MASTER THESIS REPORT

A MILP-BASED APPROACH FOR THE ANALYSIS OF COOPERATIVE RELATIONSHIPS IN THE TRANSITION OF THE ENERGY-INTENSIVE INDUSTRY

MICHELA DESIDERI PEREA

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Michela Desideri Perea

Student number: 5162432

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Graduation committee

First Supervisor	: Dr.ir. R.M. Stikkelman,	Energy and Industry
Second Supervisor	: Dr. P.W.G. Bots,	Policy Analysis
External Supervisor	: Dr. R. Bhardwaj,	TNO/Sustainable Process and Energy Systems

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Executive Summary

The Dutch energy-intensive industry relies heavily on fossil-fuelled energy sources for production processes, being responsible for one third of CO_2 emissions in the Netherlands. The road to CO_2 neutrality by 2050 requires a massive transformation of the industrial sector: sustainable supply and (re-)use of industrial heat, CO_2 capture and storage and improved efficiency and circularity are some of the routes that the transition of industry may follow. In the light of the European Green Deal, a rapid mobilization of investments is required in order to reap their benefits before 2050.

In this context, new forms of cooperation within energy-intensive industrial clusters have the potential to accelerate the delivery of innovative solutions. Multi-actor and technical dependencies offer synergetic possibilities that make collaborative decision-making of great importance in a situation of profound transformation. The challenge is to understand how to systematically manage and govern such inter-firm collaborations to favour the transition of industrial clusters, while balancing actor profit and cluster welfare. Formal governance mechanisms such as bi- and multilateral contracts play a critical role in this respect, regulating the distribution of costs and benefits of investment projects, while consolidating the exchange of the resulting products to reduce the uncertainty of flows. As a result, the adoption of different forms of contracts needs to be carefully considered when evaluating investment options for decarbonization. Although the transition of the energy-intensive industry has been studied from different angles, current approaches fall short in analysing and understanding the relation between the technical (hardware) level and multi-actor (and institutional) context of an industrial complex. However, integrated methods and tools are needed to identify optimal transition paths, while enabling a dynamic evaluation of investments decisions under diverse multi-actor configurations. This thesis addresses the problem by means of the following main research question:

"What are the implications of implementing contractual structures in optimization models to support optimal investment decisions in the decarbonization of industrial clusters?"

Answering this question requires an exploratory research design combined with a modelling approach. The initial exploratory steps involve gaining insight in the field of contractual governance using elements of Transaction Costs Economics and Game Theory. A case study analysis of the industrial cluster located in the Port of Rotterdam is conducted alongside the literature study, analysing key investment projects for decarbonization and the underlying contractual network. As part of the hard-to-electrify (and therefore hard-to-abate) sectors, the Rotterdam cluster attempts to transition to a new energy system by switching from fossil fuels to electricity, low-carbon hydrogen and green hydrogen. Thus, a focus on hydrogen as fuel and for power generation is established with respect to investments' evaluation. As a final step resulting from the exploratory approach, hypotheses on the impact of contracts on the transition of industrial clusters are formulated, together with the experimental setup required for hypotheses' testing.

The information gathered in the exploratory steps serves as input to develop a novel methodology to incorporate contractual structures in optimization models. The output of these research steps is translated into an integrated optimization model of the Rotterdam cluster using Linny-R, a software tool developed by Dr. P.W.G. Bots that applies Mixed Integer Linear Programming (MILP) optimization. Besides the quantification of results of hypothesis testing, the model provides a proof of concept of the developed methodology to include contractual structures in the analysis of investment decisions for the energy transition. In addition, the model provides measurable insights in the effects of contractual structures on the transformation of industrial clusters, specifying the cash flow of the total cluster and its distribution among individual actors as the main metric for the evaluation of the economic

performance. Optimal investment curves and resulting CO_2 emissions are finally analysed as determinants of the cash flows obtained from the model experiments. As a result, implications of the implementation of contracts in optimization models are observed and discussed.

As part of the research outcomes it is found that, without an explicit implementation of contractual agreements, results obtained from MILP may be characterized by a distorted allocation of cash flows, in which sacrifices of some actors in the form of negative cash flows are compensated by higher profits of other cluster's members. These kind of results are clearly misleading in the identification of an optimal transition path. Thus, the proposed methodology adds value to MILP-based approaches.

The model results show that contracts do have an effect on the transition of the industrial sector. In fact, adopting different contractual structures shifts investment decisions overtime, affecting the timescale of investments and the associated CO_2 reduction. Bilateral contracts seem to yield the highest benefits for the modelled system, both from an economic and environmental perspective, as contract terms are tailored to the specific needs of the contractual parties. This makes off-takers less constrained than with multilateral contracts, whose advantages can be fully observed in thick markets.

Although the findings suggest that there may not be a universal, one-size-fits-all approach in establishing a set of contracts that best supports investment projects under all possible conditions, the proposed methodology is effective in providing direction for the next steps to make decarbonization projects an investable prospect in the energy-intensive industry. More precisely, barriers identified via the implementation of contracts specify areas of need for targeted policy action, addressing the creation of greater economic incentives for the integration of investment options. With specific respect to hydrogen applications, regulated revenue support in combination with policies recognising the higher social value of low-carbon/green hydrogen products may be relevant options to take into consideration. From a managerial perspective, the methodology allows to identify and address dependencies among investment options which may strengthen or jeopardize each other. Relevant examples for hydrogen integration are the need for increased CO_2 savings and/or the need to complement green hydrogen with additional measures to capture refinery fuel gases to improve the business case of such projects. Other implications consist in the need to carefully rethink the relationship between producers and off-takers to gradually adapt it to market developments.

As a general conclusion, implementing contractual structures in MILP enables a more accurate representation of the behaviour of rational actors, allowing for a dynamic analysis of the system's behaviour. Not only the incentives arising for each contracting party are taken into account in selecting optimal transition paths, but also synergies and externalities arising from the combination of technical options are optimized. This generates more valuable insights from a multi-actor and system perspective.

This research suggests several research avenues that can be pursued. First and foremost, further research should be conducted to provide understanding of possible consequences of combining diverse policy interventions with contractual structures. It is possible that contracts will play a greater role in determining the revenue generation of investment options when more policies that provide specific economic incentives for decarbonization are introduced.

Moreover, besides incorporating a higher level of detail and improving input data, adjustments to the proposed model could be performed to simulate a shift in contractual structures that follows the (hydrogen) market developments. Moreover, additional model expansions could allow to examine the consequences of blue and green hydrogen integration on the incumbent grey hydrogen suppliers.

Finally, building upon the results of this research, the performed study could be replicated for clusters in different locations. A cross-case analysis would then reveal whether location significantly influences the identification of optimal contractual structures to support the energy transition.

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1. Introduction

1.1. Problem definition and societal relevance

In the past decades, global effort has been made to intensify transition strategies and (inter)national climate policies to comply with the established emission budget. Scientific evidence shows that, if the average global temperature is to be maintained below 2°C, the global growth trend of greenhouse gas (GHG) emissions must be stopped by 2020, and reversed as to reach half of 1990 levels by 2050 (Henriques & Stikkelman, 2017). Such reduction in GHG emissions is only to be achieved by a massive transformation of every sector of the economy, and the industrial sector has considerable potential in this respect. In fact, the energy intensive industry is still heavily reliant on fossil-fuelled energy sources for production processes, being responsible for two-thirds of CO_2 emissions in the European Union (Gerres, Chaves Ávila, Llamas, & San Román, 2019).

