2030, the high share of renewables will increase the duration and number of both the high- and low-electricity price periods, compared with the year 2023 electricity price profiles. The electricity price profiles in 2030 are much more volatile than in 2023. The phasing out of the coal-fired plants increases the demand for (expensive) flexible generation increases.

The volatility of the electricity price profile in 2030 is evident in Figures 6.2, 6.3 and 6.4, which show the electricity prices and the wind and solar power generation levels, as obtained from the EMF modelling. The electricity price is influenced differently by solar and wind power. Wind power lacks any cyclic component in its variation and has no regular pattern. Solar power, on the other hand, is cyclic in nature due to the day and night cycles.

The same price development pattern is observed in the literature paper of Toktarova et al. [59]. They have used price data from an electricity system investment model, referred to as H2D. The quantitative difference between the price levels of that model and the model used in this work, are the assumptions in the base years (2018) and geographical focus (Ireland and Southern Germany).

Some other settings and parameters influence the results of the EMF model, such as electricity imports and export behaviour, weather year and demand pattern, APX price matching, demand growth, battery storage and in later scenarios, power to heat (P2H) and gas (P2G) buffering (i.e., hydrogen). The assumptions of the input parameters of the EMF model are summarized in table 6.1. Based on the objective of this thesis, the dataset of the 2030 scenario will be used as input data for the conceptual model, as in the year 2030, the DRP and REF will be operational at the TSN site in IJmuiden.

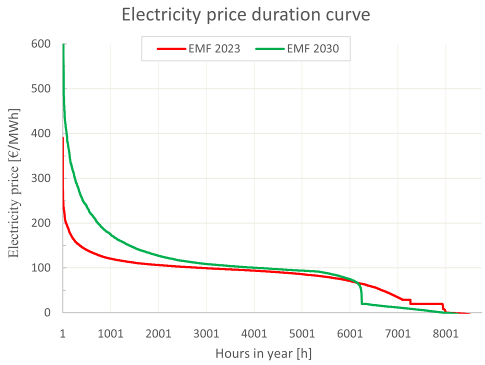


Figure 6.2.: Electricity price during a whole year on each hour (n=8760) for two different scenarios.

Scenario	Average price [€/MWh]	Total generation [GWhe]	Percentage renewable generation [%]
2023	136	109,374	45.7
2030	97	131,871	71.3

Table 6.1.: Numerical values of the scenarios depicted in figure 6.2.

The discrepancy between the electricity demand (table 2.1) and the total generation (table 6.1) is covered by import or export mechanism in the EMF model. This import and export mechanism is based on the historical electricity trading behaviour of a specific year.

6.1.2. CO2 intensity of electricity

The second input dataset from the EMF model is the CO_2 intensity per hour emitted by the electricity mix. To determine the CO_2 intensity of the electricity mix for each hour, the EMF model calculates the amount of power that was supplied by each electricity generation source based on the merit order. The variable renewable energy source or volatiles (i.e., wind & solar) and must-runs (i.e., nuclear) have a-priori-defined current load profiles that determine the 'on/off time'. In addition, the profiles of the volatiles are based on a predetermined weather pattern. The load and the weather profile are used to determine the hourly production by scaling them with the installed capacity of the respective participant.

Dispatchable generation (i.e., gas turbines) does not have a load profile defined yet, as these are calculated in the EMF model based on the residual demand.

By allocating a specific emission intensity factor to each electricity generation source, the EMF model will calculate the total CO_2 emissions for that specific hour. By dividing the total CO_2 emissions by the total generated power (renewables and conventional), an hourly-based emission factor can be determined for the whole year. A similar approach is used in the paper of Elsheikh and Eveloy[22] for the Spanish context.

The outputs of the EMF can be visualised in various ways. For instance, figure 6.3 visualises the results of the EMF model of week 39 in the 2030 scenario. Each generation source has its colour and is stacked upon each other. The demand profile (black dotted line) must be met at each hour, either by increasing the flexible generation capacity (orange), discharging batteries and buffers (green) or ultimately importing electricity. The wind (blue) and solar (yellow) generations are based on the weather year and thus a given power supply. Whenever there is an excess of renewable electricity, batteries and buffers are charged, or the electricity is exported. The separations of these electricity generation sources enable visual analysis of the impact of renewable energies on the final electricity mix. The complete hourly data sets on electricity price and CO_2 emissions are visualised in figure 6.4 and 6.5 for the 2030 scenario, respectively. The annual average CO_2 emission factor derived from the EMF v7.0 model is estimated at 0.130 tCO_2/MWe for the 2030 scenario.

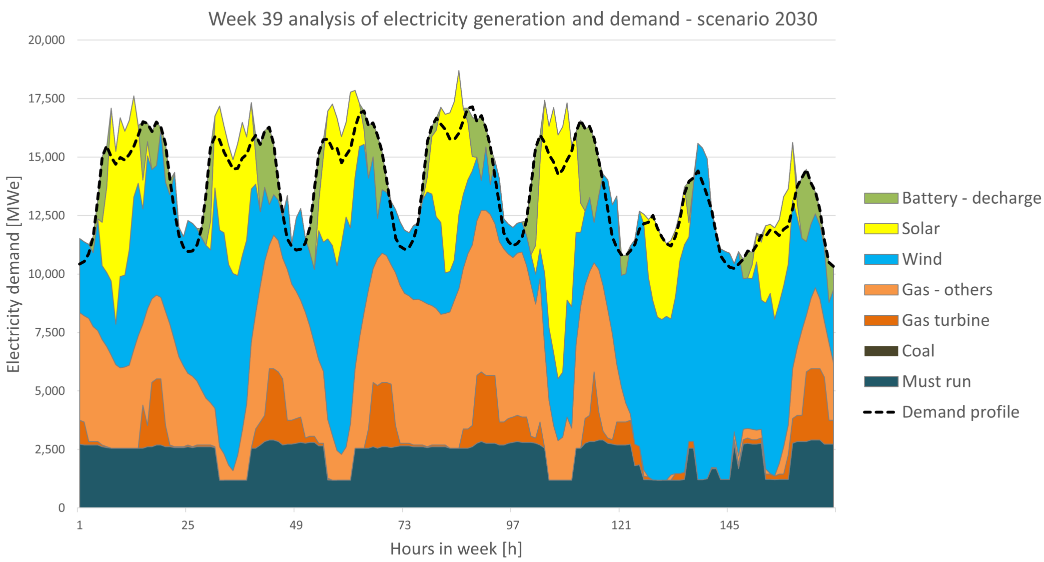


Figure 6.3.: Generation profile of week 39 in the 2030 scenario of the EMF model V7.0. There are several moments in this week where the electricity demand is fully covered by renewable energy (blue and yellow).

It should be noted that in figure 6.4, there are approximately 800 h where negative electricity prices are observed. These negative electricity prices range between 0 and -30 €/MWhe. Figure 6.5 indicated that there no are moments where the electricity generated by the Dutch electricity mix in 2030 is completely CO_2 free. This is due to the must-run installation (i.e. waste incineration facilities) producing heat and electricity, but also CO_2 emissions.

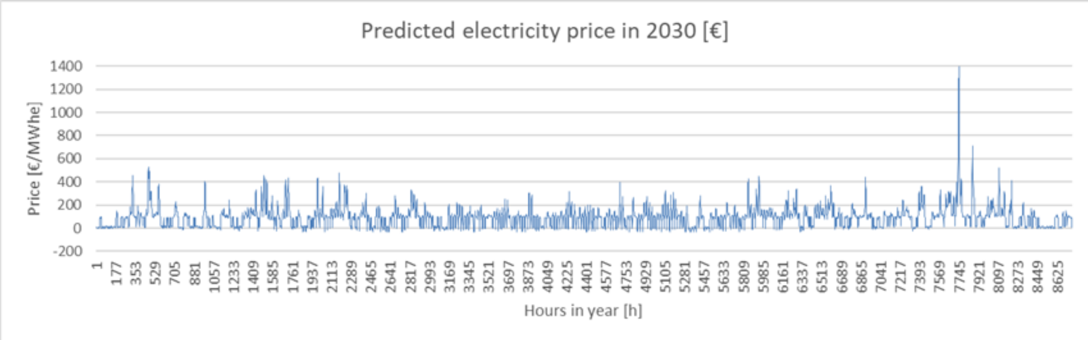


Figure 6.4.: Predicted electricity price for the year 2030 under specific model assumptions.

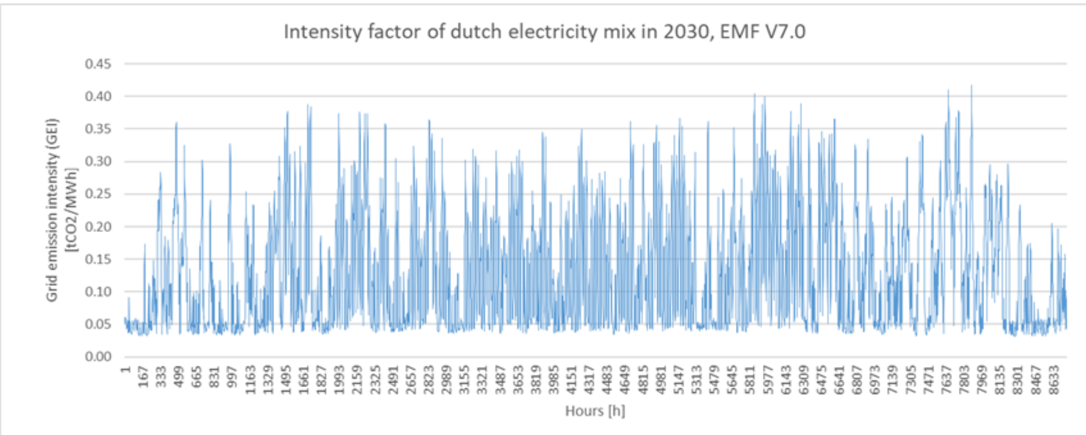


Figure 6.5.: Predicted carbon emissions of the electricity mix generation in the Netherlands in the year 2030.

Assumption	Parameter	Explanation
Scenario	2030	This is the main input of the EMF model indicating the simulated year
Weather year	2014	This is weather year is an average year where enough wind and sun were measured. The demand profile is based on this input
Generation capacity scenario	IPKA0 from TenneT	From TenneT 'leveringszekerheid rapport' [58], see chapter 2.1
Electricity demand growth	12%	Electricity demand growth compared to 2014, resulting in 149 TWh
Import scenario	2021	Imported electricity power on each time interval

Table 6.2.: Summary of the EMF model input assumptions

6.2. Material, process, and economic input parameters

Besides the two input datasets explained above, other relevant inputs have to be explored as put forth in the conceptual model. The main DRI-REF and electrolysis input modelling parameter and their range of variation for off-base case analysis are documented in subsections 6.2.1 and 6.2.2, respectively. These input parameters are sorted in relevant material, process and economic properties based on literature or data acquired for TSN. Only the most relevant values are presented in the main body of this thesis.

6.2.1. Material properties

Figure 5.3 in chapter 5.4 depicts the relevant material flows used to solve the problem situation. The materials used as input parameters are natural gas and hydrogen, used for the chemical reduction process and heating. These two materials have vastly different properties and can have different values based on their origin. For example, the values assumed for the natural gas originating from the Middle East differ from the natural gas from Groningen [64]. Slight deviations or the lack of documentation can result in significant disparities in modelling results. The assumed and most important properties are documented in table 6.3 with their respective source. The full table of properties can be found in table C.1.

Parameter	Value	Unit	Reference
NG methane	92.2	% mol	TSN
NG emission	56.1	$kgCO_2/GJ$	TSN
NG Lower Heating Value (LHV)	47.15	MJ/kg	TSN
Hydrogen LHV	120.1	MJ/kg	TSN

Table 6.3.: Assumed material properties of natural gas and hydrogen

6.2.2. Process properties

The following properties comprise of technical DRI-REF and electrolyser input modelling parameters, documented in table 6.4. The parameters are based on process information acquired from TSN and literature data. Several values are calculated through the implementation of the model and will be evaluated based on the analysed literature described in chapter 3. These calculated process parameters are used to assess the technical and economic performance of the DRI-REF process with variating hydrogen volumes, further elaborated in chapters 7 and 8.

Some parameters have an indicated range instead of a specific value. These parameters change depending on the hydrogen/natural gas composition in the feed gas and add complexity to the modelling. The majority of the analysed papers use fixed values either assumed or calculated in their modelling. However, the goal or aim of the modelling is of crucial importance. A modelling constraint in this research is that the quality of the output (Hot Metal) must remain the same irrespective of the system's inputs.

TSN has provided linear data concerning these variable values. However, based on the results of Müller et al.[44] visualised in figure 6.6, it becomes clear that the required chemical energy and carbon content are not linear with the fraction of hydrogen in the feed gas. This is because hydrogen is formed next to the carbon monoxide through the in-situ reforming of natural gas in the DRI shaft based on the reactions A.1-A.7 seen in appendix A. The references indicated in the paper of Müller et al. used for figure 6.6 could not be checked due to prohibitive access. The data is approximated and used in this research. Furthermore, the electrical efficiency and the limestone consumption of the REF process are based on the data from TSN. They are linearised based on the chemical energy composition of hydrogen and natural gas per ton of DRI.

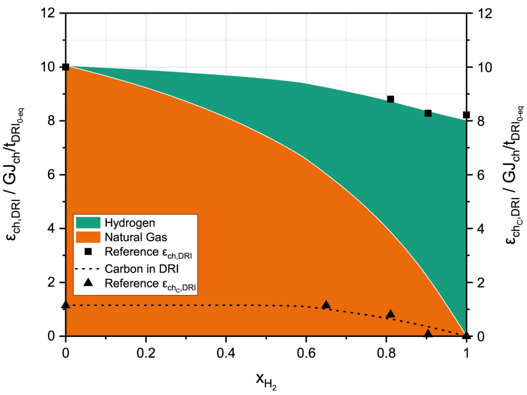


Figure 6.6.: Chemical energy fraction and carbon content based on varying hydrogen/-natural gas composition of the feed gas. Picture adopted from [44, p.10].

Parameter	**Unit**	**Value in this thesis**	**Reference**	**Value(s) in literature**	**Reference**
DRI Plant capacity	kt_{DRI}/a	3924	TSN		
DR pellet consumption	t/t_{DRI}	1.311	TSN	1.359 -	[34]
DRI electricity usage	kWh/t_{DRI}	129	TSN	78-125	[34; 44; 49]
DRI reduction SEC	GJ/t_{DRI}	7.75-8.25	TSN	8.0-10.0 (reduction + heating)	[34; 44]
DRI heater SEC	GJ/t_{DRI}	1.7	TSN	211.9 kWh/t_{HM}	[22]
DRI CO_2 emissions	$kgCO_2/kWh$	Calculated			
DRI carbon content	%	0.5-4.5	TSN	3.5	[44]
H2 consumption	kg/t_{HM}	Calculated			
Electrolyser efficiency	kWh/kgH2	47.7	Calculated	45-53	[5],
REF plant capacity	kt_{HM}/a	3672	TSN		
REF DRI consumption	t/t_{HM}	1.069	TSN		
REF carbon consumption	t/t_{HM}	0-0.0580	TSN	0.020	[22]
REF carbon charging efficiency	%	82.5	TSN	50	[65]
REF lime(stone) consumption	t/t_{HM}	0.07-0.075	TSN	0.050 (EAF process)	[22; 59; 65]
REF electrical efficiency	kWh/t_{HM}	635 713	TSN		
REF SEC	kWh/t_{HM}	Calculated			
REF emissions	$kgCO_2/t_{HM}$	Calculated			

Table 6.4.: Technical input modelling parameters and assumptions

7. Model implementation

The methodology of the technical model implementation is discussed and evaluated in the following chapter. To do this, a conceptual model has been formulated, see chapter 5. Chapter 6 provides substantiation and an overview of the input data sets and parameters needed for the technical implementation.

Based on the discussions with TSN, it was decided to implement the conceptual model in Microsoft Excel as it would best fit the current development progress of the DRI-REF system. The modelling consists of two main parts. First, the base modelling of the DRI-REF process, and the second part is directed to the implementation of various hydrogen/natural gas feed gas compositions and its effect on the material and energy balance. Both steps will be evaluated and validated based on the system performance metrics and literature sources. The final step after the technical implementation is the economic evaluation of the modelled system, which uses the modelling results along with the data set in section 6 and will be further discussed below.

7.1. Base modelling

As seen in the visualisation of the conceptual model in section 5.3, the first step is the base modelling. This process uses the input parameters in section 6.2 and handles them accordingly. The base modelling determines the energy and material demand for the DRI-REF process while using 100%NG natural gas as the feed gas.