Within the industrial sector, sustainable industrial clusters are a promising option to enhance the regional economic performance, while contributing to the energy transition. An industrial cluster consists of "a geographically proximate group of interconnected companies [...] in a particular field, linked by externalities of various types" (Porter, 2010). Specifically, industrial clusters include initially separate industries that engage in a collaborative approach to gain competitive advantage involving physical exchange of materials, energy and/or other by-products (Chertow, 2000). In North-West Europe, it is likely that the existing energy-intensive clusters will undergo a process of transformation towards a more sustainable system, rather than being built *ex novo* (Cuppen, Nikolic, Kwakkel, & Quist, 2020). This transition poses a dual challenge for the petrochemical-process industries: how to transform their production processes using more sustainable business practices, while increasing business value leveraging the advantages of cluster collaboration.

This task is further complicated by the multi-actor context: actors establish relations that are not only functional but also institutional, legal and economic. Thus, when the owner of a process makes an investment decision, its business case will strongly depend on new regulation and contractual arrangements with other cluster's members, decreasing the flexibility of the system (Cuppen et al., 2020). Moreover, changes at a unit operation's level will affect the overarching cluster level, highlighting technical dependencies that make the added value for the new option diverge from the added value for the whole cluster. Thus, a balance between competition and collaboration for the actors of the cluster must be found.

1.2. Socio-technical complexity

A cluster is a clear example of a socio-technical system. At a lower hierarchical level of aggregation, industrial clusters consist of networks of interacting enterprises, representing the elementary units of the system. We refer to them as production units (PUs). PUs are subject to competitive forces that make them engage in economic activities. At the same time, PUs interact with each other (via the exchange of materials, commodities, energy, etc.), forming a network structure (Wallner, 1999).

Aggregating PUs in a network of enterprises forms a cluster. At this level of aggregation, complexity originates from different dimensions (Verwater-Lukszo & Bouwmans, 2005). Firstly, there is physical/technical complexity resulting from the large number of interacting elements in the network. Their relations are all functional and causal but do not result in completely predictable behaviour. Second, interactions between actors that own PUs increase the level of complexity of the industrial system, as actors vary in size and create relations beyond the functional level, comprising also the institutional, legal and economic areas. Finally, the interactions between the actors and the physical system create an interconnected, complex network: in this context, multi-actor decision-making has important implications on the technical level and, vice-versa, changes in the physical system increase or decrease dependencies among the enterprises belonging to the cluster. It follows that complex patterns of interaction are created in the network due to the interplay of the system components as opposed to individual elements (Wallner, 1999).

While sizable literature focuses on technical challenges of clusters' transformation, less attention has been dedicated to changes in the multi-actor context resulting from the transition. Opportunities for inter-firm collaboration, however, may be a key enabler of decarbonization, worth being explored: the challenge is to understand what kind of dependencies may arise among the cluster members and how to govern them to favour the transformation of the cluster itself, while balancing actor profit and cluster welfare.

1.3. Scientific relevance

To improve our understanding of the scientific problem, relevant literature of the past two decades is reviewed. This section defines key concepts that characterize the multi-actor context of clusters' transition. Next, we present an overview of how this transition has been analysed and modelled so far. As a result, we identify a knowledge gap leading to our main research question.

1.3.1. Definition of key concepts

Industrial clusters (Porter, 1998) or Industrial symbiosis (Chertow, 2000) are identified as the core of this research. Analogies in the definitions provided by the authors are found in the attention to the physical exchange of materials, energy and/or by-products, and to the collaboration and the synergistic possibilities offered by geographical proximity. This also introduces the concepts of collaboration versus competition, that we use to further scope the research.

1.3.1.1. Cluster collaboration

We have discussed how multi-actor networks represent an additional source of complexity. Such complexity becomes particularly relevant in the context of the energy transition, as the system needs to undergo a radical (technical) transformation. New investment options need to be carefully evaluated, as investment costs become bigger and take more time to show satisfactory returns. Taking the words of the president of Koninklijke Hoogovens, in this context ". . . you cannot do it all by yourself. It rarely happens that I by myself say: that's how we're going to do it". This shows the importance of collaborative decision-making in a situation of profound transformation.

Mutual dependencies among the cluster's participants generate what Cooke and Morgan (1993) defined as the "network paradigm". The paradigm consists in each system element finding its new function in the system, for the sake of improving the network's performance. In this perspective, network participants must be aware of the fact that operating within a network will not entail only advantages, as a systemic perspective needs to be adopted (Wallner, 1999). It could well happen that an enterprise assumes the role of "servant of the network" to benefit of the overall system. Another interesting consequence of the establishment of networks is "co-opetition", a situation in which a company may have a competitor that simultaneously complements its economic activity, due to interactions via the exchange of materials that enhance the value of the company's services or products (de Bruijn & Heuvelhof, 2012). As a result, competing actors are aware of their interdependencies and of the potential value arising from cooperation. However, it is still unclear how can collaborative and competitive forces be balanced and governed in the transition of industrial cluster.

Several theoretical approaches have been used to shed light on this matter, the most prominent being Game Theory (Lorenzen, 2016; Melese et al., 2016). Newlands (2003) uses transaction costs economics (TCE), institutional and evolutionary economics, and several other theoretical backgrounds to offer a critical reading of the competitive and cooperative forces that characterize clusters' operations. A commonly shared conclusion is that there is a need for further research applying and exploring these concepts empirically (Lorenzen, 2016; Newlands, 2003).

1.3.1.2. Cluster governance and contractual agreements

Collaboration between cluster members needs to be systematically addressed and managed to reap its full benefits (Coletti & Landoni, 2018). Governance mechanisms play a decisive role in this context. Several definitions of cluster governance are available in literature, the most general being provided by Coletti at al. (2018). The authors refer to the governance of a collaboration as the structure through which objectives of a relationship among organisations are decided, together with the means of achieving them. These objectives span from reducing transaction costs to gaining competitive advantage in the market (Sheffi, Saenz, Rivera, & Gligor, 2019; Wei, Zhou, Greeven, & Qu, 2016). Several forms of governance can be identified, although different research streams have not established a common taxonomy to refer to each type of mechanism. Some overlap exists in literature among governance mechanisms that involve contractual arrangements, under the names of "contractual governance" or "formal governance" (Coletti & Landoni, 2018; Lowitzsch, Hoicka, & van Tulder, 2020; Sheffi et al., 2019). We narrow down the scope of our research to this governance form, and more specifically, to the contractual structures (i.e. the set of contractual agreements) in a cluster: in fact, our main interest is to understand how the interplay of economic agents can be formalised in rules that enable clusters' transformation. Contracts seem to be suitable for this purpose (Coletti & Landoni, 2018).

Contracts allow to define the rules for collaboration and facilitate the formation and reinforcement of relations among multiple actors (Sheffi et al., 2019). Inter-firm relations are characterized by complexity and dynamism: thus, contractual arrangements are often incomplete as they fail to capture the complexity of real life, which is further increased by the changing network of partners (Coletti & Landoni, 2018). In order to neutralize potential hazards, contracts need to specify key issues upfront, such as requirements from partners regarding investment costs, prices and quantities to be exchanged, and safeguard mechanisms (Coletti & Landoni, 2018).