Parts of the base model can be validated based on state-of-the-art knowledge from the literature or expert inputs. The system of interest, a DRI-REF system, has yet to be fully conceptualised in detail in the public literature. However, as mentioned in chapters 3 and 5.6, several papers have already modelled the DRI-EAF process with varying aims and depths. Therefore, the DRI process of the model implementation can be validated based on literature data, and the REF process will be validated through expert knowledge. The section will present and explain the methodology of the base modelling.

The first part of the base modelling is centred around the DRI (direct reduced iron) process, which reduces iron pellets in the shaft furnace to produce DRI. A detailed representation of the model is already presented in section 5.4. The quantities of DRI on an hourly basis are calculated based on the total plant capacities and on the acquired or assumed data, as seen in table 6.4. The DRI output is calculated on 491 t_{DRI}/h based on 8000 operations hours and 2 DRI plants with an annual capacity of 2 Mt/a. The modelled DRI process uses 1.312 $t_{DR\text{-}pellet}/t_{DRI}$, neglecting the distinction between the internal and external pellets.

Subsequently, the energy requirements are calculated per ton DRI. Based on the simplification given in section 5.6 and the information provided in chapter 6, the energy requirements are determined for base case configurations. The total energy required for the DRI process can be split into chemical energy needed for the reduction process, thermal energy for heating the feed gas, and electricity. The current assumed gas-fired heater could use hydrogen instead of natural gas or be replaced by electric heaters if technically and economically permitted. For a 100% natural gas system, 8.25 GJ/t_{DRI} chemical energy is assumed for the reduction process and 1.7 GJ/t_{DRI} thermal energy heating the natural gas. The DRI process has an assumed base electricity usage of 129 kWh/t_{DRI}, irrespective of the feed gas composition. The SEC for the DRI is calculated at 2.89 MWh/t_{DRI} for a 100% natural gas DRI-REF system. For the base case, the carbon content of DRI output is determined to be 4.5 weight percent (%wt) of the iron . The heat recovery unit (condenser) and the oversupply of hydrogen are not modelled in this thesis. This is done because the CO_2 removal system is not modelled, which is one of the systems that could utilise this recovered heat. However, modelling these components would only increase the specific energy consumption. In most cases, the heat recovery unit has an assumed efficiency of 70% [48]. The oversupply of hydrogen to the DRI process is determined based on the value $\lambda = 1.5$ [65]. λ is defined as the moles of H_2 supplied to the moles necessary for the complete conversion reduction of iron ore in the shaft.

The second part of the base modelling is directed to the REF process. Similar to the first part, the material balances are determined first for the base case, the 100% NG case. It is assumed that all the DRI is converted to Hot Metal (HM) with an annual capacity of 3672 kt_{HM}/a. The hourly production capacity is 459 t_{HM}/h based on the same operating hours as the DRI process. Consequently, 1.069 t_{DRI} is needed to produce one ton of hot metal. This value is essential for further emission and economic calculations as they will be levelized on the hot metal output. Furthermore, the lime consumption is 0.070 t/t_{HM}, and no additional carbon atoms are added in the base case. The REF has a carbon electrode consumption of 0.002 t/t_{HM}. Other materials such as dolomet, bauxite, reverts, and scrap are excluded from the modelling as these materials either have no influence on the energy balance or still have an unknown effect. Based on the paper of Vogl et al. [65] it is known that scrap metal significantly reduces the energy requirements of the EAF. However, whether the same should happen with the REF process is still being determined. Therefore, this parameter is excluded from this research.

The REF process's energy requirements are simplified to solely electrical energy. The REF part of the modelled system is based on crude data, and the lack of literature data hampers validation. However, it is assumed that the REF has an SEC of 0.635 MWh/t_{HM} for the base case and increases as hydrogen is added to the feed gas, as explained in section 6.2.

7.1.1. Emission calculations

The emission modelling method for the base case and subsequent modelling additions is limited to CO_2 calculations. The material and energy demand resulting from the modelling and simulation configurations can be used directly for the emissions calculations. The emission calculation can be separated into material, natural gas, and electricity emissions.

The material emissions consist of lime(stone) and graphite electrode emissions. No additional carbon is added in the base case because the natural gas provides the necessary carbon atoms. The chemical reaction formulas are based on the molecular weights. The added lime(stone) results in 0.44 tCO_2/t_{lime} considering the flow to be pure lime (CaO). Graphite electrodes emit 1 mol of CO_2 per mole of carbon consumed according to the chosen consumption rate, resulting in 3.66 $tCO_2/t_{electrodes}$. For the natural gas emissions, 56.1

$kgCO_2/GJ$ is calculated based on the natural gas composition documented in table C.1. It is assumed that all carbon atoms in the natural gas are converted to CO_2, as explained in section 5.7.

Since TSN is not generating electricity, it imports electricity from a third party. This research assumes that the electricity is directly sourced from the Dutch electricity grid. The emissions associated with electricity production are part of scope 2 emissions viewed from TSN. Nevertheless, this thesis estimates the potential emissions created/negated using electricity (and hydrogen) in the DRI-REF process. The electricity consumption in the base case consists solely of the DRI and REF electricity consumption. Electricity consumption for hydrogen production is thus excluded in the base case, as no hydrogen is used. The given hourly electrical CO_2 intensity is used to estimate the hourly CO_2 emissions of the electricity consumption. Chapter 6 discusses how this input dataset determines this hourly parameter. The yearly average electricity CO_2 emissions intensity is assumed to be 0.130 tCO_2/MWe for the assumed 2030 scenario elaborated in section 6.1.2.

7.2. Technical key performance indicators

In this section, the KPI are explained. The KPIs are used to measure or quantify the outputs and determine the performance of the intended simulation. However, the KPIs are often built upon, which means that KPIs will also be an output of the model. The modelling KPI are determined throughout the implementation of all steps: base modelling, hydrogen modelling and economic modelling. The KPIs are used to display most of the results of the modelling part and support the content of the results chapter.

The aim of these modelling KPIs is to transform the model's outputs– the simulation of different hydrogen feed gas compositions in the DRI-REF process over an entire year - into usable results. The modelling KPIs can be sorted into technical performance and economics KPIs. The different KPIs are defined based on the literature review conducted in chapter 3.

The technical performance of the DRI-REF simulations is assessed using the following KPIs:

The DRI-REF process SEC, in MWh/t_{HM}, which is the ratio of the total annual electricity consumption for electrolysis and the DRI and REF process, the energy required for the DR pellets and feed gas pre-heating, and the chemical energy required for the reduction process, to the annual hot metal production [22]:

$$SEC_{DRI-REF} = \frac{\sum_{h=1}^{n} W_{E.total}}{m_{HM,a}} \tag{7.1}$$

Where n is the number of operating hours taken as 8000h [22], and the annual hot metal output (m_{HM}) is set to the output of TSN, which consists of two times a typical large-scale plant production capacity of 2 million tons per annum (MTPA) [22]. The specific values are documented in table 6.4 in the Data Chapter.

The emissions evaluation of the DRI-REF process is based on the specific CO_2 emissions of the considered configuration. The specific CO_2 emission for each considered configuration is the sum of annual electricity, material, and thermal emissions, divided by the annual hot metal production (tCO_2/t_{HM}):

$$EE_{DRI-REF_{Consideredroute}} = \frac{\sum_{h=1}^{n}(EE_{mat} + EE_{elec} + EE_{heat})}{m_{HM,a}} \quad (7.2)$$

Where EE_{mat} refers to the material emissions from the DRI and REF processes, EE_{elec} refers to the emissions from the electricity consumption from the electrolysis, DRI and REF processes. The EE_{heat} defines the emissions from the heater which can be based on natural gas, hydrogen or ultimately electricity, respectively.

To further demonstrate the effect of various hydrogen feed gas compositions on the $EE_{DRI\text{-}REF}$, a stacked area graph highlights the magnitude of change over the different compositions presented in chapter 8. Furthermore, to quantify and evaluate the performance of various hydrogen feed gas compositions, the specific CO_2 mitigation potential is applied:

$$\phi_{CO_2} = \frac{SpecificCO_2Emissions_{NGroute} - SpecificCO_2Emissions_{H_2route}}{SpecificCO_2Emissions_{NGRoute}} \quad (7.3)$$

The specific CO_2 emission mitigation potential allows for assessing which CO_2 reduction is achievable for the considered route compared to the base case. The specific emission mitigation potential can be directly calculated from the process modelling of section 7.1. Up and downstream operations are excluded. Therefore, the conducted emission analysis does not meet the requirements of a life cycle analysis.

The above-mentioned technical KPIs are all based on the yearly averages. The results will be visualised in a time-series graph to demonstrate the hourly variations. In addition, a boxplot graph is used to understand better the hourly variability of the hot metal price and associated emissions. These will be further elaborated in chapter 9.

7.3. Hydrogen implementation

The hydrogen implementation modelling process has several steps as hydrogen affects several aspects of the base model and requires the following component: the electrolyser. Figure 5.1 in the conceptual model visualised the system's boundaries with the considered inputs and flows. Each step calls for a separate implementation, and at the centre are the base model's material and energy reaction formulas. The output of the base model and the hydrogen implementation will be validated based on literature data in section 7.4.

The main methodology for the hydrogen implementation is to select a hydrogen fraction in either the feed gas for the DRI process or feed gas pre-heating. The conceptual model chapter already explains several boundary conditions and simplifications concerning its implementation. The applied methodology is based on a top-down approach, meaning that the output of the REF process and the hydrogen fraction determines the required hydrogen, energy, and material demand. This approach is chosen as it enables investigation of the demand for hydrogen, energy and materials based on the best achievable production rates. Other methods, such as the bottom-up approach, start with the available electrolyser capacity or renewable energy for green hydrogen production to investigate the opportunities [source]. Although both methods are common, they require a different modelling approach.

The literature reviewed on model-based assessments of low-carbon steelmaking via the DRI route is mainly limited to a 100% hydrogen feed gas composition. A few studies have considered the effect of varying hydrogen composition [44]. Therefore, the hydrogen modelling is implemented so that all possible hydrogen fractions can be investigated and compared based on the output parameters and KPIs. This requires the implementation of formulas for the parameters affected by variation in hydrogen fraction. Due to the sheer complexity of the iron and steelmaking process, early stages of hydrogen-based steelmaking and limited time for this research project, several simplifications are made based on the limited data acquired from TSN.

7.3.1. Electrolyser modelling

As the conceptual modelling indicates, the electrolyser is situated within the chosen system boundaries. The conceptual model shortly elaborates on the common industrial types of electrolysers. The works by Toktarova et al.[59], Bhaskar et al.[5], Otto et al.[47], and Vogl et al.[65] are not considering a particular type of electrolyser technology. Based on the aim of this thesis, it is chosen not to select a specific type of electrolyser as this would increase the complexity of the model. However, as indicated by Müller et al.[44], different types of electrolysers, especially the technology allowing high-temperature electrolysis, allow for unique features of heat integration and co-electrolysis of H_2O and CO_2. Chapter 9 provides a discussion and the limitations of this choice.

The first step in the electrolyser modelling is determining the energy demand to produce hydrogen. Hydrogen has a LHV of 0.120 GJ/kgH_2 and a Higher Heating Value (HHV) of 0.142 GJ/kgH_2. For a 100% efficient electrolyser, 39.4 kWh/kgH_2 of electricity would be required based on the HHV. The efficiency of the electrolyser system is taken in this thesis and is assumed to be 70%. This is in line with 2030 projections for the PEM electrolysers [42; 53; 65].

7.3.2. Hydrogen effects on the DRI process

Increasing the hydrogen volume fraction in the feed gas for the reduction process influence several parameters, as introduced in section 5.4. First, the chemical energy required for the reduction process decreases as the volume fraction of hydrogen increases. Based on the data from TSN and Müller et al.[44], it is assumed that 0.5 GJ less chemical energy would be required at 80% volH2. Second, the substitution of chemical energy source, hydrogen, or natural gas, in relation to the volume fraction is not linear, as TSN suggested. TSN has provided data for 80% hydrogen volume fraction in the feed gas. At this hydrogen volume fraction, 5.02 GJ chemical energy is provided by the hydrogen (65% of the total chemical energy), which correlates with the findings of Müller et al.. Furthermore, it is assumed that the heater natural gas energy substitution is linear to the hydrogen energy.

7.3.3. Hydrogen effects on the REF process

Several inputs of the REF process, as indicated in section 6.2.2, are affected by the variations in DRI feed gas composition. For example, hydrogen is not a direct input of the REF, but it changes the composition of the output of the DRI process. This results in a relationship between input parameters for the REF based on the carbon content of the DRI and the hydrogen volume of the DRI feed gas.

The energy consumption of the REF process is assumed to have a linear relationship starting at 635 kWh/t_{HM} for 100% NG feed gas composition up to 755 kWh/t_{HM} for 80% hydrogen volume fraction. Furthermore, the lime consumption has a linear increase up to 0.0747 t/t_{HM}. Carbon is added to the REF process to keep the carbon content of its output constant. It is assumed that the added carbon has a linear increase up to 0.0580 t/t_{HM} at 80% hydrogen DRI feed gas fraction. The emissions for the added carbon in the REF are determined to be 0.642 tCO_2/tcarbon while assuming a charging efficiency of 82.5%, meaning that 82.5% of carbon enters the hot metal, see Table 6.4, whereas the rest is converted to CO_2.

7.4. Model validation

Only the electrolyser and DRI modelling steps can be validated for the technical implementation of the model. As discussed in the problem situation in section 5.1, the REF process has yet to be documented in the context of steel manufacturing based on the analysed literature. As such, it is challenging to fully validate the conceptualisation and technical implementation of the REF process. However, the electrolyser and DRI implementation and base modelling result can be validated based on the literature data.

There are several validation methods identified based on the analysed literature. For instance, Müller et al.[44] uses real operation data of a natural gas-based DRI reduction process to validate their model findings. Another method that Elsheikh and Eveloy[22] uses, is using the process inputs from Bhaskar et al.[6] and compares the key modelling parameters. Lastly, the paper of Jacobasch et al.[34] compares their key modelling parameter with several other papers based on specific ranges.

Due to the simplifications applied in this thesis, it is decided to validate the outputs of the modelling based on comparing the end results with literature data. Therefore, the key model findings are compared to several papers in table 7.1. The modelling assumptions from the mentioned papers are used to compare the key findings thoroughly. For instance, the electricity emissions (scope 2) are excluded from the outputs if they are not included in the results of the indicated papers. Additionally, the feed gas composition of the mentioned papers below are adopted. For example, the paper from Elsheikh and Eveloy[22] uses a 100% hydrogen feed gas composition, whereas Jacobasch et al.[34] uses 100% natural gas feed gas composition.

One thing to note, is that the electricity consumption of the REF process is significantly higher than the EAF process in the mentioned papers. This results in an overall higher energy consumption of the system of interest. Furthermore, the DRI hydrogen consumption depends on two main assumptions, the electrolyser efficiency and the efficiency of the DRI process. This thesis uses a more conservative estimation than other papers.

The required energy of the DRI changes as the hydrogen feed gas fraction increases. The SEC of the DRI process is comparable with the data presented/reported in the literature . The emission from carbon and lime are purely based on the consumption quantity, which is slightly higher in this thesis as seen in section 6.2.2. Finally, the specific CO_2 emission of the whole modelled system is comparable with the results from other papers, especially that from Müller et al.[44]. The slight differences between the papers are mainly based on the difference in energy consumption, auxiliary systems such as carbon capture units, or the assumed emission intensities of the inputs, e.g., NG composition and electricity.

Parameter	**Unit**	**This work**	[22]	[5]	[44]	[65]	[34]	[49]
DRI H2 consumption	Kg/t_{DRI}	62.3	59.3	59.3			60.7	62.4
DRI SEC (100% H2 – 100% NG)	MWh/t_{DRI}	2.68-2.89	2.60 (100% H2)		2.79 (100% NG)		2.68 (100% NG)	
Emissions from carbon and lime	$kgCO_2/t_{HM}$	77		73		53		
Specific total CO_2 emissions (100% H2 – 100% NG)	$kgCO_2/t_{DRI}$	84 - 635	124 - /		70 - 625	53 - /	39 - 435	

Table 7.1.: Validation of the present DRI-REF model prediction with the literature results.

8. Economic evaluation

Future steel production should be both economically and technically viable to be competitive. Besides the technical implementation and introduced KPIs, the economic evaluation is presented in this chapter. The economic evaluation of the modelled system can be done based on the modelling results after its technical implementation. This chapter puts forth the applied methodology for the economic evaluation of the implemented conceptual model.

The economic evaluation aims to help answer the main research question; the overall evaluation will be solved based on a series of sub-research questions. The economic evaluation will answer the following sub-research question.