However, the effect of these elements on clusters transition has not been clarified yet (Coletti & Landoni, 2018).

1.3.2. Modelling the transition of industrial clusters

Different energy system models are used as instruments to support strategic decision-making in the transition to a sustainable system. Although such transition is studied from different angles, current approaches fall short in analysing and understanding the relation between the technical (hardware) level and multi-actor (and institutional) structure of an industrial complex. Models usually put the spotlight only on technological details, or policy parameters, or focus on transition pathways: only a few assess all these elements in an integrated manner (Fleiter et al., 2018; Lessard, Habert, Tagnit-Hamou, & Amor, 2020; Melese, Heijnen, Stikkelman, & Herder, 2015; Raimbault et al., 2020; Romero & Ruiz, 2014). For instance, Fleiter et al. (2018) point out that "models with high level of technology detail are . . . less comprehensive in their consideration of policy instruments" and models able to overcome this shortcoming, fail in optimizing the technical performance of the system. It is evident that conventional modelling approaches are unable to integrate all these perspectives and, as a result, fail in recognizing future uncertainties deriving from the interactions between technical and multi-actor components of clusters' transition over time (Melese et al., 2015).

Specifically, in a context where every actor strives to transform its production processes and/or to introduce new assets, potential externalities produced by their interaction should be factored in when analysing investments. This would enable greater coordination of multi-actor decisions, thus enhancing synergetic effects of the activation of new assets, or anticipating and preventing situations in which different investment options would be mutually damaging. An analysis of such dynamic behaviour would therefore provide added value to the investments' evaluation and signal possible investment paths to be pursued for a successful transition.

An investment path entails, by definition, a planning of investment options over time. Such investments generate cash flows depending not only on pricing and exogenous variables, but also on the introduction of other assets which may strengthen or jeopardize each other. As part of the research scope we strive to support the identification of such transition paths in the context of the energy-intensive industry. Among the available methods, optimization offers an agile approach to the problem: given a set of investment options, an underlying solver evaluates different moments for the activation of each investment, returning an optimal transition path consisting of the most economically-convenient assets to be invested in and the respective timing for each investment. Such insightful outputs would hardly be obtained without optimization, using traditional investment evaluation methods: the latter usually require the timing of investment options as exogenous variables which, in turn, affect the calculation of cash flows, ultimately returning a measure Net Present Value for each option. As a result, the identification of an optimal investment path would only be possible by benchmarking the results of multiple manual iterations in which the timing of each investment's activation is gradually shifted.

Optimization models have inspiringly been applied to optimize investment portfolios. Several studies focus on applications for industrial clusters, although pursuing research objectives that do not completely align with our scope, spanning from optimal risk sharing to collaboration for cross-plant precaution investments (Jamal & Montemanni, 2018; Y. Melese et al., 2016; Reniers, Cuypers, & Pavlova, 2012). The challenge is to build upon such approaches by providing a methodology that captures the interrelations between the physical and multi-actor levels over time in the same, integrated model.

Several knowledge gaps are identified as a result of this literature scan. First, we found that there is only little understanding of the effects of clusters' governance on the transition of the industrial sector. Specifically, contractual governance has been recognized as a relevant mechanism to formalize the interplay of the cluster's participants via structured sets of rules: however, the extent to which contractual agreements can facilitate the transformation of industrial clusters has not been clarified yet. Finally, we have discussed how conventional energy system models are unable to provide insights on how the physical and multi-actor complexity of the system should evolve overtime to create favourable conditions for clusters' transformation. These knowledge gaps are summarized and addressed in the following main research question (MRQ):

"What are the implications of implementing contractual structures in optimization models to support optimal investment decisions in the decarbonization of industrial clusters?"

This research will provide further understanding on this matter by exploring the effects of different contractual structures on investment decisions in multiple decarbonization options. We strive to create this insight by using a modelling technique that will optimise the cluster's investment path over a time-span of 30 years. As a result, the research approach described in the next section is selected as the most effective in completing this study.

1.4. Research approach

This research adopts an exploratory research design combined with a modelling approach. The research cycle below effectively summarizes the adopted approach.

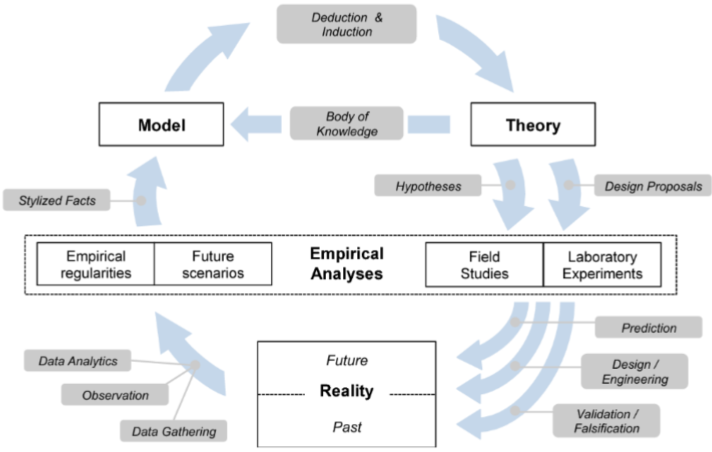


Figure 1. Research cycle (Krämer & Schnurr, 2017)

The initial exploratory steps involve gaining insight in the field of contractual governance. To this end, existing theories such as Game Theory and TCE will be used to gain a preliminary understanding of empirical regularities, resulting in an initial classification of contractual structures based on theory. Such categorization will be extended by observing how contractual structures are implemented in practice, analysing key investment projects for the decarbonization of clusters by means of a case study. As a final step resulting from the exploratory approach, hypotheses on the impact of contracts on the transition of industrial clusters will be formulated. In this way, the exploratory approach lays the groundwork for this research (Saunders, Lewis, Thornhill, & Bristow, 2019).

The next step is translating the information gathered in the exploratory phase into an integrated optimization model. This will force us to conceptualize this information and formalize it via a mathematical model. The conceptualization and formalization steps consist in identifying and designing the necessary building blocks to include contracts in optimization models. Thus, this research phase constitutes the core of our proposed, novel methodology to model contractual structures, bridging the technical and institutional levels in investments' evaluation. Such methodology will be tested via a stylised model, providing a proof of concept. Lastly, the model will produce a quantification of results from hypotheses testing, providing measurable insights in the impact of contractual structures on the transformation of industrial clusters. As a consequence, we will be able to deduce what are the implications of incorporating contracts in optimization models.

Combining the exploratory and modelling approach brings the advantage of extending the applicability of the research, by using the flexibility of the exploratory approach along with the quantitative insights provided by the modelling approach. Naturally, both approaches have shortcomings which have to be recognized. Insights gained from application of an exploratory approach are not easily generalizable (Saunders et al., 2019). This aligns with one of the pitfalls of the modelling approach: no matter the model, it still remains a representation of the system rather than the system itself. As a result, outcomes of the model may be misaligned with the behaviour of the real system: determining how to implement the findings into the real system after applying the modelling approach deserves special attention (Bryden, 2007).

1.5. Research sub-questions and methodology

Each phase of the research cycle in Figure 1 is now further specified into research activities, linked to research sub-questions (SQs) and to suitable research methods for data gathering, as summarized in the Research Flow Diagram (RFD) in Figure 2.