Sub-RQ: *What is the levelized costs of the DRI-REF process in the NL for a given energy market condition?*

8.1. Economic KPIs

A discounted cash flow analysis is conducted to calculate the LCOP for the considered route. The LCOP is calculated using equations 8.1 and 8.2, adopted form Bhaskar et al.[5].

$$LCOP_{consideredroute} = \frac{(C_{Capex} * ACC) + C_{Opex} + C_{maint} + C_{labour} + C_{emission}}{m_{HM,a}} \tag{8.1}$$

Where the levelized cost of production ($LCOP$) is calculated based on the total capital investments and annuity factor (C_{Capex} and ACC), annual operational costs (C_{Opex}), maintenance ($C_{Maintenance}$), labour (C_{Labour}) and emissions costs ($C_{Emissions}$), respectively. These variables are explained in more detail in the sections below. The annuity factor is calculated using equations 8.2:

$$ACC = \frac{(r * (1+r)^n)}{((1+r)^n - 1)} \tag{8.2}$$

Where r refers to the discount rate and n represents the plant life. The considered literature in chapter 3 applying economic calculations use discount rates between 5 and 10%. This thesis will use a discount rate of 7.5% and a plant life of 20 years, which is widely reported in the literature considered [48]. The complete list of economic variables and assumed values are documented in table 6.4.

Based on the results of the modelling implementation presented in the previous chapter, the CO_2 mitigation cost (M_{cost}) in €/tCO_2 can be calculated for different hydrogen configurations, compared to the purely natural gas-based DRI-REF process. The CO_2 mitigation cost can be calculated using equation 8.3 [5; 22].

$$M_{Costs} = \frac{LCOP_{H_2route} - LCOP_{NGroute}}{EE_{NGroute} - EE_{H_2route}} \tag{8.3}$$

The numerator represents the difference in LCOP of the h_2 and DR(CH_4) modelled systems with similar assumptions. The LCOPs are calculated using equation 8.1. The EE_{route} represents the sum of direct and indirect emissions from the DR(H_2)-REF and DR(CH_4)-REF system and is calculated in tCO_2/t_{HM}.

8.2. Captial costs

To calculate the LCOP, the CAPEX of the DR(H_2)-REF system need to be approximated. The CAPEX comprises values for the electrolyser, DR shaft and the REF.

The electrolyser CAPEX is based on the estimation of an PEM in 2030. The reported specific investment costs are 0.585 €/kW installed capacity for both PEM and alkaline electrolyser technology [42]. The electrolyser installed capacity was calculated based on the hydrogen flow rate for each feed gas scenario and the corresponding efficiency. Only the electrolyser stacks are assumed to be replaced after 80000 h of operations. These stacks represent 60% of the system costs [5].

Economic data for the DRI is assumed from the literature, see table 6.4, whereas TSN provides the economic data for the REF process. Furthermore, it is assumed that capital expenses for the DRI and REF processes are equal for each considered hydrogen fraction in the feed gas. Table 8.1 summarises this thesis's capital costs assumptions and the literature's values.

Parameter	**Unit**	Value in this thesis	Values in literature	Reference
DRI capex	€/t_{DRI}	280	200-300	[5; 22; 65]
REF capex	€/t_{HM}	224		TSN
Discount rate	%	7.5	5-10	[5; 22; 65]
Plant life DRI & REF	Years	20	20	[5; 48]
Plant life Electrolyser	Years	10	10	[5; 65]
Electrolyser CAPEX	€/kW	700	585 - 1200	[5; 22; 42; 65]

Table 8.1.: Capital expenses assumptions applied in this thesis

8.3. Operational costs

Direct and indirect overhead costs must be considered to calculate the OPEX. The following section elaborates on each considered parameter for the operational costs. The parameters are summarised in table 8.2 with indicated cost ranges found in the literature.

8.3.1. Direct operational costs

The direct operational costs considered in this thesis include the procurement of base materials and commodities (electricity). The direct costs correlate directly with the output quantity of the modelled system. The considered raw materials and commodities are the following:

- Iron ore pellets
- Lime
- Anthracite (coal)
- Graphite electrodes (for the REF)
- Electricity
- Hydrogen production
- Natural gas
- Carbon emission tax

Iron ore pellets, lime, coal, and graphite electrodes are internationally traded commodities with fluctuating market prices. The costs of these commodities are assumed to be fixed over an entire year. The corresponding cost values are based on literature findings. For iron ore pellets, a cost of 100 €/t is assumed. For lime, a cost of 100 €/t is assumed. In the REF process, graphite electrodes are consumed at a determined rate indicated in section 6.4, costing approximately 4000 €/t.

The electricity costs are determined using the EMF v7.0 model described in section 6.1.1. The assumed natural gas price in the analysed literature dramatically differs from the current gas prices. In the last few years, major global events have affected gas and coal prices in Europe and the Netherlands. In 2022 in the EU, coal and gas prices have reached the highest levels in decades, as seen in figure 8.1. A large increase in gas prices contributes to an increase in coal usage for electricity generation and, consequently, increase the demand for carbon emission allowances.

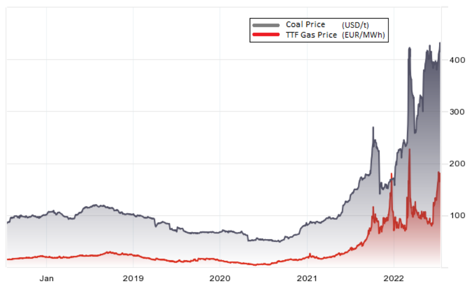


Figure 8.1.: Coal and gas prices. Own adaptation based on data from Source [61]

An important aspect to note is that the gas price strongly impacts the electricity price. In fact, according to a Q&A session with the

EU Commission Communication on Energy Prices, the impact of the gas price increase is nine times larger than the impact of the increase in carbon price [40]. Although the market is expected to calm down in the coming years [37], the price estimations remain structurally higher and more volatile than before. Based on multi-year contracts, the gas price is assumed to be or 20 €/GJ.

The last considered direct operational expenditure is the emissions price. Direct emissions from the modelled system are used to calculate the hourly emission costs and subsequently aggregated on a yearly basis. The price for CO_2 emissions has risen sharply in recent times, even before the gas price surge. For example, in mid-February 2021, this price was about 16.5 €/tCO_2; a year later, the price was about 95 €/ton. The market is currently very volatile, partly due to the Ukraine crisis, an increase in the use of coal and speculations.

Figure 8.2.: EU ETS prices. Own adaptation based on data from [60]

The tightening of the climate targets to a 55% CO_2 reduction by 2030 will further reduce the available CO_2 rights. Companies can buy, receive, or trade emission allowances as they see fit within the cap. However, price developments in the CO_2 market are challenging to predict. Insufficient rights can, for example, lead to very high (temporary) price peaks. In this thesis, a price of 110 €/tCO_2 is assumed for the year 2030 [38].

8.3.2. Indirect operational costs

The indirect overhead costs considered in this thesis are labour, operational, maintenance, and stack replacement costs for the electrolyser. Contrary to the direct operational costs, these indirect costs do not correlate with the output quantity of the system. Labour costs are included at 30 €/t_{HM}. Operational and Maintenance (O&M) costs are assumed to be a percentage of the CAPEX, commonly done in the analysed literature [5; 34]. The annual O&M costs for each component are 3% for the DRI process, REF [22] and 2% for the electrolysis plant [22] . The direct and indirect OPEX assumptions are presented in table 8.2.

Parameter	Unit	Value in this thesis	Values in literature	Reference
Pellets	€/t	100	84.18-122	[5; 34; 48; 65]
Lime	€/t	100	100-110	[22]
Added carbon	€/t	50	50.67 180	[22; 34]
Graphite electrodes	€/t electrodes	4000	4000 – 4503.52	[34; 65]
Natural gas price (2030)	€/GJ	20	(116.8 €/t)	[34]
Emission penalty (2030)	€/tCO_2	110	22.5 - 150	[22; 37]
Electricity price	€/MWh	varies	54 - 76.8	[34]
Labour cost	€/t_{HM}	30	20 - 53.2	[5; 34; 65]
DRI, REF O&M costs	% of CAPEX	3	1.5-3	[5; 34; 65]
Electrolyser O&M costs	% of CAPEX	2	2	[22]
Electrolyser efficiency	kWh/kgH_2	47.7 (calculated)	45 - 53	[5]
Stack replacement costs	€/kW	300	250 - 1250	[5; 34]
Stack lifetime	h	80.000	60.000 - 100.000	[5; 34; 65]

Table 8.2.: Direct and indirect OPEX parameter assumptions used in this thesis with literature values and references

9. Results

This chapter presents the results of the technical model and the economic evaluations, described in chapters 7 and 8, respectively. The results are mainly based on the different hydrogen volume scenarios in a predefined energy market, geographical location, and system of interest, with the hydrogen volume scenarios modelled on hourly bases. A holistic overview is provided where the results are initially aggregated on a yearly basis. Most of the results are obtained from the technical and economic KPIs defined in Sections 7.2 and 8.1. In order to evaluate the impact of the electricity price and the CO_2 grid intensity in more detail, the results are presented on an hourly basis for four distinct scenarios specifying the hydrogen to NG ratio for the reducing gas.

To provide clarity in this chapter, only four distinct hydrogen volume scenarios are presented on an hourly basis. The settings and properties of these scenarios are elaborated on in more detail in section 9.1.1. As explained in the research approach, the chosen co-feed boundary is based on the maximum operating conditions in the near future, 0vol% up to 80vol% H_2.

It is important to note that all the results of the hydrogen volume scenarios displayed in this chapter are primarily based on data sets from the EMF model v7.0 with one specific set of settings. These and future data sets are described in detail in chapter 6.1. Changing the settings of the EMF model would result in a change in both the electricity price and associated CO_2 emissions, which would lead to additional scenarios. Therefore, one specific data set is used to keep the results more focused and enable comparisons between the different scenarios. The effects of this choice and its limitations are discussed in chapter 10.

This chapter is structured in the following manner: first, the specific input parameters for each distinct scenario are discussed in section 9.1. Then, the first results, discussing the energy consumption of the system of interest, are described in section 9.2. After that, the emissions and economic modelling results are presented on yearly and hourly bases in sections 9.3 and 9.4, respectively. Next, section 9.5 compares the scenarios based on the CO_2 mitigation potential and costs. Lastly, section 9.6 elaborates on the flexibility analysis and results of changing the feed gas composition based on certain conditions.

9.1. Setup of input parameters

9.1.1. Hydrogen volume scenarios

The chosen hydrogen volume scenarios are primarily based on the envisioned technological transition at TSN. In 2030, the planned DRI-REF installations will begin to operate on natural gas to start the DR process. Therefore, the first scenario, the base case, will use 100% natural gas and 0% hydrogen. The two subsequent scenarios have an increment of 10% hydrogen volume in the co-feed of the feed gas, 10vol% and 20vol% H_2, respectively.

The fourth and last presented scenario is the current maximum hydrogen volume that is technically proven (80 vol% hydrogen – 20 vol% natural gas) [44]. This last scenario is currently not feasible in 2030 for numerous reasons, with the availability of electrolyser capacity, hydrogen costs and cheap electricity being the most prominent reasons. Nevertheless, this last scenario indicates the possible outcomes if TSN uses this hydrogen volume.

9.1.2. Scenario specific inputs

As discussed in chapter 5.5.2, several inputs have an indicated range depending on the hydrogen volume. Now that we have defined four specific scenarios, we can evaluate in more detail the used input parameters for each scenario, with the numerical values for the various inputs given in table 9.1.

The first set of specific inputs is related to the hydrogen demand and assumed electrolyser capacity. The hydrogen demand is based on the hydrogen volume in each scenario. The electrolyser capacity is linearly scaled based on this hydrogen demand. Anthracite, otherwise known as coal, is added to keep the carbon content of the output constant. The coal charge is increased as more hydrogen is added to the system. The lime charge on the other hand, is scaled linearly with the hydrogen volume. As explained in the conceptual modelling in section 5, the modelled gas heater is assumed to have the same hydrogen volume as the main scenario. To elaborate, in the scenario where 10vol% hydrogen is used for the reduction process, the heater will also use 10vol% hydrogen. The REF's electricity consumption depends on the added cold material in the process. These values are obtained from TSN and are presented in the table below.

Input name	**Unit**	**0vol% H_2**	**10vol% H_2**	**20vol% H_2**	**80vol% H_2**
Chemical energy demand	GJ/t_{DRI}	8.25	8.17	8.09	7.63
Thermal energy demand	GJ/t_{DRI}	1.70	1.70	1.70	1.70
Heater feed gas	$GJ\ H_2/t_{HM}$	0	0.17	0.34	1.36
Hydrogen demand	$kg\ H_2/t_{DRI}$	0	8.02	15.87	63.02
Electrolyser capacity	GW	0	0.2	0.4	1.7
Anthracite (coal) charge	t_{carbon}/t_{HM}	0	0.0092	0.0182	0.0673
Lime charge	t_{lime}/t_{HM}	0.0703	0.0710	0.0717	0.0757
REF electricity demand	KWh/t_{HM}	635	647	659	731

Table 9.1.: Summary of specific input parameters used for each specific hydrogen volume scenario

9.2. Energy consumption

The first result category is the energy consumption of the system of interest. The energy consumption of the DRI process (100vol% NG and 100vol% H_2) is validated by comparing its value with literature papers with similar configurations (see chapter 7.4). The energy consumption for the whole system of interest with the various hydrogen volumes is presented in this section.

Chapter 7.2 discussed the technical KPIs where the SEC is presented first. This KPI sets the basis for all the other results. Therefore, this metric must be understood to understand all the results fully. First, a stacked area graph is presented in figure 9.1, where the hydrogen volume scenarios are set out against the SEC [MWh/t_{HM}]. Second, a table summarizing all the values of the SEC breakdown is presented in table 9.2.

The energy consumption is specified for the six energy demand sources, as seen in figure 9.1. On the x-axis the hydrogen volumes are indicated with a fraction number ranging from 0 to 0.8. '0' means 0vol% hydrogen configuration, and '0.8' means 80vol% hydrogen in the system of interest. On the y-axis, the SEC expressed in MWh/t_{HM} is shown. The chemical, thermal and electrical energy consumption values are converted to MWh/t_{HM} to add them up. The energy demand breakdown contains the following sources: Electricity consumption of the DRI and REF processes, natural gas consumption of the DRI reduction and heater processes, hydrogen consumption of the DRI reduction and heater processes, and, to conclude, additional electricity consumption for the hydrogen production due to efficiency losses.

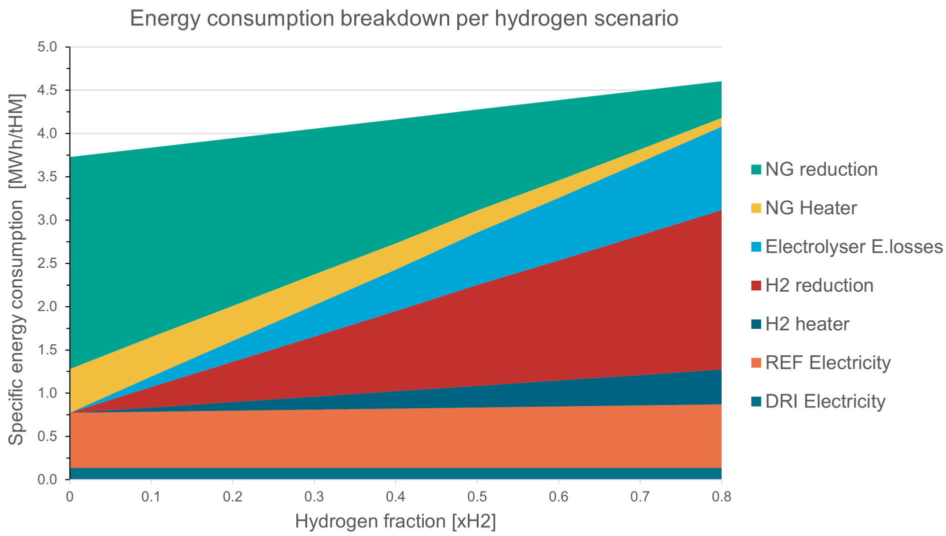


Figure 9.1.: Energy consumption per type of demand source per hydrogen volume scenario

The results indicate that the energy consumption increases by 0.9 MWh/t_{HM} (+20.9%) when the maximum percentage of hydrogen is introduced in the system of interest compared to

0vol% hydrogen. The primary reason for this is the energy loss of the electrolysis process, even though the chemical energy demand slightly decreases. The base case has an electricity consumption of 0.78 MWhe/t_{HM} with a linear increase to 3.67 MWhe/t_{HM} for the 80vol%H_2 scenario. The electricity consumption in the base case is dominated by the electricity consumption of the REF process. The increase in electricity demand is due to the choice of including an electrolyser within the system boundaries. Excluding the electrolyser from the system boundaries would change the results significantly, as in this case, hydrogen will be imported and used for chemical or thermal energy. Furthermore, natural gas consumption decreases as more hydrogen is introduced. Therefore, the energy consumption in the 80vol%H_2 scenario is mainly based on hydrogen and electricity consumption. This shift in energy sources can have implications in various ways on the CO_2 emissions and economics of the modelled system of interest. The following sections present and discuss these effects.

Input name	**Unit**	**0vol% H_2**	**10vol% H_2**	**20vol% H_2**	**80vol% H_2**
Electrolyser electricity losses	MWh/t_{HM}	0,00	0,12	0,24	0,96
DRI Electricity		0,14	0,14	0,14	0,14
NG reduction		2,45	2,19	1,94	0,42
H_2 reduction		0,00	0,24	0,47	1,84
NG Heater		0,50	0,45	0,40	0,10
H_2 heater		0,00	0,05	0,10	0,40
REF electricity		0,64	0,65	0,66	0,73
Total energy consumption		**3,73**	**3,84**	**3,95**	**4,60**

Table 9.2.: Summary of the yearly aggregated energy consumption sources for four different scenarios

9.3. Emissions

Similar to the energy consumption section, the hourly results for the CO_2 emissions are aggregated on a yearly basis for each hydrogen volume scenario. This is shown in figure 9.2, where the y-axis is now changed to emissions per ton hot metal output, expressed in tCO_2/t_{HM}. Again, the x-axis remains the same, with the fraction of hydrogen increasing from 0vol% up to 80vol%.

Based on the energy and materials consumption sources during the production process, we can determine the total emissions of the system of interest. The different emissions sources are seen in the legend in figure 9.2, divided into material CO_2 emissions (Electrode, Lime, Anthracite (coal)), electricity CO_2 emissions (DRI, REF and Electrolyser), and lastly, natural gas CO_2 emissions. The electricity emissions are part of the indirect emissions (scope 2). To clarify, the emissions from the electricity production are not from Tata Steel, as TSN only consumes electricity and does not produce electricity, as indicated in the contextual information chapter. Therefore, the presented results will distinguish between direct and indirect emissions.

Before the results of figure 9.2 are discussed in detail, the key parameters and assumptions must be clarified again, as they fully shape the results. First, the electrolyzer efficiency has

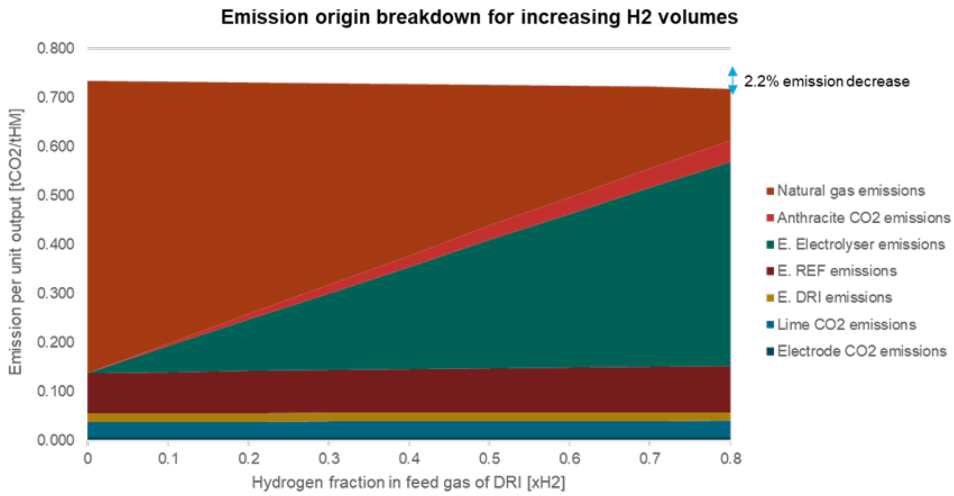


Figure 9.2.: Average emissions for various hydrogen fractions for the modelled DRI-REF process in 2030

an assumed energy consumption rate of 47.6 kWh/kgH_2. Natural gas has an emissions intensity of 56.1 kgCO_2/GJ, which TSN provides. Lastly, electricity has an emissions intensity of approximately 0.13 tCO_2/MWh, which results from averaging the hourly electricity emissions from the EMF model, as documented in chapter 6.1.2. It should be noted that changing these parameters and assumptions will change the emissions results significantly, so the conclusion can be different. The electrolyzer efficiency and the emission intensity of natural gas will remain constant in this thesis to reduce the number of variables. However, the electricity emission intensity varies over time, as previously explained. The effect on the CO_2 emissions of the hot metal is further explained below.

The main changes in emissions sources can be seen in figure 9.2. As the volume of natural gas decreases for increasing hydrogen volumes, we see a decrease in the associated CO_2 emissions (-82.8% decrease in NG emissions). However, since more electricity is used for hydrogen production, the indirect electricity emissions also increase (+429% indirect emissions increase). Additionally, a slight increase in Anthracite (coal) emissions is observed to compensate for the increase in hydrogen volumes and to keep the carbon fraction constant in the HM at around 4-4.5 wt%. Substituting natural gas with hydrogen barely (-2.2%) decreases the total CO_2 emissions under the assumed conditions. This is because the emission intensity of the electricity is still relatively high compared to a 100% renewable electricity generation mix, as is often assumed in the analyzed literature (see chapter 3). The determined yearly average of the electricity emission intensity factor is approximately at the breakeven point in 2030, as no significant decrease in direct and indirect emissions is observed. A sensitivity analysis is performed and documented in chapter 10.2.2 to illustrate the effect of changing the average electricity CO_2 intensity factor on the total direct and indirect emissions. Table 9.3 summarizes the values with the different H_2 volume percentages.

	Unit	0vol% H_2	80vol% H_2
Total emission	tCO_2 / t_{HM}	0.735 (100%)	0.719 (100%)
Direct emissions		0.635 (86.4%)	0.190 (26.4%)
Material emission		0.038 (5.2%)	0.084 (11.7%)
Natural gas emission		0.495 (67.3%)	0.085 (11.9%)
Electricity emissions		0.100 (13.6%)	0.529 (73.6%)

Table 9.3.: Summary of the CO_2 emissions source for the base case and 80vol%H_2 scenario.

9.3.1. Hourly emission results

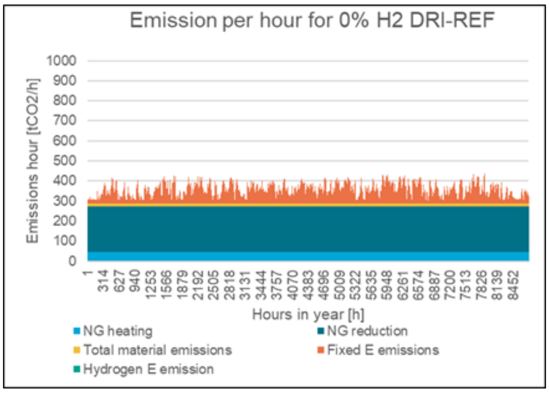
The following sub-section will present the hourly results for the emission modelling. Figure 9.3 (a-d) illustrate the total emissions on an hourly basis for an entire year. On the x-axis, we can see the 8760 hours in a year and on the y-axis, the emissions per ton hot metal output, expressed in tCO_2/t_{HM}, are indicated. The four distinct hydrogen volume scenarios are presented, as explained in section 9.1.1.

The electricity emissions have a specific variation over an entire year, as seen from the four scenarios in figure 9.3. As the hydrogen volume increases, so does the variation in total emissions. Especially the CO_2 emissions associated with the electricity consumption for the electrolyser show increasing fluctuations. This leads to the conclusion that the H_2-based DRI-REF system is sensitive to electricity emissions intensity factor, comparable to the DRI-EAF system discussed in the analysed literature. Lastly, the H_2-based process has higher indirect emissions in several hours of the year than the purely natural gas-driven system.

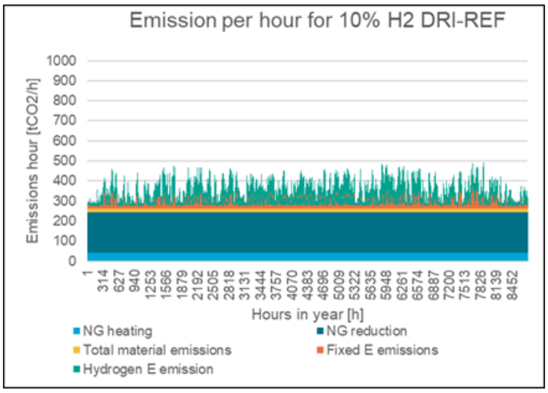
The hourly results of the four hydrogen volume scenarios are interpreted with the help of two statistical graphs, the histogram and the boxplot. For example, Figures 9.4a and 9.4b presents two of the four scenarios, the scenario with 0 vol% and the one with 80 vol% hydrogen, in the histogram format. On the x-axis, the CO_2 emissions are expressed in tCO_2/t_{HM} and on the y-axis, the frequency is expressed in how many times a certain level of emissions has appeared for an entire year. The column widths represent a 0.005 tCO_2 incremental step. The highlighted grey areas in both figures indicate the emission range of the (conventional) DR(CH_4)-EAF route (0.6-1.2 tCO_2/t_{HM}) and the current coal-based BF-BOF route (1.7-1.9 tCO_2/t_{HM}) [34; 44; 49]. The large emission range in the DR(CH_4)-EAF route originate from the different technological principals and operational efficiency between company and countries.

There are a few observations from the hourly figures and histogram graphs. The first aspect that strikes from the histogram figures is that in both scenarios there is a bulk in emissions frequencies, centred on the left-hand side of the histograms. This bulk in frequency can be interpreted as the moment when the electricity mix is (almost) wholly covered by renewable energies (solar/wind). This can be seen in figure 6.3, where the weekly results of the EMF model are illustrated. As observed, at the end of the week, the electricity demand is fully covered by renewable energies, mostly from offshore wind. This 'bulk' (highest frequencies) shifts to the left in a and b, which can be interpreted as decreasing percentages of renewable energy generation in the electricity mix. This shift of hot metal CO_2 emissions towards the higher emitting moments is more pronounced as more hydrogen is introduced to the system because of increasing electricity demand, as explained in section 9.2.

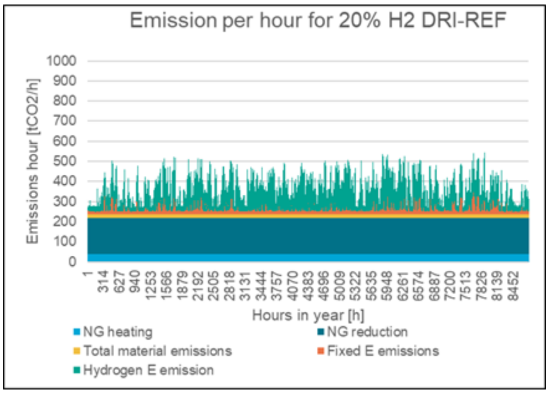
A second aspect observed in figure 9.4 is the increase in the spread between the lowest and highest emitting moments as more hydrogen is introduced to the system of interest. This



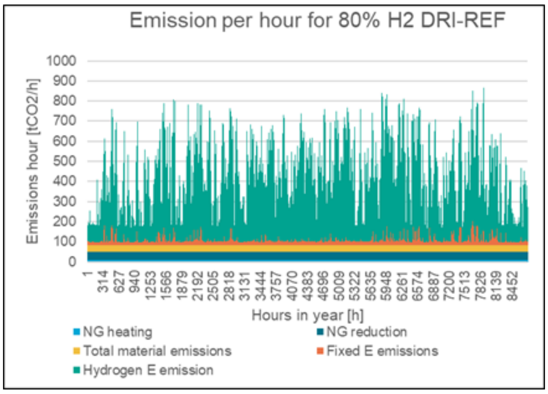
(a) 0% H_2 Scenario



(b) 10% H_2 Scenario



(c) 20% H_2 Scenario



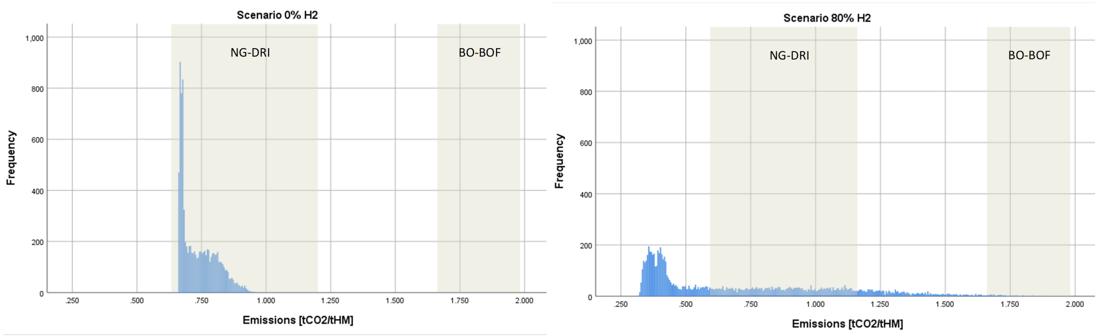
(d) 80% H_2 Scenario

Figure 9.3.: Four distinct H_2 scenarios were the electricity CO_2 emissions intensity varies over time

developed is seen in scenarios with increasing hydrogen volumes because the electricity consumption becomes a large part of the total systems energy consumption. From figure 9.2 and 9.4, we can conclude that the improvements in emissions towards the lower-emitting zones are almost entirely negated (-2.2%) by the increase in emissions towards the higher-emitting zones.

In the most extreme cases ($\geq$1.65 tCO_2/t_{HM}), the emissions from the 80vol% hydrogen scenario match the emissions of the BF-BOF coal-based production process. This is happening in approximately 88 hours over an entire year. On the other hand, the scenario with 0%H_2 does not reach this level of CO_2 emission due to the limited electricity consumption. Section 9.6 will analyse and elaborate on the possible flexibility options by switching between NG and H_2 use in the DRI-REF system, analysing the hybrid (NG/H_2) operational case.

The boxplot (figure 9.5) summarises the histograms and the hourly emissions figures. In general, we observe an increase in emissions in higher end as well as a decrease in the lower end with increasing hydrogen volumes. The average decreases by 2.2% from the base case based on 100%NG to the 80vol% H_2 scenario. In table 9.4 the numerical values of the boxplot are presented. The interquartile range is 0.112, 0.173, 0.232 and 0.591 tCO_2/t_{HM} for the scenario 0%H_2, 10%H_2, 20%H_2 and 80%H_2 respectively. Additionally, the 25th per-



(a) 0% H_2 Scenario

(b) 80% H_2 Scenario

Figure 9.4.: Two H_2 scenarios were the electricity CO_2 emissions intensity varies over time

centile decreases from 0.675 to 0.399 for the increasing hydrogen volumes. On the other hand, the 75th percentile increases from 0.787 to 0.990 tCO_2/t_{HM}. The developments in the interquartile range confirm that increasing electricity consumption, due to the energy source replacement by hydrogen, strongly increase the spread of CO_2 emissions over the course of an entire year. Section 9.5 will discuss the last technical KPI and compare the (specific) CO_2 mitigation potential of the different scenarios.

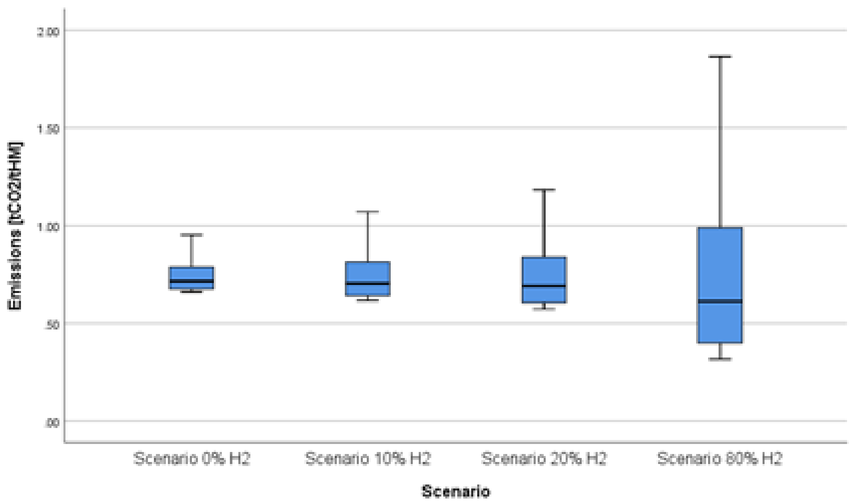


Figure 9.5.: Hourly CO_2 emissions per ton hot metal grouped in their respective hydrogen volume scenario.