The MRQ is broken down into the following research SQs:

1. *"Which contractual structures can be identified, based on different forms of collaboration among contractual parties?"*
2. *"What are possible impacts of different types of contractual structures on clusters' transition, according to literature?"*
3. *"How can the effects of contractual structures be tested in a structured manner?"*
4. *"How can investment decisions be effectively represented in optimization models?"*
5. *"How can contractual agreements be effectively represented in optimization models?"*
6. *"What is the effect of adopting different contractual structures on investment decisions for the transition of industrial clusters?"*

The first three SQs are related to the exploratory phase of this research. Identifying a classification of contractual structures requires knowledge on the state-of-the art in the field. The best suited method to conduct this analysis is a desk research, making use of existing textual sources as input data for a literature review. One limitation of the literature review is its full reliance on previously published studies, whose quality determine answers and conclusions to the research questions (Snyder, 2019). Thus, based on the selection criteria, one could end up missing studies containing relevant insights (Snyder, 2019). This limitation is overcome in this research by conducting a case study analysis alongside the desk research. Case study analysis is chosen as a suitable method in the light of its exploratory power (Yin, 2012). In this way, patterns observed in practice can be included in the analysis and add to the theoretical findings from the literature review process, thus providing an answer to SQ1.

The cluster located in the Port of Rotterdam is selected as a case study to provide relevant insights in decarbonization options currently under evaluation. The Rotterdam cluster is chosen due to its strategic location in North-West Europe, which is of high potential for increased industrial cooperation, according to Cervo et al. (2019). Given its potential to become a hub for several energy vectors (i.e. chemicals, electricity and gas), the Rotterdam cluster is regarded as a suitable location for this research. For simplicity, only part of the cluster will be considered, given time constraints and the complexity of real dynamics. Publicly available reports and grey literature will serve as input data for the case study analysis, as well as to define the system boundaries.

Based on the analysis of the existing clusters' relations, insights about possible impacts of contractual structures on investment decisions will be obtained. These insights provide an answer to SQ2 and will be used as input data for SQ3. Here, hypothesis will be formulated and an experimental setup will be designed based on a discussion of previous results.

The combined output of these sub-questions will be used as input to build a simplified model of clusters relations. Importantly, SQ4 and SQ5 will provide guidance on the conceptualization and formalization of investment- related constraints and on the representation of contractual agreements in optimization models. The resulting model will be used as a testing tool in SQ6, to support, adjust or reject our hypotheses (SQ3). The model will cover a time-span of 30 years, from the present time to 2050. This choice is due to the availability of data and to the fact that the coming 10 years represent a key period for increased R&D activity, piloting and final investment decisions for decarbonization technologies. As a consequence, such technologies are expected to have reached maturity before 2050.

The model will be based on Mixed Integer Linear Programming (MILP), which has inspiringly been applied in several studies for optimizing clusters' performance (Jamal & Montemanni, 2018; Pedrozo, Rodriguez Reartes, Chen, Diaz, & Grossmann, 2020; Pirim, Eksioglu, & Glover, 2018). This will obviously entail some degree of simplification of the actual (non-linear) relations in a cluster, but hopefully will be representative of the real dynamics. As previously argued, this limitation cannot be completely overcome in this research, but we should note that the final MILP model serves as a proof of concept of the effects of contracts on the energy transition, not as a predictive model of future cluster's developments.

The model will be developed in Linny-R, a dedicated software tool for industrial process optimization relying on a MILP solver. This tool can model production systems as a cluster of processes, and allows for nested modelling (i.e. processes within firms within clusters). It allows to visualize the impact of an (institutional) intervention on the cluster performance, both from a technical and economic perspective. Moreover, it allows optimising cash flows for the total cluster or for selected companies. All these features make Linny-R inherently suitable for incorporating institutional elements such as contracts. However, it is worth noting that contractual structures have never been implemented in Linny-R, to the best of our knowledge. Hence, this adds an appreciable element of novelty to this research, which will provide an innovative design for the inclusion of contracts in MILP.

The effects of different contractual structures on investment decisions in decarbonization options will be analysed by comparing optimal investment paths, selected by the optimization. Besides assessing the optimal sequence for investments, the effects of contractual structures on investment decisions will be quantified by benchmarking the cluster's performance on the basis of the total cluster's cash flow and its distribution among cluster members. As a result, an answer to the main research question will be provided.

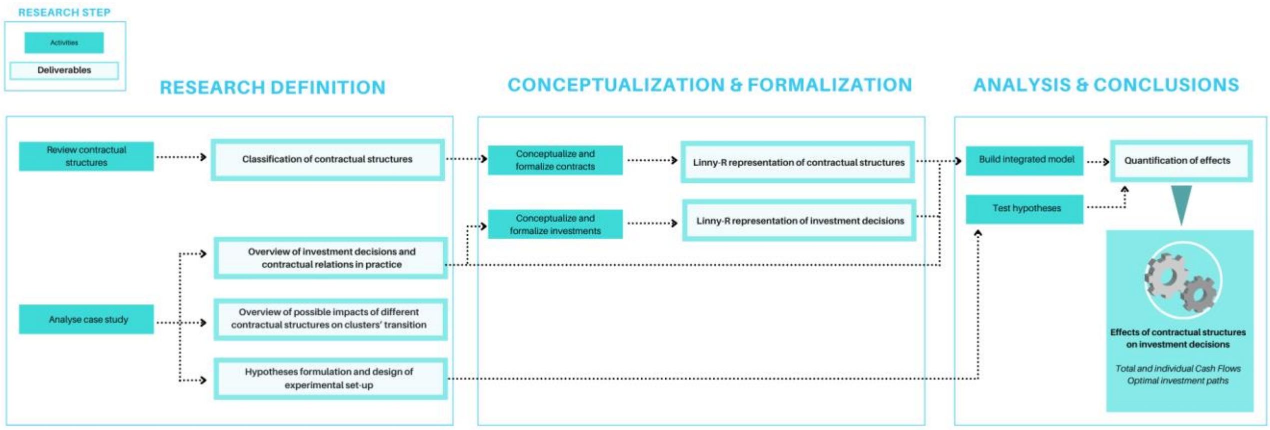


Figure 2. Research Flow Diagram

1.6. Research structure

This thesis is structured as follows. Chapter 2 specifies the theoretical lens through which contracts are analysed, and presents a preliminary categorization of contractual structures based on scientific literature. Chapter 3 explains how contractual structures are operationalized in practice by means of an analysis of major investment projects in the Rotterdam cluster. Chapter 4 conceptualizes and formalizes the information gathered in the previous chapters to identify a methodology that incorporates investments and contracts in optimization models. In Chapter 5, an example of application of the proposed methodology is provided via a stylised model of the Rotterdam cluster, used as a testing tool to evaluate the effects of contracts on the transition. Results of such simulations are presented and discussed in Chapter 6. Lastly, Chapter 7 concludes this research by presenting the main contributions of this thesis and highlighting future research opportunities.