Statistical results of the boxplot hydrogen scenarios					
		0% H_2	**10% H_2**	**20% H_2**	**(80% H_2)**
N	Hours in year	8760	8760	8760	8760
Mean (tCO_2/t_{HM})		.735	.734	.732	.719
Std. Deviation		.068	.105	.141	.359
Minimum emission (tCO_2/t_{HM})		.659	.616	.573	.316
Maximum emission (tCO_2/t_{HM})		.958	1.077	1.194	1.892
Percentiles	25%	.675	.640	.606	.399
	50% (Median)	.715	.702	.690	.612
(tCO_2/t_{HM})	75%	.787	.813	.838	.990

Table 9.4.: Summary of the boxplot figure 9.5 values on the hourly CO_2 emission per scenario

9.4. Economics

With the energy consumption and emissions modelling results, the economic performance can be determined. The methodology for calculating the LCOP is explained in chapter 8 and the determination of the electricity price is documented in chapter 6.1.1. Identical to the sections above, the hourly costs are aggregated on a yearly basis for the different hydrogen fraction scenarios. Several key parameters and assumptions must be highlighted to fully understand the economic modelling results.

First, the installed electrolyser capacity is assumed to scale with the hydrogen demand, as explained in chapters 8.2 and 9.1.2. The increase in capital costs is a direct result of an increase in electrolyser capacity. Second, the assumed natural gas price is 20 €/GJ (2030), and the CO_2 price is assumed to be 110 €/tCO_2. Changing these parameters has a direct and indirect effect on cost calculations. Third, the average yearly electricity price assumed for the 2030 scenario is 97 €/MWh and a direct result of the EMF v7.0 modelling, explained in detail in chapter 6.1.1. A sensitivity analysis is performed in section 10.2 to demonstrate the effect of this parameter on the LCOP.

The LCOP are split into several categories as can be seen in the legend of figure 9.6. The CAPEX comprises of the annuities of the DRI, REF and electrolyser facilities. The indirect OPEX are the O&M and labour costs whereas the direct OPEX is based on the emissions, other materials, electricity, and natural gas costs.

The most notable results of the costs modelling are the increase in electricity costs of 320 €/t_{HM} (Δ+426%) and the decrease in natural gas costs of 175 €/t_{HM} (Δ-82%) as the hydrogen volume increases to 80vol%. The primary reason for this development is the substitution of natural gas for hydrogen demand. Furthermore, due to the decrease in natural gas consumption, so does the decrease in the emissions produced by TSN onsite. This decrease in direct emissions results in a 49 €/t_{HM} (Δ-71%) reduction in emissions tax, amounting to 195mil€ mitigated on a yearly basis. Furthermore, the capital investment increased by approximately 53 €/t_{HM} (Δ+202%) due to the increase in electrolyser capacity. Lastly, the total LCOP increases by 209 €/t_{HM} (+34.9%). The most important results are summarised in table 9.5.

The LCOP composition will change significantly with increasing hydrogen volumes in 2030. For the base case, natural gas costs and other material costs dominate the LCOP, as indicated in table 8.2. Other material costs, O&M costs and labour costs remain approximately the same

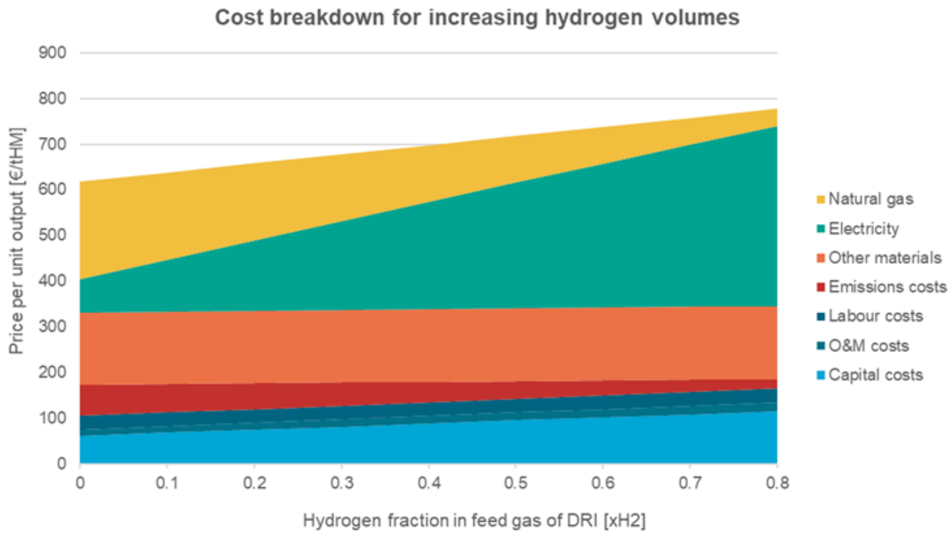


Figure 9.6.: Average LCOP for various hydrogen fractions for the modelled DRI-REF process in 2030

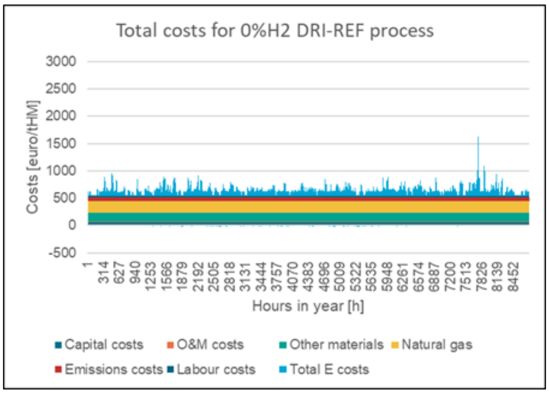
	Unit	0vol% H_2	80vol% H_2
Total LCOP	€/t_{HM}	598 (100%)	807 (100%)
Natural gas		213 (35.6%)	38 (4.7%)
Electricity		75 (12.5%)	395 (48.9%)
Other material		156 (26.1%)	178 (22.0%)
Emissions tax		69 (11.5%)	20 (2.5%)
Capital costs		42 (7.0%)	127 (15.7%)

Table 9.5.: Summary of the CO_2 emissions source for the base case and 80vol%H_2 scenario

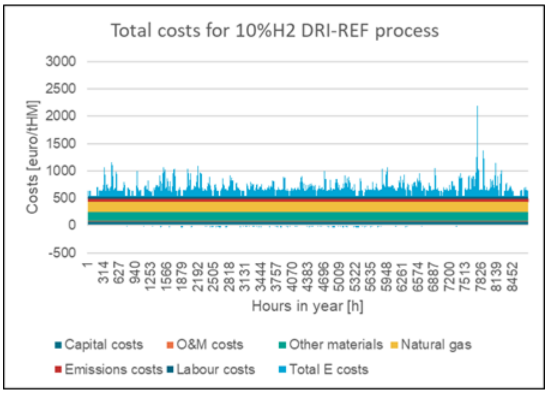
for all scenarios. The other material costs consist mainly of the DR pellet (iron ore) costs. On the other hand, the 80vol% H_2 scenario is mainly dominated by the electricity costs, other material costs and the annuity of the electrolyser. According to Jacobasch et al.[34], there is a difference in the annuity for different electrolyser technologies, and the difference in technological maturity can explain this. Therefore, the different electrolyser technologies can influence the presented proportions in table 9.5, but not in a significant manner so that the interpretation of the result changes. This is because the LCOP of the different electrolyser technologies is expected to converge in the coming decades[34]. Furthermore, the hydrogen costs differ per electrolyser technology since they directly depend on electrolyser efficiency. In sum, the economic evaluation results suggest that the DR(CH_4)-REF route in 2030 under the assumed energy market circumstances has the lowest LCOP of 598 €/t_{HM}.

9.4.1. Hourly costs breakdown for different various hydrogen volumes

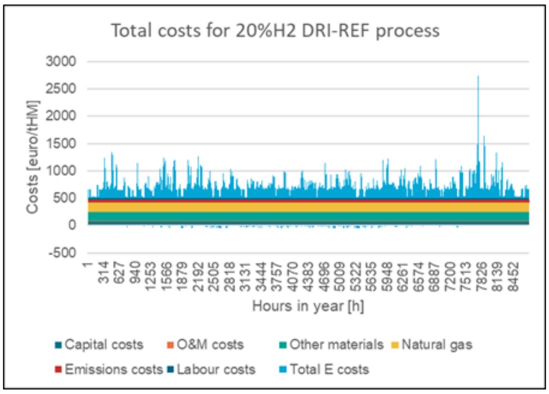
Similar to the documentation of sub-section 9.3.1, the hourly production costs are plotted over a full year for four different hydrogen volume scenarios. As discussed in the conceptual modelling, it was chosen to limit the parameters that change over an entire year. The electricity price and associated emissions are the only parameters that change on an hourly basis during a specific scenario. The hourly results can be seen in figure 9.7 for four different scenarios.



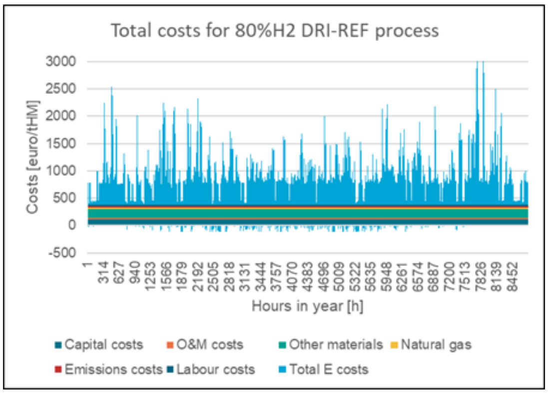
(a) 0% H_2 Scenario



(b) 10% H_2 Scenario



(c) 20% H_2 Scenario



(d) 80% H_2 Scenario

Figure 9.7.: Four distinct H_2 scenarios were the electricity price varies over time

The electricity price is the only parameter that fluctuates on an hourly basis during the entire year. The other parameters such as the CAPEX, indirect OPEX and natural gas costs are constant on a hourly basis but are different per specified scenario. The changes of these parameters are already explained in section 9.1.2.

The effect of increasing the hydrogen volume on the LCOP can clearly be seen from the hourly results. The hourly variability increases significantly, resulting in a multiplication of LCOP can be observed on certain hours, as shown in figure 9.7d. However, the contrary can also be observed in moments where the electricity price is low or even negative. Although the yearly aggregated data would suggest that a full natural gas-based process would be the most cost-efficient, there are some cases throughout the year where the electricity price is below the breakeven point. This breakeven point is determined by a sensitivity analysis documented in chapter 10.2. The effect of alternating between NG and H_2 is further documented in the flexibility analysis in section 9.6.

Figure 9.8 presents a boxplot where all the data is visually summarized and table 9.6 provides the numerical values.

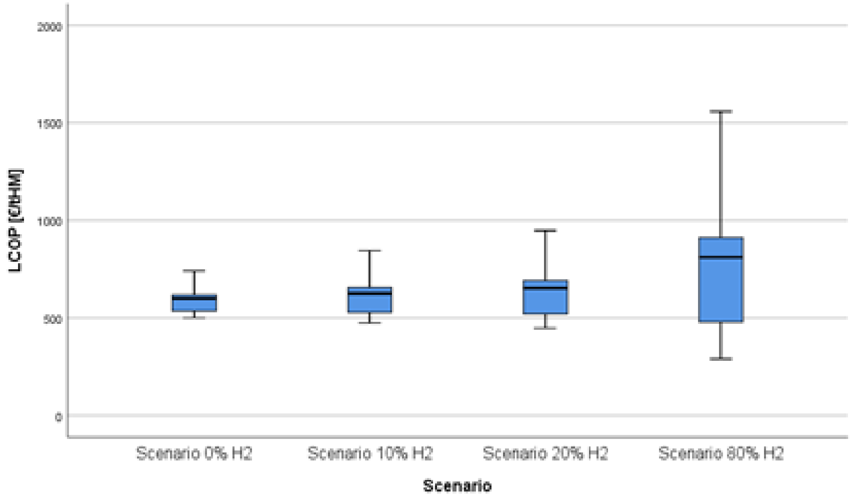


Figure 9.8.: Hourly costs calculation per ton hot metal grouped in their respective hydrogen volume scenario.

Statistical results of the boxplot					
		0% H_2	**10% H_2**	**20% H_2**	**80% H_2**
N	Hours in year	8760	8760	8760	8760
Mean (€/t_{HM})		598	625	651	807
Std. Deviation		70	107	144	367
Minimum costs (€/t_{HM})		500	474	447	290
Maximum costs (€/t_{HM})		1605	2179	2742	6120
Percentiles (€/t_{HM})	25%	536	529	522	479
	50%	599	626	653	811
	75%	618	655	692	911

Table 9.6.: Summary of the boxplot figure 9.8 values on the hourly CO_2 emission per scenario

The interquartile range of the LCOP is 82, 126, 170 and 432 €/t_{HM} for the 0%H_2, 10%H_2, 20%H_2, and 80%H_2 scenarios, respectively. Comparable to the emissions results, the 25th percentiles decreases and the 75th percentiles increase for increasing hydrogen volumes. Although the mean increases from 598 to 807 €/t_{HM}, there are more number of cheaper hours for the 80%H_2 scenario than for the 0%H_2 scenario. This increase in spread could potentially be beneficial to decrease costs. How alternating between NG and H_2 in the feed gas affects the total LCOP is further discussed in section 9.6.

Now that the emissions and the LCOP for the base case (100vol% NG) and the 80vol% H_2 scenario are determined, the CO_2 mitigation potential and cost can be calculated. The following section will compare the four scenarios based on the last KPIs.

9.5. Scenario comparison

To contextualise the results presented in sections 9.3 and 9.4, the CO_2 emission mitigation potential, ϕCO_2, and emission mitigation cost, M_{costs}, are used to evaluate the performance. These two KPIs are introduced in sections 7.2 and 8.1. To enable comparison with literature findings, it is chosen to use a 100%H_2 scenario for further comparisons. The 100%H_2-DRI-REF route is compared to the 100%NG-DRI-REF route and the current coal-based BF-BOF route. Additionally, the 100%NG-DRI-REF route is compared with the BF-BOF route. These mentioned comparisons are performed with the direct emissions and with the total emissions, thus including the indirect electrical emissions. This provides insights into the performance of the system of interest for TSN and the effective performance from a national viewpoint.

Figure 9.9 presents the (specific) CO_2 emission mitigation potential of the various production routes. In the case of 100%NG and 100% H_2, the specific CO_2 mitigation potential amounts to ϕCO_2 = 0.62 and 0.95, respectively, while the CO_2-intensive BF-BOF route is assumed to emit 1.65 tCO_2 /t_{HM} [34; 44]. This corresponds with a reduction of 1.02 and 1.57 tCO_2/t_{HM}, respectively. The specific ϕCO_2 of the comparison between 100% H_2 to the 100% NG route amounts to ϕCO_2= 0.87, which results in a reduction of 0.55 tCO_2/t_{HM}. These results are promising because it would mean that most of the CO_2 emissions are reduced when TSN is transitioning from the coal-based BF-BOF route to the intermediate NG-DRI-REF route to the final H_2-DRI-REF route. Especially the hydrogen-based production process has the potential to emit very low quantities of CO_2. These results are compared with findings from the literature in chapter 10 to substantiate the results in this thesis.

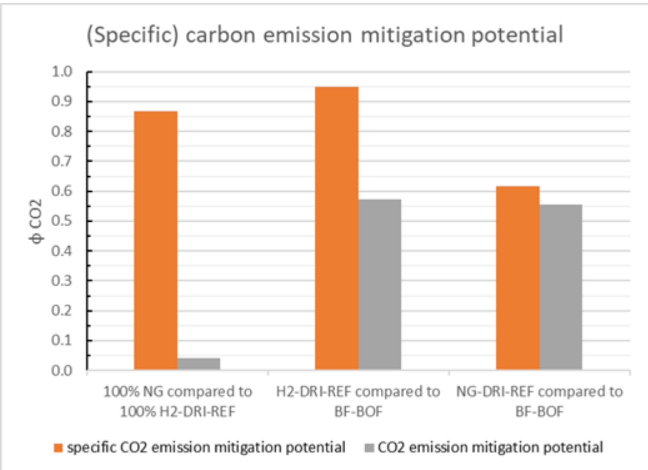


Figure 9.9.: (Specific) CO_2 emissions mitigation potential compared to the BF-BOF process and the DR(CH4)-REF process.

However, calculating the CO_2 mitigation potential for the total emissions leads to vastly different results. In the case of 100%NG and 100% H_2 process, the CO_2 mitigation potential amounts to ϕCO_2 = 0.55 and 0.57 compared to the BF-BOF route. This corresponds with a reduction of 0.91 and 0.94 tCO_2/t_{HM}, respectively. The calculated ϕCO_2 are almost equal, meaning that both production routes would decrease the total emissions by the same amount under the assumed energy market conditions in this thesis. These results can also be seen from the emissions modelling results in section 9.3.

The total ϕCO_2 of the comparison between the 100% H_2 and the 100% NG route would result in ϕCO_2= 0.04, which gives a reduction of 0.03 tCO_2/t_{HM}. This decrease in CO_2 mitigation potential, from 0.87 to 0.04, between the NG and H_2-based process is worrying. This indicates that the CO_2 emissions benefits of using hydrogen by 2030 under the assumed energy market conditions are almost negated by the CO_2 emissions originating from the electricity mix.