2. Contractual structures: theoretical context

This chapter presents and interprets scientific theories that are relevant to the research objective, in order to specify the theoretical lens through which contracts are analysed. After presenting the method to review scientific literature (Section 2.1), the theoretical relevance of the problem is discussed from an Institutional Economics perspective with the aid of the four-layered framework by Williamson (2000) (Section 2.2). The scheme allows to position the coordination issue addressed in our first sub-question in the theoretical debate. Section 2.3 addresses SQ1 via the Institutional Analysis and Development (IAD) framework by Ostrom (2010). As a result, an overview of existing contractual structures that shape inter-organizational collaboration is provided (Section 2.4), using solid theoretical foundations and partially answering SQ1.

2.1. Reviewing literature for contracts' classification

Industrial clusters present unique opportunities for collaboration, even between rival firms. Petrochemical industries are in fact highly integrated at several stages of the value chain, yielding competitive advantages over firms operating on an isolated basis: benefits resulting from this configuration include the optimization of capital investments, increased assets' utilization, exploitation of economies of scale and several other advantages (The European Petrochemical Association, 2007).

Challenges arising from the new competitive landscape in the industrial sector are calling for increased cooperation among industrial entities, pushing beyond existing synergies and complementarities among firms in a cluster. As the integration of fluctuating energy sources calls for new flexibility options, novel technical possibilities are being explored by industries –an example being the conversion of molecules into electricity and vice-versa. In addition, various technical options for the abatement of CO_2 emissions are being evaluated and implemented by industrial entities, which are increasingly seeking collaboration to jointly realize such investments (Y. Melese et al., 2016).

In the light of the above, we seek to provide understanding of these dynamics, through a critical reading of different scientific theories. To this end, a review of scientific literature is performed. Papers were selected by means of electronic journal databases, such as Scopus, Science Direct and Google Scholar. Initially, the string {"economic organizational theories" OR "institutional economics" OR "transaction cost economics" AND contracts AND (collaboration OR cooperation OR competition)} was used for a preliminary search to improve understanding on the theoretical background regarding contractual structures in an inter-organizational setting. Subsequently, additional search terms were added to this query, examples being {"structural governance" or "relational governance"} or {multi-actor AND theory AND "petrochemical industry" OR "chemical industry"}. From here, forward and backward snowballing techniques were used to select papers regarding game theory and its applications to the energy-intensive industrial sector. Papers were scanned and selected based on the criteria "the article provides an overview of the theoretical context surrounding the use of contractual structures in inter-organizational settings", "the article specifies behavioural assumptions of actors involved in a contractual agreement" or "the article distinguishes interfirm collaboration and competition in industrial clusters from a theoretical perspective".

The string {("industrial clusters" OR "petrochemical industry") AND "joint investment" AND contracts} was used to identify contractual options available to industries and their key differences. Patterns were searched among these papers, based on the criteria "the article specifies relevant variables present in contractual arrangements underlying investment projects". These papers were subsequently used to apply the IAD framework.

Below we provide a schematic representation of the structure of this chapter including relevant literature that was used to address each section.

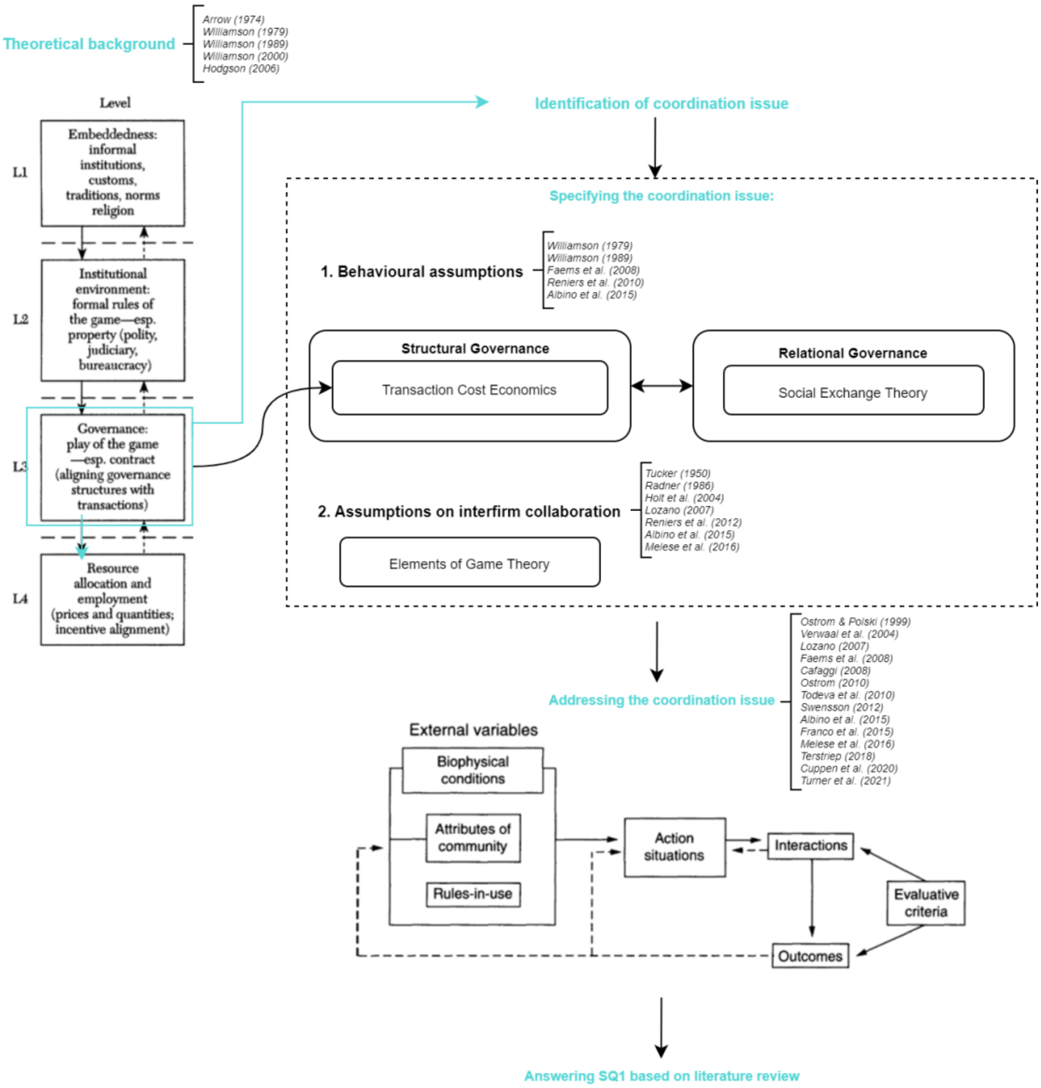


Figure 3. Structure of literature review, Chapter 2

2.2. Theoretical relevance

2.2.1. Identifying the coordination issue: Williamson's scheme

Economic organizational theories have made a major contribution to the analysis of inter-organizational coordination needs. To thoroughly explain organizational choices and rules, Williamson (2000) structured the rules that coordinate the activities of actors into a four-layered framework of economic analysis (Shafritz, Ott, & Jang, 2016). After providing an explanation of his four-layer scheme, we operationalize it in order to specify which coordination issue should be addressed as a first step towards solving our research problem.

Williamson's scheme provides a lens to study the complex economics of "institutions", defined as "systems of established and embedded social rules that structure social interactions" (Hodgson, 2006). According to Williamson (2000), institutions can be categorized in four layers of social analysis, as shown in Figure 4. Higher and lower levels interact with each other, imposing constraints on the ones below, and feeding back into the levels above (Williamson, 2000).

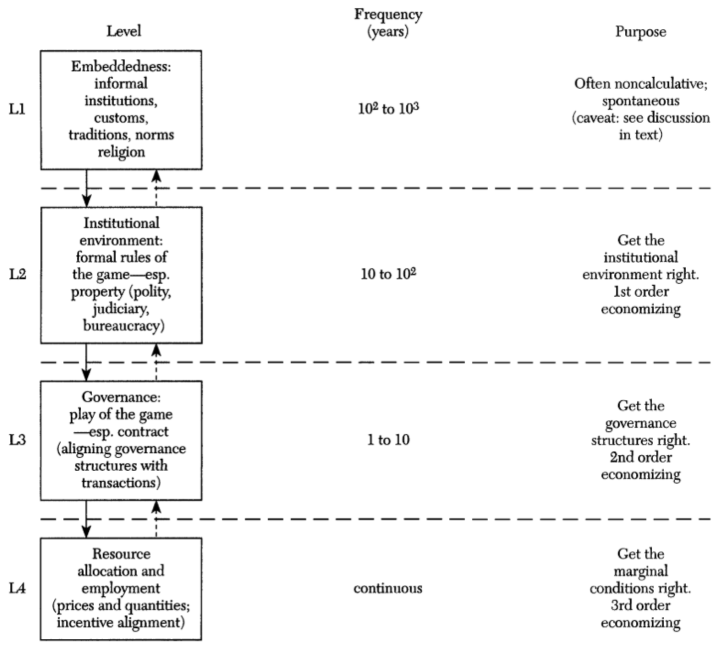


Figure 4. Four-layer scheme of the Economics of Institutions by Williamson (2000)

The first level is the "social embeddedness" level, which includes informal institutions such as norms, customs and traditions. They have mainly spontaneous origins and, as they stem from evolutionary patterns, they change very slowly (i.e. centuries or millennia), shaping the way society behaves. Because of these features, institutions at this level are regarded as given for most economists (Williamson, 2000).

The second level is the "institutional environment" level, where formal institutions are located, including laws and property rights. These institutions represent the "rules of the game" within which economic activities are organized and stabilized. Changes occur at rare windows of opportunity, or "defining moments" such as civil wars or financial crisis, in the timeframe of decades to centuries (Williamson, 2000). In the 1960s, the claim that the legal system would create order by defining and enforcing property rights was widely accepted. However, many transactions did not fit in this context. Thus, the need of moving beyond the rules of the game, towards the "play of the game" arose.

With this premise, the governance of contractual relations walked in during the 1970s. This corresponds to the third layer of Williamson's scheme, namely the "governance" level, which specifies the conditions under which actors engage in transactions and cooperate. Transaction Cost Economics (TCE) operates in this layer, under the constraints imposed by the rules of the game. According to this theoretical framework, governance is aligned with transactions in "an effort to craft order, thereby to mitigate conflict and realize mutual gains", by reshaping actors' incentives (Williamson, 2000). This theory analyses the comparative costs of task completion under alternative governance structures, and adopts a contractual perspective, focusing on institutions that serve to harmonize trading between parties with otherwise adversarial interests (Williamson, 1989).

This influences the fourth level of institutions, namely the "resource allocation and employment" level, which entails the examination of costs, benefits and outputs of individual actions (i.e. marginal analysis), resulting from contracts specified in the level above. Neoclassical economics and agency theory operate at this level. Agents base their decisions on price and output adjustments and, since these elements continuously change depending on market conditions, this is the fastest changing institutional level (Williamson, 1979).

Our research is well positioned in the governance level of Williamson's scheme (L3), as we aim to test the effects of different contractual structures on the optimal investment path to decarbonize the petrochemical industry. This in turn influences the level of resource allocation and employment (L4), since adjustments to prices and outputs are typically the variables constrained in contractual agreements. The overarching coordination issue positioned in L3 and L4 is addressed in our first sub-question: *SQ1: "Which contractual structures can be identified, based on different forms of collaboration among contractual parties?"*

Before attempting to provide an answer, we need to define key concepts mentioned in SQ1: having specified which behavioural assumptions apply to contractual parties and how collaboration is defined in theory, we will address the coordination issue arising from this sub-question.

2.2.2. Specifying the coordination issue: behavioural assumptions

Transaction Cost Economics (TCE) is the organisational theory operating on L3 of Williamson's scheme. As such, it is used as a starting point for the identification of assumptions that apply to economic agents. TCE relies on the behavioural assumptions of (i) bounded rationality and (ii) self-interest seeking agents. The former refers to economic actors as "intendedly rational, but only limitedly so" (Williamson, 1989). As such, individuals are assumed to have complete and transitive preferences, that allow them to state which option they prefer from a set of alternatives. According to rational choice theory, rational agents perform their own analysis of potential costs and benefits of a decision, to determine which action to pursue in order to achieve the best outcome. Nevertheless, contractual parties have limited cognitive capabilities and do not have perfect foresight.

This assumption is coupled in TCE with the self-interest-seeking assumption: according to Williamson (1989), individuals intrinsically aim to maximize their profits, thus tend to act opportunistically in order to realize gains (Williamson, 1989). Thus, a central function of formal governance mechanisms (i.e. contracts) is to harmonize interests of involved actors, that would otherwise lead to pursuit sub-goals antagonistically (Williamson, 1979).

The assumptions of TCE constitute the essence of the "structural perspective" of the governance of inter-organizational relations, which proposes contracts as main governance mechanism to mitigate opportunism. In other words, according to the structural perspective, contracts constitute safeguarding devices that create a predictable collaborative environment, mitigating transaction hazards and facilitating coordination among involved actors (Faems, Janssens, Madhok, & Looy, 2008).

This perspective is opposed to the "relational perspective" of governance, which instead relies on social exchange theory to explain collaborative patterns: opportunism and contractual hazards are neglected in this perspective, which places more emphasis on informal governance mechanisms, such as trust. This constitutes the main safeguarding mechanism of a collaboration.

Table 1 presents the characteristics of the two perspectives. Both of them have been criticized, as the former does not take into account the social context beyond transactions, while the latter holds an excessively optimistic view of human nature (Faems et al., 2008). Hence, relying on one perspective alone does not suffice to fully capture the behaviour of contractual parties (Reniers, Dullaert, & Visser, 2010).

Table 1. Structural and Relational perspectives on Alliance Governance, adapted from (Faems et al., 2008)

Characteristic	Structural Perspective	Relational Perspective
Focus of analysis	Single transaction	Inter-firm relationship
Theoretical basis	Transaction cost theory	Social exchange theory
Main assumptions	Partners act opportunistically Alliance performance is driven by the quality of the initial structural design	Alliance performance is driven by the quality of the ongoing relational process
Proposed governance mechanism	Complex contracts	Trust
Criticism	Under-socialized view of human actions	Over-socialized view of human actions

In our research, we attempt to bridge these two perspectives, by combining assumptions from both structural and relational governance. A socialized view of human actions is given its relevance, postulating that being part of an industrial cluster presupposes a basis of trust among industrial entities –as their processes are highly integrated and connected on different stages of the value chain. In fact, the existence of strong social ties among industries effectively increases cohesion and reduces opportunistic behaviour by companies (Albino, Fraccascia, & Giannoccaro, 2015). Still, industries will seek profit maximization, according to the behavioural assumptions of TCE of (i) bounded rationality of actors and (ii) self-interest seeking agents. Thus, industries will decide whether to opt for a competitive or collaborative strategy based on which one yields the highest benefits. This choice may potentially give rise to opportunistic behaviour. To this end, we consider contractual arrangements as the proposed governance mechanism to cope with potential opportunistic behaviour in interfirm relationships, consistently with the premises of the structural perspective. The subsequent section further defines the concepts of cooperation and competition in the context of industrial clusters.