The CO_2 emissions mitigation costs (M_{costs}), otherwise known as the carbon abatement costs are used to determine the economic performance of the various routes. First, the 100% H_2 route is compared to the 100%NG and coal-based BF-BOF routes. Lastly, the 100%NG route is compared to the BF-BOF route. Then, the M_{costs} is calculated using equation 8.3 introduced in chapter 8.1, and the results are presented in figure 9.10. For the BF-BOF route, a LCOP of 450 €/t_{HM} is assumed as the literature indicates that it could vary between 400-500 €/t_{HM} [5].

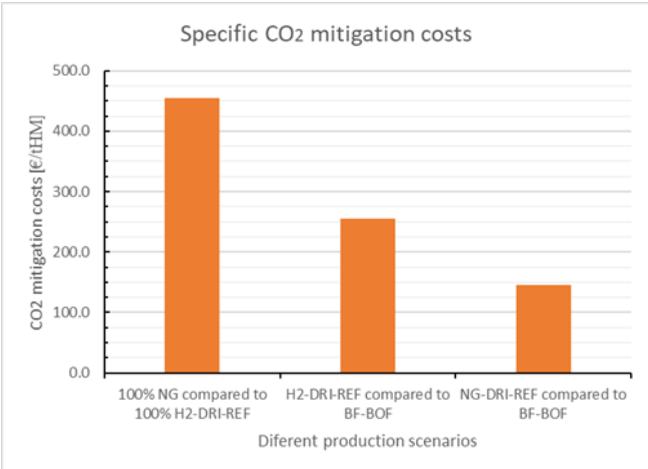


Figure 9.10.: Specific CO_2 mitigation costs of different process compared to the BF-BOF and the DR(H_2)-REF route.

The NG-DRI-REF route would result in 1.02tCO_2/t_{HM} avoided at the cost of M_{costs} = 146 €/tCO_2. However, the long-term goal should be achieving the maximum possible CO_2 abatement. This would require the currently developed direct reduction process using only hydrogen produced using the electrolysis process. According to the results of this study, transitioning from the 100%NG to the 100%H_2-based route would reduce the direct emissions by 0.55 tCO_2/t_{HM} at the cost of 455 €/tCO_2. This high price is mainly attributed to the assumed average electricity price of 97 €/MWh, which is considerably higher than the assumptions made in the analysed literature. Chapter 10 provides a discussion and compares the results with the analysed literature.

9.6. Flexibility analysis

This section will present the results of the flexibility analysis, which is different from a sensitivity analysis in the sense that the analysis must adhere to certain restrictions. The flexibility of the system is based on the possible change in the co-feed composition of the reducing gas. This means that natural gas is replaced by hydrogen and vice versa to optimise costs and generate the least CO_2 emissions. The system's requirement to switch from feed gas composition constrains the moments where this switch can occur, thus requiring a separate flexibility analysis.

The hydrogen and natural gas feed gas can be interchanged based on specific requirements, which are explained now. For the emissions modelling, the average yearly emissions of the electricity mix have been determined and set at 0.13 $tCO_2/MWhe$. We have observed that this value is approximately the breakeven point of the emissions of the hot metal, as seen in figure 9.2. Therefore, this average value is used as a target for determining whether to use H_2 or NG. The consecutively hours below or above this target are sorted in their respective categories, seen in table 9.7. The categories are the counts of the consecutively hours under 12 h, between 12 h and 24 h, 24 h and 48 h and finally, all the moments when the associate electricity mix emissions are 48 h or more above or below the predetermined target. The same methodology is applied to the electricity price, where the breakeven point is determined to be 32 €/MWh. This breakeven is illustrated in the sensitivity analyse in chapter 10.2. Furthermore, the total amount of hours within the categories are listed. The results are presented in table 9.7 and are elaborated below.

Times above target - Duration	**<12h**	**12h<24h**	**24h<48h**	**>48h**
Emission counts above 0.13 $tCO_2/MWhe$ [-]	145	125	19	6
Price counts above 32 €/MWhe [-]	50	121	36	25
Emissions hours above target [h]	795	1927	661	394
Price hours above target [h]	260	2267	1246	2471
Times under target - Duration	**<12h**	**12h<24h**	**24h<48h**	**>48h**
Emission counts under 0.13 $tCO_2/MWhe$ [-]	163	84	29	20
Price counts under 32 €/MWhe [-]	181	23	19	10
Emissions hours under target [h]	931	1232	974	1845
Price hours under target [h]	742	369	624	780

Table 9.7.: Results of the quantity and duration of hours within a category that electricity price and associated CO_2 emissions are under a predetermined target.

The results of table 9.7 can be interpreted in the following manner. There are 145 moments throughout the year where the associated electricity mix emissions are less than 12 h consecutively above the predetermined target of 0.13 tCO_2/MWh with an average of 5.5 hours. There are in total 795 h in the year where this condition is met. The same can be said for the electricity price, where 50 moments are identified where the electricity price is less than 12 h consecutively above the target of 32 €/MWh.

Ideally, the changeability between NG and H_2 happens within the hour. However, in practice, this is not the case. The exact values for the ramp-up of hydrogen volume are not known or regarded as sensitive information. The work of Toktarova et al.[59] has taken a ramp up and ramp down of 12 h for the DRI process operating on full hydrogen. This thesis is assuming a 24 h duration for the complete switch from 100% natural gas towards 80vol% hydrogen and vice versa. Due to time constraints, only the full NG or 80vol% H_2 scenario are considered. No intermediate process configurations are considered. This constraint is applied to the flexibility analysis, which results in the following:

A DRI-REF process that can switch between H_2 and NG with the above-mentioned constraints could decrease its direct and indirect CO_2 emissions to 0.701-0.686 tCO_2/t_{HM}. This is lower than the emissions of a 100%NG-DRI-REF process with 0.735 tCO_2/t_{HM} and that of the 80vol% H_2-DRI-REF process with 0.719 tCO_2/t_{HM} (indirect emissions included). Using the interchangeability of the feed gasses could decrease the emissions up to 0.05 tCO_2/t_{HM} (6.5% decrease). In the ideal scenario where the feed gasses can be changed instantly, a CO_2 emission of 0.601 tCO_2/t_{HM} is calculated. Future research could apply an optimisation algorithm with intermediate feed gas compositions to determine a more precise decrease in CO_2 emissions of the system of interest. However, electricity with no associated CO_2 emissions can decrease emissions to 0.190 tCO_2/t_{HM} (80vol% hydrogen), which is significantly lower than the optimised feed gas process.

Switching between NG and H_2 based on the electricity price breakeven point results in a production price between 590-697 €/t_{HM} calculated with the above-mentioned constraints. The LCOP for the 100%NG-DRI-REF process is determined in section 9.4 and set at 598 €/t_{HM}. The 80vol% DR(H_2)-REF process has a LCOP of 807 €/t_{HM}. With instantly changing feed gasses an idealistic LCOP of 570 €/t_{HM} is calculated under the electricity market condition and process characteristics applied in this thesis. We can observe that the calculated LCOP of the 100%NG process is close to the lower end of the optimisation range. This indicates that using H_2 is more expensive for the large majority of hours in the year. Comparable to the emissions flexibility analysis, future research could apply an optimisation algorithm with intermediate feed gas compositions to determine a more precise decrease in LCOP of the system of interest. Also, if the EU ETS price increases, there will come a point where H_2 becomes more interesting - considering the relationship with the electricity price, which is also partly determined by the EU ETS prices (and NG price).

10. Discussion

This chapter summarises and discusses the research findings. These findings are based on the overall research project as the modelling part. After this, this research project's model and dataset validation is discussed, particularly the methodology and data use.

This research project carried out several research activities. At the project's core, the modelling and simulation methodology is used to explore and evaluate the performance of hydrogen in an ironmaking process within a predefined electricity market mix. Additionally, a literature review is conducted as well as background knowledge of the Dutch energy market developments towards 2030 and the envisioned technological transition of TSN. In the following two subsections, the general research findings and the findings based on the model are summarised.

10.1. General research findings

The problem that this thesis is trying to solve is currently ongoing in many energy-intensive industries worldwide, especially the iron & steel industry, which must decarbonise their production processes within a specific timeframe. This problem is presented in the introduction with the following findings: The energy demand, particularly the renewable energy, of the I&S industry is so high that our current (Dutch) energy system is not suitable for a complete transition towards sustainable steelmaking. Furthermore, incremental changes in performance gain within the current steelmaking techniques would not reach the CO_2 emissions reduction goals fast enough. However, recent technological development does suggest that the I&S industry can decarbonise within the time frame specified by the Paris Agreement. However, the performance of these technological development depends mainly on the national energy system developments.

Choosing the TSN case study is no surprise, as this company is the largest I&S producer in the Netherlands and emits 6.5% of the national CO_2 emissions. Furthermore, TSN is a prime example of a company that has recently decided to use the carbon avoidance route to transition from the conventional coals-based BF-BOF production process towards a hydrogen-based production process based on electrolysis. However, a direct transition towards hydrogen-based production is not feasible yet as this process is not yet fully developed, and the required hydrogen quantities are not available or price competitive. Therefore, the natural gas-based ironmaking process will act as an intermediate process in the near future. Furthermore, TSN case is unique as the chosen technical configuration is different from the major steelmaking route, illustrated in figure 5.1.

The energy market developments in the Netherlands, documented in section 2.3, provide a clear overview of the renewable energy capacity developments up to 2030. In 2020 the offshore wind capacity amounted to 2.5 GW, with the desire to grow to 21 GW in 2030 [43]. Although large quantities of offshore wind and solar generation are being built, a flexible electricity generation capacity is still needed based on natural gas (14.5 GW in 2030) [58]. This result in increasing fluctuations in electricity price, but also in the associated CO_2 emissions. It is estimated that the electricity mix will decrease its emission from 0.328 [21] to approximately 0.130 tCO_2/MWh in 2030 with the IPKA0 scenario and to 0.96 tCO_2/MWh if the total 21 GW offshore wind capacity is installed, which is still considerably higher than the conservative assumptions made in the literature papers. The implication of these findings suggests that, if only using electricity from the electricity mix, there will still be considerable indirect CO2 emissions (scope 2) by the year 2030 and onwards. Companies such as the recent start-up H2 Green Steel or the test facility of SSAB located in countries with a natural landscape (e.g. North Sweden) that can facilitate hydropower have an advantage when producing 'green'-steel with hydrogen due to the availability of constant and abundant renewable electricity [5; 34; 44]

Additionally, the electricity procurement methods are expected to change from the current 12-month valid GoO to a time-bounded GoO certification. Also, the geographical boundary wherein they can be traded will be limited, explained in section 2.3.2. These findings further accentuate the need to understand how the transition of TSN would perform in the Dutch energy system in 2030 on an hourly basis with hydrogen as a feedstock.

Next to the background research findings, the literature review's most important findings are summarised here. These literature findings shaped the modelling methodology and, thus, the model findings. The analysed literature all qualitatively agree that the emissions and economic performance of hydrogen-based DRI ironmaking are highly dependent on the electricity price and the use of low-emitting electricity sources. However, on the quantitative level, there are still significant discrepancies between findings due to the assumption of specific energy consumption, the carbon intensity of the electricity, energy/material losses and hydrogen DRI reactive requirements. However, the majority of this literature research assumes artificially low electricity prices. Additionally, it is found that none of the papers uses variable electricity price with associated electricity emissions to determine the performance of a DRI process within the local energy system. Lastly, most papers either assess a full hydrogen-based or natural gas-based process without considering the intermediate process configurations. These findings shape the methodology and content of the modelling.

10.2. Model findings

The modelling findings of this thesis project are based on the simulation results presented in chapter 9. The results are split into three parts, energy consumption, CO_2 emissions and economic results. Furthermore, four hydrogen volume scenarios are chosen for the simulation on an hourly basis, with their specific input parameters explained in chapter 9.1.

10.2.1. Specific energy consumption findings

First, the energy consumption of the DRI-REF process will be discussed. Based on the assumed material and process properties documented in chapter 6.2, the specific material, electricity, and thermal energy consumption can be determined for various hydrogen volumes. It was found that the DRI-REF system has a SEC of 3.73 MWh/t_{HM} for a full natural gas process with a linear increase to 4.60 MWh/t_{HM} for an 80vol%H_2 process. The analysed literature has SEC values ranging between 3.48 MWh/t_{LS} [65] to 4.25 MWh/t_{LS} [5] for DR(H_2)-EAF systems. These results are comparable if the additional electricity consumption of the REF process is accounted for. The increase in SEC is mainly attributed to the increase in electricity consumption due to the inherent energy losses in the electrolysis process. It was found that for the 80%H_2 scenario, a 1.7 GW electrolyser is needed, which resulted in 0.96 MWh/t_{HM} electricity losses. This value can decrease in the coming decades if the electrolyser technology is further developed, giving the hydrogen economy a boost.

This increase in electricity demand cannot be counterbalanced by the higher efficiency of the H_2-based direct reduction process compared to the NG-based direct reduction process. Furthermore, a relatively small increase in electricity consumption of the REF process (0.09 MWh/t_{HM}) is given for the 80vol%H_2 process due to the declining carbon content of the DRI. For a 100%H_2-based DRI-REF process, the electrolysis process consumed 78% of the total energy for the direct reduction process. Comparable findings are found in the paper of Bhaskar et al.[5], which state that 75.8% of their SEC was a result of water electrolysis. The findings mentioned above only consider the ironmaking process without the further energy demand in the pelletising process and in secondary metallurgy, casting and rolling. For pelletising and rolling, 0.61 MWh/t of fuel and 140 KWh/t of electricity are required irrespective of the production route [65].

The implications of the shifting energy source (coal to natural gas to electricity) can have a major effect on the costs and CO_2 emissions. Due to the large energy consumption of the I&S industry, the production systems must be placed in a broader context, meaning that the I&S system and the energy system must be modelled together to better understand and determine the economic and environmental impact. Currently, we observe that several high energy-intensive companies with rigid consumption processes are moving towards countries with large quantities of renewable energy generation with storage capacity. A good example is Sweden, where hydro-power is used to produce excessive quantities of renewable electricity.

10.2.2. Emission findings

The second subject of the model findings is centred around the CO_2 emissions and the performance of different hydrogen volumes in the system of interest. There are several important findings discussed here which are the following: On a yearly basis, the CO_2 emissions between a full NG-based process and the 80%vol H_2 process amount to a 2.2% decrease in emissions, including the indirect electricity CO_2 emissions. This is assuming that the electricity comes fully from the modelled 2030 electricity mix with a carbon intensity of 0.13 tCO_2/MWhe. This electricity CO_2 emission intensity is approximately the breakeven point between the use of natural gas and 80vol% hydrogen in the modelled system of this thesis, as can be seen from the sensitivity analysis in figure 10.2. A breakeven of point of 0.36 tCO_2/MWh for the electricity carbon intensity is found for the comparison with the current coal-based BF-BOF process and the 80vol% hydrogen route. The determined electrical CO_2 emission intensity originates from the settings and calculations performed in the EMF v7.0 model, which is fully explained in chapter 6.1. On the other hand, the direct carbon emissions of the DRI-REF system show a decrease of 70.1% from 0.635 tCO_2/t_{HM} to 0.190 tCO_2/t_{HM} with increasing hydrogen volumes. To achieve the 2050 decarbonisation goals, a complete carbon-neutral process is needed. This could be achieved with measures such as the use of bio-coal with CCS.

However, it should be noted that if the indirect electrical emissions are included in the calculations, the emission reduction potential is greatly diminished. For the 0%H_2 scenario, the direct emissions accounted for 86.4% of the total emissions. On the other hand, for the 80%H_2 scenario, the direct emission accounted only for 26.4% of the total emissions. This indicates a significant displacement of carbon emissions from the TSN boundary towards the electricity generators in the Netherlands, also observed in figure 9.9. This displacement of carbon emissions is accentuated by increasing hydrogen volumes because of increasing electricity consumption and the characteristics of the electricity generation capacity. Comparable direct emissions values are found in the papers of Elsheikh and Eveloy[22], Jacobasch et al.[34], Müller et al.[44] and for comparable systems, discussed in chapter 7.4. The slight discrepancies in results originate from the difference in assumptions of material consumption.