2.2.3. Specifying the coordination issue: inter-firm collaboration

Achieving CO_2 neutrality in the petrochemical industry is no easy task, as technical, institutional and multi-actor dependencies need to be taken into account. The parties involved are subject to constraints and pursue different goals, thus potential conflicts might arise within the actor network (Lozano, 2007). This endogenous uncertainty resulting from strategic behaviour is coupled with exogenous uncertainty, related to technological constraints, market fluctuations or regulatory changes (Y. Melese et al., 2016). In such context, parties become afraid of "betting on the wrong horse" and need to weigh the costs and benefits of collaboration against the ones of competition. Given these premises, the decision to engage in inter-firm collaborations can be framed as a multi-motive game (Y. Melese et al., 2016).

Sizable literature on deterministic game theory models has addressed the allocation of value from cooperation, and some of them have inspiringly been applied to inter-firm collaboration in chemical clusters for several purposes. In this study we apply concepts of game theory to analyse which strategies can be undertaken by industries to work towards the energy transition, in the attempt to provide a definition of collaboration in industrial clusters.

Game theory is a discipline that models and interprets decision making in strategic games. It conceptualises multi-actor decision making in terms of three components: players, strategies, and payoffs. Player *i*'s strategy is defined as "a rule for choosing an action at every point that a decision might have to be made", while player *i*'s payoff function specifies the utility of the chosen strategy (Reniers et al., 2012). In such games, a single decision is made by each player without knowing decisions made by others prior to their own move.

Two broad categories of games can be distinguished in game theory: zero sum and non-zero sum games. In a zero sum game, actors choose their strategies aiming at profit maximization: however, what is won by one actor is lost by the others, so that the arithmetical sum of gains and losses is zero (Lozano, 2007). Non-zero sum games, on the other hand, allow gains minus losses to be larger than zero, since the importance is reaching the system's optimum in which the total gain is maximized and all actors win (Lozano, 2007).

Conceiving the transition of chemical clusters as a zero sum game is clearly unrealistic, given the complex interrelations of activities and exchanges among stakeholders (Lozano, 2007): applying a zero-sum game to chemical clusters would mean optimizing investment decisions for one actor solely. Thus, alternatives that would be beneficial for the whole industrial configuration would be ignored.

This strategy is not viable in a cluster setting due to the continuous interaction between companies whose operations are integrated in subsequent stages of the value chain.

Non-zero sum games are best suited to deal with such a diverse, complex environment (Lozano, 2007), as they allow to search for the common interest of the cluster, exploiting the various complementarities of the system to achieve the optimal sustainable strategy for all actors. Hence, in this research we adopt this theoretical lens to analyse the choice between collaboration and competition in the transition of industrial clusters.

A class of problems that attempts to compare outcomes of competition and collaboration is the family of "social dilemmas": here, the socially desirable outcome can only be achieved by direct collaboration among players. One of the best known problems belonging to this family is the Prisoner's Dilemma (PD) (Tucker, 1950), a situation in which two rational players both fail to achieve the optimal collaborative outcome because they have no means to build trust. Thus, they opt for a "best response strategy" to hedge themselves against the risk deriving from the other player's choice. Note that the best response strategy is chosen by both players only because of no possible cooperation: uncertainty about the other player's move makes each player chose the strategy that is his best response to whatever the other might choose. However, had the players been able to exchange information and cooperate, they would have earned a higher payoff.

In light of the above, the PD allows to distinguish between "non-cooperative" and "cooperative" outcomes (Radner, 1986). The non-cooperative outcome results from the best response strategies of the players, in which all players maximise their individual payoff, anticipating that the other players will do likewise. In this setting, Nash equilibria can be identified. These are equilibria because, given the possible strategies of the rivals, each player has no incentive to deviate from his strategy, or else it would lower his payoff. As a result, no external means of enforcement is needed to maintain this equilibrium, since it is in the self-interest of each player to maintain their positions (Holt & Roth, 2004).

On the other hand, a cooperative outcome that yields higher payoffs is defined as "Pareto optimal". Although also this strategy is regarded as rational (as it leads to the mathematical optimum for the system) (Radner, 1986), it cannot materialize in reality without the correct enforcement mechanisms in place. The cooperative outcome, in fact, is not an equilibrium and is going to be unstable in ways that can make cooperation difficult to maintain (Holt & Roth, 2004). Thus, institutions are needed to transform games from prisoner's dilemmas into games in which cooperation is a sustainable equilibrium (Holt & Roth, 2004).

The transition of energy-intensive industrial clusters can be seen as an example of the prisoner's dilemma. Players are represented by industries of the cluster, who make investment decisions in cleaner technologies. When choosing their strategies, industries can either jointly invest in a project and cooperate, or make investment decisions individually, obtaining different monetized payoffs. A Nash equilibrium or a Pareto-optimal outcome can result from such strategies.

We assume that a Nash equilibrium is achieved in the cluster when each industry chooses its strategy to balance its investments' gains and costs with its environmental performance (for instance, quantified through monetized emission levels) to maximize its payoff, being constrained by the strategies of the other players. In this way, a non-cooperative outcome is obtained, in which industries make their own investment decisions without considering the impact that the combination of these decisions (i.e. the resulting strategy) would have on the overall cluster. Thus, we conclude that Nash equilibria are obtained as a result of competitive strategies in a non-zero sum game. As a result, we define competition in a cluster as a non-cooperative strategy in which no agreement is needed as enforcement mechanism, and in which each industry seeks to maximize its payoff subject to the constraints of investment decisions made by other players.

In contrast, a Pareto-optimal outcome is obtained when all the industries choose their moves collectively, such that the resulting strategy generates the highest total payoff (i.e. the sum of the payoffs for the individual players). However, this does not imply that every industry will be better off: the payoffs of some players might be so high that can amply compensate the negative payoffs of some of other industries. In case of unevenly shared benefits of cooperation, a misalignment incentive problem arises (Albino et al., 2015). Thus, a Pareto-optimal outcome can materialize in reality only when the companies are willing to negotiate and reach an agreement both on their strategies and on how to redistribute the obtained payoff, modifying the incentives of individual firms and pushing each other to behave in a way that is desirable for all parties. Such a situation is stabilized by means of contracts as external enforcement mechanisms, which specify how the involved actors share pains and gains of the cooperative strategy, as a result of a joint investment decision. In this study, we refer to this situation as a collaboration among industries, namely a cooperative strategy in which contracts are needed to distribute benefits and costs resulting from investment decisions that maximize the overall profit of involved industries.

The main conclusions on how inter-organizational relations can be presented in terms of Game Theory are schematized in the figure below.