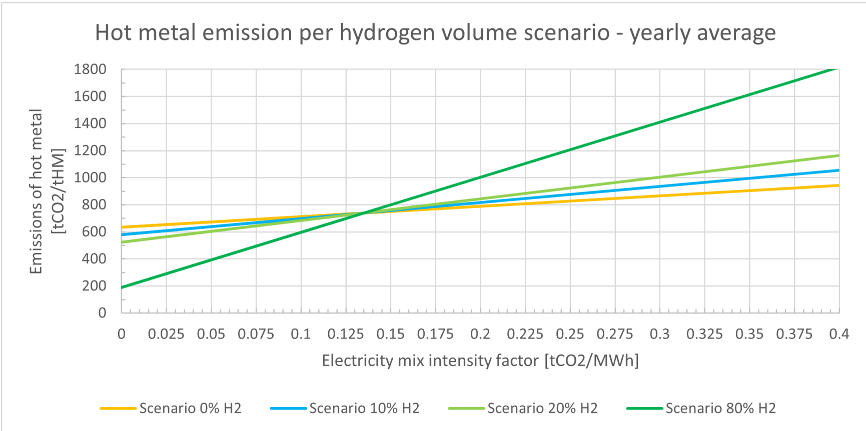


Figure 10.1.: Sensitivity analysis for different hydrogen scenarios of the hot metal emissions for increasing electricity CO_2 intensity.

Second, the hourly modelling findings of the CO_2 emissions provide valuable insights into the performance of the system of interest on an hourly basis. The variability of the generated electricity coming from renewable energy sources is reflected in the CO_2 emissions of the DRI-REF system, depicted in chapter 9.3.1. Increasing hydrogen volumes magnify this influence in the system of interest. The findings of the boxplot indicate that the CO_2 emissions interquartile range increases from 0.11 tCO_2/t_{HM} to 0.59 tCO_2/t_{HM}.

The increase in CO_2 emission spread or the IQR for higher hydrogen volumes increases the complexity of estimating the CO_2 footprint of the output over a period or given time. Additionally, the spread in emissions originates from the weather pattern observed. In this thesis, 2014 is used as a weather scenario year, explained in section 6.1.2. Using different weather scenarios will change the results significantly, further elaborated in the research limits in section 11.2.4. Thus, as more hydrogen is introduced in the (any) system, that said system will be more dependent on the weather pattern in the Dutch context. This is because is the Dutch electricity mix, as the IPKA0 scenario dictates, is dominated by variable electricity generation such as wind and solar.

Furthermore, the findings of the histograms indicate that the most common emitting moments are centred around the lower end of the spectrum but with a longer tail as more hydrogen is introduced into the system. This means that TSN could use specific flexibility measures to decrease electricity consumption during the most polluting hours of the year, thus decreasing the total CO_2 emissions of the system.

One of such measure is the flexibility potential, discussing the performance gains when switching from the energy source, presented in chapter 9.6. Using the variable feed gas composition by switching between natural gas and hydrogen could decrease emissions by an additional 6.5%, considering that 24h are needed to switch from one feed gas to the other entirely. In the ideal case where the switch can happen instantaneously, a decrease of 18% is calculated compared to the full NG production. This indicates that a significant amount of CO_2 emissions can still be reduced. However, these are emitted within the 24h time constraint. There are approximately 2700h in a year where the electrical emissions have less than 24 consecutive hours above the breakeven point between the NG and H_2 use. In these hours, TSN should not produces hydrogen based on electrolysis with the electricity coming from the grid but use other means, such as material or energy storage options. On the other hand, in 2030 there are almost 5000h when it is beneficial to use electricity from the Dutch electricity grid seen from an environmental point of view.

The implication of the emission findings in this study can be translated to other sectors and companies within the same energy market characteristics as the Netherlands. As the renewable energy supply in the Netherlands will be volatile due to its large percentage of renewable energy generation coming from wind and solar, companies with large flexibility potential can thrive in this environment. This is because these companies could serve and help balance the electricity grid by applying the demand response, thus reducing the strain on the grid and reducing curtailment and reducing the starts of the natural gas electricity generation. However, energy-intensive companies such as TSN which are notoriously known for demand response will have much harder and increasingly complex business cases in the future when hydrogen in introduced into their systems. Even if large hydrogen storage will be accessible in the future, the accompanying costs will increase the business case of hydrogen-based steel production compared to companies with readily accessible constant and cheap renewable energy.

10.2.3. Costs findings

The LCOP of the modelled system increases based on the hydrogen volume from 598 €/t_{HM} to 807 €/t_{HM} with an average electricity price of 97 €/MWhe. It is found that the composition of the LCOP changes significantly, especially the OPEX calculation. The most notable change happens in the decrease in natural gas costs and the increase in electricity costs. For the 80vol%H_2 scenario, the electricity costs can reach up to 49% of the total LCOP, accentuating the need for constant cheap electricity. The increase in LCOP accounts for the CAPEX and direct and inderct OPEX of the electrolyser, the DRI and REF plant, presented in detail in section 8.3. Figure 10.2 presents a sensitivity analysis to determine the influence of the electricity price on the LCOP of the hot metal. A breakeven point of 32 €/MWhe is calculated where hydrogen-based production becomes economically competitive with NG-based production on a yearly average. This breakeven point is a factor 3 lower than the estimated electricity price in 2030 generated from the EMF model.

The most interesting findings of the economic calculations are based on the hourly results. Comparable to the hourly emissions calculations, the hourly electricity price variations are reflected in the LCOP. This effect is increased with increasing hydrogen volumes, as seen in chapter 9.4.1. These results can also be derived from the boxplot, where the interquartile

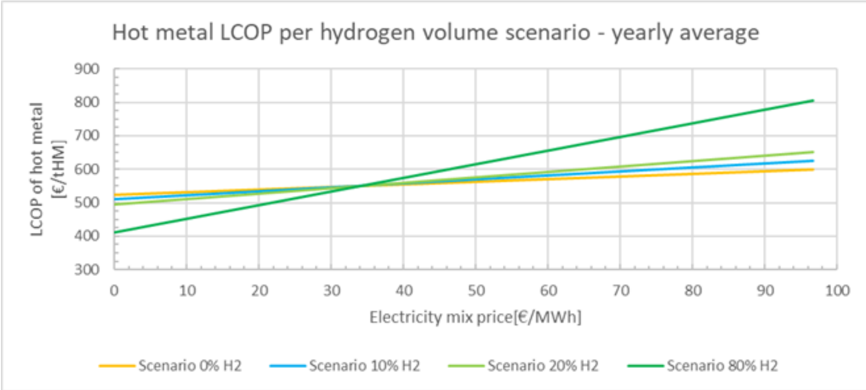


Figure 10.2.: Sensitivity analysis for different hydrogen scenarios of the LCOP for increasing electricity prices.

range increases from 82 €/t_{HM} to 432 €/t_{HM}. The implication of these results can be significant when TSN transitions towards hydrogen-based production. The current coal-based production process has a relatively small electricity consumption compared to the hydrogen-based process, thus minimising the effects of electricity price swings from the electricity mix. However, the hydrogen-based process has a huge dependency on the electricity price from the electricity market, as seen from the results. This dependency on the electricity price increases the need to understand the electricity market and demands a specific ability to predict the electricity price in the future, as it can severely affect the LCOP. The LCOP of the H_2-based process shows comparable findings with the work of Bhaskar et al.[5], which determines a LCOP of 714 $/t with an electricity price of 60 $/MWh.

Additionally, the calculated LCOPs for the NG and H_2 route in this thesis are within the IEA's 2035 projections, with DR(CH_4)-EAF (i.e., 410-600 $/$t_{HM}$) and DR($H_2$)-EAF (i.e., 510-830 $/$t_{HM}$)[33]. It should be noted that the IEA assumed a gas price of 2-9 $/GJ, whereas this thesis assumes an NG price of 20 €/GJ due to recent global developments. This difference in NG price considerably influences the LCOP of the 0%H_2 scenario, as NG has a share of 35.6%. This is less the case for the 80%H_2 scenario, which has a 4.7% share in LCOP.

The economic improvement potential of interchanging NG and H_2 is limited. As stated earlier, the LCOP of the NG-based production is 598 €/t_{HM}. The calculated price range of the flexibility analysis lies between 590-697 €/t_{HM}. In the ideal case where the switch between NG and H_2 can be performed instantaneously, a LCOP of 570 €/t_{HM} can be achieved. There are approximately 6200 hours when the electricity price exceeds the breakeven point. This indicates that in 2030 under the assumed renewable generation capacities given in table 2.1, the electricity price is still approximately 70% of the time above the breakeven point. However, there are already 1400h where is electricity dips under the 32 €/MWh with 24 consecutive hours or more. These hours could be exploited as they will hopefully increase as more renewable energy generation capacity is installed during the coming decades.

The implication of the LCOP findings and especially the costs for the DRI production with hydrogen are crucial for the strategic decision-making for TSN. There are already several iron production companies that have started their iron production in locations with readily available cheap renewable electricity. The green-DRI produced in these places can be produced much cheaper due to the constant low electricity costs for hydrogen production.

Figure 10.2 illustrates the results of these low electricity prices with increasing hydrogen penetrations. In the Netherlands, the electricity price and emission intensity will not be as stable, which results in increased costs and (scope 2) emissions. It is not inconceivable that TSN could displace their iron (DRI) production towards a geographical location with a steady and cheap renewable electricity supply and shipping the green-DRI towards Ijmuiden for further processing and steelmaking.

It should be noted that the findings of this thesis are based on the electricity price and associated CO_2 emissions data sets of the EMF model. Therefore, the complete data sets need to be validated and compared with other comparable data sets, explained in the following section.

10.3. Model and data set validation

Several validation steps are performed to substantiate this thesis's input data and datasets. First, the assumed material, process, and economic parameters are compared with literature values in sections 6.2.2 and 8.3, respectively. The technical implementation results are validated in section 7.4 by comparing the results of several papers used in the literature review. The DRI hydrogen consumption, DRI-specific energy demand, material emissions and direct total CO_2 emissions are all within an acceptable range. Minor differences are observed, attributed to the slight deviation in energy and material assumptions.

The hourly simulations depend on the assumed electricity price and associated CO_2 emissions. It is, therefore, imperative to validate the values and the shape of these data sets. The basic modelling methodology of the EMF model is briefly explained in chapter 6.1, where the workings of the merit order are explained. Due to the importance of the data sets used in this thesis, the EMF data sets need to be validated with external data sets. Unfortunately, due to the difficulty of finding readily accessible data, only one data source is found to compare the EMF results. Therefore, the associated electricity CO_2 emissions data set is compared with the historical data acquired from Electricitymaps.com for 2020 [62]. The year 2020 is chosen because the data set from the Electricitymaps does not make futuristic predictions. As such, we can validate the methodology of the EMF v7.0 model for futuristic estimations by comparing the prediction made for 2020, as seen in figure 10.3. The associated numerical values are presented in table 10.1. Both data set profiles are sorted and plotted against the hours of the year.

Data set source	Unit	N	Mean	Std. Deviation
Electricitymaps.com: 2020	$kgCO_2e/MWh$	8760	385	68
EMF V7.0: 2020 reference		8760	375	92

Table 10.1.: Summary of the two considered data set sources seen in figure 10.3.

The mean CO_2 intensity of the electricity mix in the EMF 2020 scenario is 0.375 tCO_2/MWh with a standard deviation of 92. The data from Electricitymaps estimates the average yearly emissions of 0.363 tCO_2/MWh with a standard deviation of 68. These two data sets have a 3.2% difference in mean. The high standard deviation can be attributed to the high number of data points. To compare these values with other sources, the estimation of the international energy agency (IEA) indicates an emission intensity of 0.392 tCO_2/MWh (2019) and 0.328 tCO_2e/MWh (2020) for the Netherlands [33] . Next to the slight differences in average

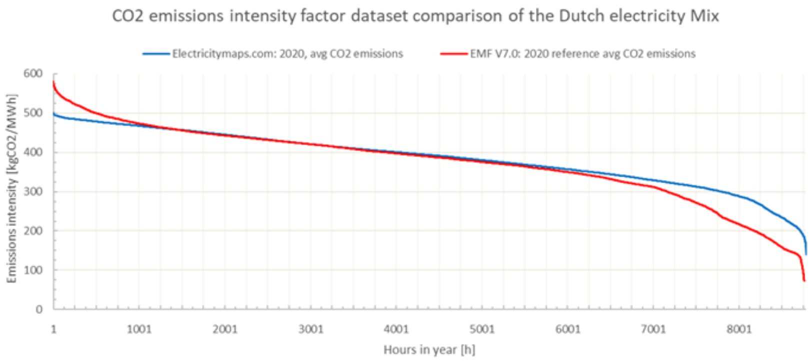


Figure 10.3.: Two CO_2 emissions intensity curves over an entire year for the year 2020, originating from the EMF model and Electricitymaps [62].

yearly electricity emissions, the profile of these emissions over a year is just as important. We can observe that, for most hours, both data sets match almost perfectly, with exceptions in the extremities. The data set of the EMF model provides higher and lower results for the electrical CO_2 intensity of the Dutch energy mix. The deviation in the data points can be attributed to the different calculation methods. One of the main characteristics of the Electricitymaps model is that it calculates the emissions from every country in Europe and adjusts the import and export behaviour of electricity. This mechanism is considerably simplified in the EMF v7.0 model. However, due to the low average difference between the two data sets and the visually matching data set profiles, it is assumed that the EMF model does provide reliable hourly data.

11. Conclusion

This chapter concludes this thesis by answering the research questions and presenting the academic relevance. Furthermore, a reflection is provided on the generalisability of the methodology used in the thesis, and to conclude, recommendations and a personal reflection are presented.

11.1. Main research question

Multiple research questions were formulated at the beginning of this thesis which supported the research. The main research question is formulated based on the identified knowledge gap, documented in section 3.4. From this main research question, several sub-research questions are formulated to support the main question. This section answers the main research question and then the sub-research questions. The main research question is:

How do various hydrogen volumes affect the technical, economic and decarbonisation performance of a DRI-REF process in the Netherlands in 2030?

The goal of this research is projected in the main research question, which is to explore the performance of hydrogen in a DRI-REF system in 2030. This goal is answered by analysing the energy consumption, CO_2 emissions and economic performance of various hydrogen volumes for a grid-driven system in the Netherlands. These three subjects provide the necessary information to determine the system's performance for specific hydrogen volume scenarios. The transition towards an H_2-based process significantly changes the energy demand of the DRI-REF system and shifts the primary energy source to electrical energy. This development increases the reflection of the electricity price and associated CO_2 emissions in the KPIs of the DRI-REF process. Under the assumed Dutch energy market developments, the CO_2 intensity of the electricity mix is approximately 0.130 $tCO_2/MWhe$, which is also the breakeven point between the NG and H_2-based process in 2030. On the other hand, the electricity price is a factor 3 higher in 2030, with an identified breakeven point of ≈ 32 €/MWhe. Additionally, there is a more extensive hourly spread for the H_2-based process in LCOP and total CO_2 emissions compared to the conventional NG-based process, which increases the uncertainty and risk of estimating future performance.

Cheaper and cleaner production hours are observed for the H_2-based DRI-REF process compared to the DR(CH_4)-REF process. However, switching between H_2 and NG to reduce LCOP or total CO_2 emissions has limited potential due to process restrictions. However, these results could change if a hydrogen storage system is included into the modelling. Furthermore, although an H_2-based grid-driven DRI-REF process could be beneficial from an environmental point of view in 2030 in the Netherlands, the increase in production costs could hamper the deployment of such systems. Through this research, it becomes clear that to assess future H_2 systems with higher precision, it would require energy market data with short time intervals to determine the potential and limitations in any geographical location. Also, it becomes clear that determining the business case of hydrogen based steelmaking, the whole supply chain needs to be modelled, including the energy system and storage options.

11.1.1. Sub-research questions

The main research question is split into several sub-research questions that facilitate answering the main research question. These sub-research questions are answered throughout the thesis and are summarised in this section.

What are the energy market and hydrogen capacity developments in the Netherlands up to 2030?
This question explores the energy market developments in the Netherlands and supports the substantiation and decision-making of the research methodology. The gathered insights are discussed in detail in sections 2.2 and 2.3. The transition from the conventional NG-based DRI technology towards an H_2-based process is a stepwise process, dependent on the availability and cost-effectiveness of 'green' hydrogen. The first transition step of TSN could provide a CO_2 reduction between 3.1 to 4.4 Mton per year when operating on natural gas. To increase the energy transition, the Dutch government increased the deployment of offshore wind generation capacity to 21 GW by 2030. Although there is an increase in local hydrogen production capacity developments, the large-scale roll-out is still awaiting due to economic considerations. There are several future energy generation scenarios available, each with its characteristics. This thesis uses the conservative IPKA0 scenario of Tennet [58] for the energy market modelling explained in chapter 2.3.1. Additionally, the current renewable energy procurement methods are expected to change towards time-related with a geographical correlation between electricity production and use.

How can the DRI-REF process be modelled to assess the technical and economic performance under various hydrogen volumes?
The main research approach in this thesis is a modelling and simulation approach. The formulation process of the conceptual model is carried out in chapter 5 following the theoretical framework of [51]. The conceptualisation process uses the following main elements: identifying the problem situation, determining modelling objectives and constraints, defining inputs and outputs, determining the model content and lastly, identifying the assumptions and simplifications. Based on this conceptual model, the required data can be acquired and implemented into the technical modelling, as documented in chapters 5.5 and 7.1.1. Detailed material and process were acquired from TSN and are validated with literature findings. Additionally, the outputs of the EMF modelling are used to provide high temporal granularity. These data sets are validated with an external source, discussed in chapter 10.3. With the technical model, the different hydrogen volumes can be simulated to assess the technical and environmental performance of the system of interest. The limitations of the modelling are reflected on in chapter 11.2.4.

What is the levelized cost of the DRI-REF process in the NL under given energy market conditions?

The economic evaluation methodology of the DRI-REF system for different hydrogen volumes is described in detail in chapter 8. The economic KPIs and assumptions are defined based on the literature review findings. Chapter 9.4 presents in detail the hourly and yearly levelized cost of production for different hydrogen volume scenarios. The LCOP of the hot metal varies with different hydrogen volumes, starting at 598 €/t_{HM} for 0%H_2 towards 807 €/t_{HM} for the 80%H_2 process. This increase in 35% LCOP for the 80%H_2 scenario can be attributed to the shift in energy carrier, increasing the electricity cost and capital costs which comprise of 48.9% and 15.7% of the total LCOP, respectively. The high data granularity of the technical modelling enables insights into the electricity market behaviour and its effects on the LCOP of the DRI-REF process. The interquartile range increases from 82 to 432 €/t_{HM} as the hydrogen volume increases. These findings provide valuable insights into the behaviour of the system in the Dutch context and the importance of using data with high temporal granularity. Cost estimations can vary significantly on an hourly basis as the system uses more hydrogen and, thus, consumes more electricity.

How does purely grid-driven H_2-DRI-REF compare with the conventional NG-DRI-REF process technically and economically?
The last sub-research question is answered using the technical model and the economic evaluation. The *results* chapter, especially section 9.5, provides a detailed answer to this question, and these results are then discussed in chapter 10.2. The H_2-based DRI-REF process could decrease direct emissions by 1.57 tCO_2/t_{HM} (ϕCO_2 = 0.95) compared to the current BF-BOF process, whereas the NG-based DRI-REF process can reduce the emissions by 1.02 tCO_2/t_{HM} (ϕCO_2 = 0.62). A crucial observation is that these reduction potentials decrease considerably if indirect electrical CO_2 emissions are considered. Especially the CO_2 mitigation potential from the NG to the H_2-based process, decreasing from ϕCO_2 = 0.87 towards ϕCO_2 = 0.04. This decrease implies that in 2030 under the assumed energy market conditions, a significant amount of CO_2 emissions will be displaced from the hot metal production process towards the electricity producers.

The specific CO_2 emissions mitigation cost of M_{costs} = 146 €/tCO_2 is identified for the NG-DRI-REF process. This emission mitigation cost increases towards M_{costs} = 255 €/tCO_2 when 80%H_2 is used in the process due to the significant increase in electricity and capital costs.

11.2. Reflection

This section presents a reflection on the completed research project. This is done by discussing the relevance of the research findings from an academic and practical perspective. Furthermore, recommendations are offered with a discussion of future work and improvements. To conclude, a personal reflection is given.

11.2.1. Academic relevance

This thesis uses the modelling and simulation methodology to model the behaviour of a DRI-REF process and simulate different hydrogen volumes as feedstock. In addition, a literature review is conducted to identify an academic knowledge gap. The identified knowledge gap is that it is unknown how a DRI-REF process performs under varying hydrogen volumes in the Dutch context in 2030.

TSN is transitioning from the coal-based blast furnace production route towards the DRI-REF process. Ultimately, the chemical energy used to reduce the iron ore will come from hydrogen instead of natural gas. For other companies in the iron and steel industry where a similar transition is taking place, the research findings of this thesis could contribute to the insights of hydrogen-based ironmaking and improve future model estimations by showing the variability in hourly results. The effect of variating hydrogen volumes is analysed and measured using performance indicators such as energy consumption and economic and environmental metrics. These metrics provide a complete image of the behaviour of such systems in a specific environment. This thesis is the first to model a process with the DRI-REF combination with hourly energy market data.

Moreover, the contribution is significant as this thesis uses accurate and interconnected data acquired from TSN. The usage of this data improves the accuracy of the performance calculations and, thus, contributes to future research in the H_2-based DRI process assessments. In many cases in the literature, the facility capacities, energy, and material consumption values are approached less accurately or based on literature findings. The holistic approach towards determining hydrogen performance is also relevant in this field of research. Incorporating local energy market circumstances provide insights into the competitiveness of hydrogen-based ironmaking due to the more focused analysis. This approach contributes to the existing body of research in this field and could make future assessments and analyses more robust and realistic.

11.2.2. Practical & societal relevance

This thesis project is supported by Tata Steel Netherland, a large iron and steel manufacturer in the Ijmuiden region. Additionally, the energy market forecast model used in this thesis is acquired from BlueTerra, an independent consultant company for industry and large business markets specialising in energy savings and sustainable energy. Therefore, the practical relevance of this research project is also important.

Modelling on an hourly basis in 2030 provides valuable insights into the hydrogen-based DRI-REF process and the effects on the decarbonisation efforts. This precision gives industry experts and other stakeholders information that has not been available before, which can improve strategic decision-making and estimation for material and energy storage options, for example. Furthermore, the simulations of the various hydrogen volumes provide insight into the energy demand and how important the electricity mix characteristics become in the Dutch context. Using values for the CO_2 intensity of the electricity mix near zero can be seen as unrealistic. This thesis provides insights to managers specialising in process flexibility, highlighting the connection between the Dutch energy mix characteristics and the new steel process. A emphasise is being put on a system where no hydrogen (energy) and material storage is used.

Reflecting on the societal relevance of this research project, it becomes clear that outcomes temper the decarbonisation goals if the indirect electricity CO_2 emissions are included in the calculations in the assumed system in this thesis. On the other hand, even with the conservative renewable energy capacity IPKA0 scenario (see section 2.3.1), the CO_2 breakeven point is already attained in 2030 for this specific process. This is quite surprising and positive news for the hydrogen business case. Furthermore, the environmental performance of a fully grid-driven DRI-REF process would improve even further if the full 21 GW of offshore wind capacity is installed. Decarbonising TSN is vital, but decarbonising the whole system is even more important. However, decreasing the CO_2 emissions of TSN and remaining competitive will become increasingly more difficult in the future. This is because the electricity mix in the Netherlands is dominated by variable renewable energy sources, which increases the difficulty to balance the electricity grid, thus increasing costs in certain hours.

Furthermore, the timeframe where TSN wants to decarbonise is closely linked to the availability of renewable energy. This thesis has used the Tennet IPKA0 scenario, which uses 11.5 GW of offshore wind energy. According to the EMF model simulation results, if 21 GW offshore wind energy were to be used instead, the electrical CO2 intensity would decrease only by approximately 25%. This implies that there are still considerable emissions from the electricity mix, increasing the scope 2 emissions. This can put additional pressure on TSN to reach its economic and decarbonisation targets.

Lastly, the implications of the flexibility analysis indicate that there are 2500-2700 hours where interchangeability of NG and H_2 operations is not possible due to process restrictions for either cost or emissions optimisation. These hours could still be utilised if, for example, more flexible access to hydrogen is provided. This could be done with hydrogen storage options which are currently being researched. This thesis provides an indication of the quantitative values of the operational hours, improving the business case of hydrogen storage and improving the requirements of this system. This means that in the Netherlands and comparable energy systems around the world, the flexibility capacity of the Iron and Steel industries must be increased by various technological solutions in the future to achieve cost reduction and decarbonisation targets.

11.2.3. Recommendations

Recommendations are given based on the research findings and their relevance to TSN. The findings of the simulations show the importance of having detailed energy market data as more hydrogen is being used in the production system. This shift towards hydrogen increases the variability in production costs and indirect CO_2 emissions, which has unknown consequences. Additionally, electricity price fluctuation will increase as more renewable energy generation capacity is introduced to the energy system through wind or solar energy. It is thus recommended to invest in and improve the knowledge base of energy system modelling and how this could affect the future production process. The Dutch national electricity mix is unique in the sense that it will become an off-shore wind-dominated energy system. In other words, strategic decisions should include the characteristics of the local energy system because this can affect the company's future competitiveness. Furthermore, the year-to-year weather variability can influence the economic and environmental performance of the modelled system. This research was limited to only one weather year scenario. However, it is strongly recommended to include at least the years from 2010 onwards to research the variability within the scenario years to sharpen the electricity price and associated CO_2 emissions estimations.

It is expected that future iron and steel companies that use green hydrogen produced from volatile renewable energy sources, such as wind or solar, need more flexibility or storage measures to cope with the energy generation fluctuations. This investment in additional storage options puts pressure on the competitiveness compared to other companies that have access to other sources of renewable energies such as hydro, thermal or even nuclear energy.

11.2.4. Limitations and suggestions for suture research

This section reflects on the limitations of this research project and provides suggestions for future research. These limitations are based on the research choices and the assumptions documented in sections 5.6 and 5.7. The documented limitations affect the results and findings of this thesis and originate mainly from the conceptual model and the technical implementation.

The first simplification presented is centred around the calculation methodology of the material and energy balances. As motivated, it was chosen to perform the calculation based on the findings of the literature, grey literature or data received from TSN. The implication is that the results are more holistic and have low complexity due to the limited number of parameters that can be adjusted. Furthermore, as already indicated, future research could add the detailed Shomate equations [11] to calculate the specific heat and enthalpy of different streams as done in several literature papers. This increase in detail could increase the realistic component and enable process optimisations such as minimising energy requirements.

The second simplification is based on the electricity procurement methodology. This simplification uses the Dutch electricity mix as the electricity source and predicts the electricity price and associated CO_2 emission for the entire year of 2030. From a methodological perspective, the analysis of the EMF model uses historical weather data to determine the values of the dataset. However, in practice, weather patterns or reports are available shortly in advance and with uncertainties. This limits the system's reaction to changing weather conditions. Therefore, the results in this thesis provide a lower limit than achievable in practice. It is recommended to include real-time weather reports or data sets and perform optimisation calculations to research the flexibility of the system to changing weather conditions.

One assumption, in particular, greatly impacts the simulations' results. The energy data sets from the EMF model have crucial importance in this thesis and are validated with external sources in section 10.3. To recap, the EMF model is using the weather year of 2014 to make a prediction on the electricity price and associated CO_2 emissions for 2030. The year 2020 is chosen to compare the different data sets due to limited data access, further explained below. One of the limitations of this EMF model is that it uses one weather scenario for its calculations. Although 2014 is comparable in terms of temperature [32] to 2020, there are still some deviations in the wind and solar hours that in turn affect renewable energy generation. Furthermore, there are significant variations in weather behaviour [8] which can lead to different results. The paper of Pimm et al.[48] analysis the offshore wind capacity factors for the last 40 years in England and finds a difference of approximately +-12.5% from the median. Suppose these different weather conditions are not considered in the strategic choices or facility scaling modelling. In that case, it could have significant consequences for the environmental and economic performance of the system. As can be seen from the results of the hourly variations in sections 9.3.1 and 9.4.1, increasing the hydrogen volume increases the dependence on electrical energy, and thus its price and associated CO_2 emissions. It is, therefore, essential to incorporate the weather variability and estimated future weather trends to reduce risk and improve estimations for long-term decarbonisation strategies.

The last discussed simplification in section 5.6 excludes the energy or material storage capabilities and the scrap material. Based on the literature findings, these capacities and parameters can significantly influence the results and findings of the modelling. The development model in this thesis is a predictive model without any process real-time optimisations over a year, increasing process material and energy demands. Due to the required modelling complexity and process knowledge for the implementation, it was chosen to omit these aspects in the modelling. However, future research should incorporate energy or material storage options as they can improve process performance significantly, according to the literature. Also, scrap material could be added to temporarily reduce the need for DRI production, thus temporarily reducing the energy demand. Future research could look into recent developments by company Rondo Energy which have potentially enabled cheap high-temperature energy storage, which could reduce the need for natural gas, hydrogen or electricity for the 1.7 GW energy needed in the gas pre-heater, seen in figure 5.4. Future research should improve understanding of these thermal storage options, which can improve the flexibility of the DRI-REF system.

11.2.5. Personal reflection

This thesis is the final step in obtaining a Master in Management of Technology (MoT) from the TPM faculty at the Delft University of Technology. The research process has been very challenging, especially the beginning of the research formulation process. In addition, the iron and steelmaking processes were new to me, which increased the complexity of this research even further. It has been a great pleasure to work with the people of TSN and especially enable connections within the company boundaries and outside.

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A. Process reactions of the DRI process

The internal reforming process in characterised by the reaction presented in this appendix. The first reaction is the reaction of natural gas (CH4) with injected oxygen (O2), resulting in the partial oxidation of methane happening inside the DR-shaft.

$$CH_4 + 12\,O_2 \rightleftharpoons 2\,H_2 + CO \qquad \Delta h_0 = -71.0 kJ/mol \tag{A.1}$$

Iron ore is fed to the shaft furnace at the upper part, resulting in a counter-current flow of a solid downstream and a gaseous upstream. DRI is leaving the shaft in the lower part in case of hot DRI (HDRI) production. Within the shaft furnace various reactions occur in parallel. In the upper part of the shaft, iron ore is reduced in a multi-stage process and can be summarised by :

$$Fe_2O_3 + 3\,CO \rightleftharpoons 2\,Fe + 3\,CO_2 \qquad \Delta h_0 - 23.6 kJ/mol \tag{A.2}$$

$$Fe_2O_3 + 3\,H_2 \rightleftharpoons 2\,Fe + 3\,H_2O \qquad \Delta h_0 = -98.0 kJ/mol \tag{A.3}$$

The reduction gases H2 and CO are either already present within the injected reduction gas or result from the internal steam reforming of methane according to

$$CH_4 + H_2O \rightleftharpoons CO + 3\,H_2 \qquad \Delta h_0 = +206.2 kJ/mol \tag{A.4}$$

or internal dry reforming of methane according to

$$CH_4 + CO_2 \rightleftharpoons 2\,CO + 2\,H_2 \qquad \Delta h_0 = +247.0 kJ/mol \tag{A.5}$$

In parallel to this, water-gas shift reaction occurs. Metallic iron, a product of the reduction process, acts as a catalyst for the reforming reactions. In the area of the gas injection, methane encounters reduced metallic iron, resulting in the carburisation of the DRI according to:

$$3\,Fe + CH_4 \rightleftharpoons Fe + C + 2\,H_2 \qquad \Delta h_0 = +74.6 kJ/mol \tag{A.6}$$

$$3\,Fe + C \rightleftharpoons Fe_3C \qquad \Delta h_0 = +25.1 kJ/mol \tag{A.7}$$

B. Energy Market Forecast Model V7.0

Name	Production		Avg. Price	Full load hours	Starts
[]		[%]	[€/MWh]	[u]	[]
Offshore wind	43,552	33.0%	70.26	3755	
Onshore wind	34,394	18.5%	57.14	2772	
Sun-PV	26,103	19.8%	53.08	848	
Must run - SV	1,774	1.3%	148.85	2063	
Must run - industry	4,769	3.6%	108.74	7226	
Must run - other	11,808	9.0%	120.20	6256	
Gasmotor	2,463	1.9%	167.93	2964	362
Gasmotor - d/n	1,877	1.4%	208.69	1018	267
Gas - other	15,131	11.5%	187.82	1961	275
P2H	6,934			3467	
P2G	11,735			1956	
Totaal	131,871	100%	96.77		

Table B.1.: Summary of the EMF v7.0 simulation run on the 2030 scenario

C. Material properties

Conversion factors natural gas		
Component	**Units**	NG
Molar weight	kg/mol	17.5
Density	kN/nm3	0.8
LHV	kJ/kg	47149.6
	kJ/kmol	826253
	kJ/nm3	36863
	Mol weights	**mol %**
Hydrogen	2.02	0
Nitrogen	28.01	1.4
CO	28.01	0
CO2	44.01	1.2
Methane	16.04	92.2
Ethane	30.07	4.1
Propane	44.1	0.8
Iso-Butane	58.12	0.1
Butane	58.12	0.2
Hexane	86.18	0.1
Emissons	kg CO2/GJ NG	56.1
	g CO2/MJ NG	56.1
	kg CO2/Nm3 NG	2.068

Table C.1.: Natural gas assumptions and conversion factors provided by TSN

Factsheet Hydrogen		
Mass & Volume		
Nm^3/kg	0.08994	
kg/N	11.12	
Energy density		
kg/MJ	142	HHV
kg/MJ	120.1	LHV
kg/kWh	39.4	100% efficiency
Nm3/MJ	12.8	
L(700b)/MJ	9.2	

Table C.2.: Hydrogen gas assumptions and conversion factors provided by TSN

Colophon

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