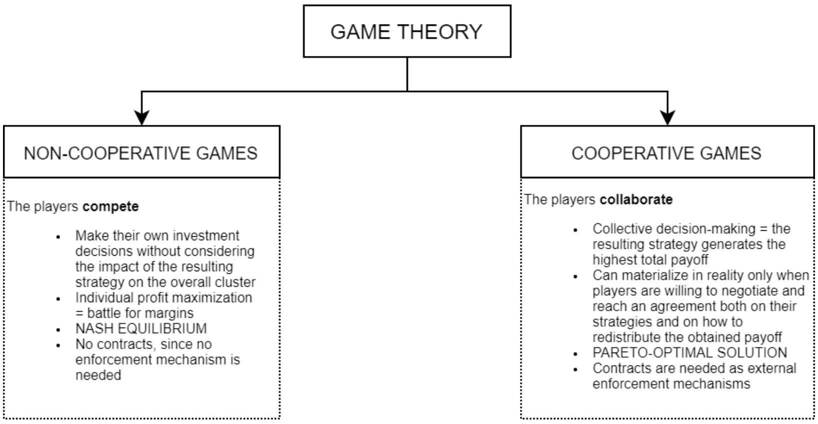


Figure 5. Overview of players' strategies based on Game Theory

2.3. Addressing the coordination issue

Having specified key assumptions and definitions underlying the coordination issue, we have concluded that a collaboration of industries needs contracts to solve the misalignment incentive. We now need to understand which contractual options are available to the players, and what are their key differences. To this end, we will first identify which variables are present in all contractual agreements and how do they differ from a contractual structure to another.

The Institutional Analysis and Development (IAD) framework by Elinor Ostrom suits this purpose since, according to the author, it "should identify the major types of structural variables that are present in all institutional arrangements, but whose values differ" (Ostrom, 2010). After providing an explanation of the IAD framework, we will apply it to differentiate contractual agreements that support investment decisions in decarbonization options.

2.3.1. The Institutional Analysis and Development Framework

The core of the IAD framework is an action situation influenced by external variables, namely (i) biophysical conditions, (ii) attributes of a community and (iii) rules-in-use. The biophysical conditions refer to the good that is produced, exchanged and consumed by the actors. Attributes of a community represent the cultural context: as such, they include common understanding of activities and preferences about strategies (Ostrom & Polski, 1999). Finally, the rules-in-use are formal and informal rules that affect the behaviour of actors involved in the action situation: more specifically, they establish who may or may not take specific actions in a given interaction (Ostrom, 2010). The external variables affect the action situation, creating patterns of interactions and outcomes that are evaluated by the actors involved, and feedback both on the external variables and on the action situation (Ostrom, 2010). A schematic representation of the IAD framework is displayed below.

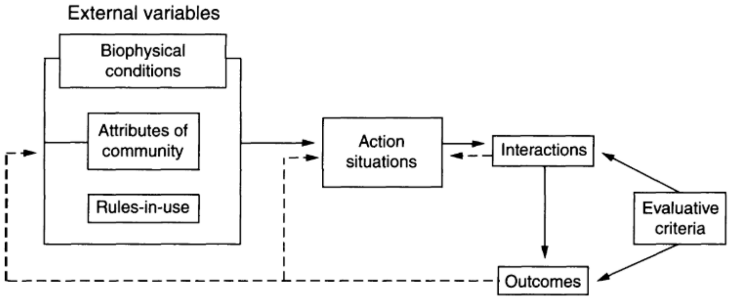


Figure 6. Institutional Analysis and Development framework (Ostrom, 2010)

The action situation (or action arena) consists of a conceptual space where participants ponder alternative decisions, take actions and experience the consequences of these actions (Ostrom & Polski, 1999). Ostrom (2010) identifies seven internal working parts of an action situation, which are "overtly consistent with the variables that a theorist uses to analyze a formal game"(Ostrom, 2010). In order to specify the structure of such game, the analyst needs to specify (i)the characteristics of the actors or participants involved, (ii) the positions roles that actors hold in this situation, (iii) a set of actions that participants can take, (iv) the level of information available to each actor, (v) the level of control actors have over decisions to take action, (vi) the possible outcomes of actions and (vii) the costs and benefits incurred by participants as a result of a linkage of actions or outcomes. The relations between these seven working parts are shown in Figure 7.

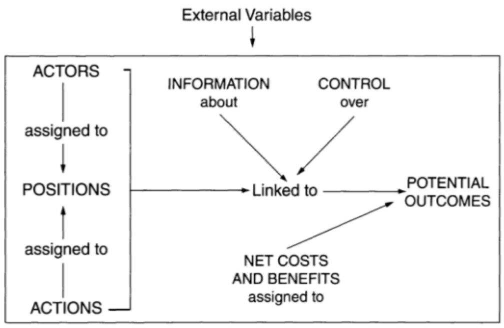


Figure 7. Internal structure of action arena (Ostrom, 2010)

2.3.2. Applying the IAD framework to the transition of energy-intensive industrial clusters

In order to address collective action problems and identify its possible outcomes, we first need to specify the set of external variables affecting the action arena.

Biophysical conditions

In this project, we will evaluate investments in infrastructure along with processing units for different products. Each feedstock/product obviously requires specific investments for its processing and integration, however all of them present common characteristics, such as high asset specificity and long asset lifetime (Todeva & Fu, 2010; Verwaal & Hesselmans, 2004). An investment is said to be asset-specific based on the extent to which that asset can be redeployed to alternative uses without losing its productive value significantly (Williamson, 1989). Generally, such investments are specific to a particular transaction and cannot be fully recovered from alternative uses. According to TCE, asset specificity elicits governance structure responses (Williamson, 1989): more specifically, long-term contracts are generally employed as a safeguard mechanism, to protect highly specific investments (Verwaal & Hesselmans, 2004). Moreover, when a company invests in a new technology, it does so envisioning its utilization for a long period of time. Together, long-term contracts and long lifetime of assets have created inertia in innovating production processes.

Attributes of community

The social embeddedness and the climate of trust in an industrial is an important factor for nurturing and sustaining cooperative exchange (Albino et al., 2015). Asset-specific investments foster the development of interfirm collaborations beyond cluster complementarities, to share and reduce risks and costs of decarbonization initiatives, while obtaining financial rewards (Franco & Haase, 2015).

Rules-in-use

When the owner of a process makes an investment decision, its business case will strongly depend on the rules-in-use, such as new regulation and contractual arrangements in place, decreasing the flexibility of the system (Cuppen et al., 2020).

The external variables described above influence the action situation, which is now further specified to unravel possible outcomes stemming from the interactions in a cluster setting.

Action situation

The actors involved in the action arena consist of the petrochemical industries of the cluster which, as concluded in Section 2.2.2, act according to the model of human choice of TCE. Companies hold the positions of players that seek profit maximization, consistently with the assumptions of game theory. In a competitive setting, each player makes investment decisions in the attempt to maximize its own profit while being constrained by other players' strategies. If a cooperative strategy is chosen, on the other hand, investment decisions are taken by actors in such a way that the resulting strategy yields the highest total payoff. Subsequently, contractual agreements need to make such investments attractive for all the companies involved (Lozano, 2007; Turner, Race, Alabi, Katris, & Swales, 2021).

Given these premises, actors can either compete or collaborate to develop a portfolio of options to abate CO_2 emissions, and they can take several system-level actions. Considering value chains as the backbone, firms in the cluster can form linkages on a vertical, horizontal and lateral level, as shown in Figure 8. The vertical dimension entails collaboration among complementary firms, connected by input-output relations –such as suppliers, service providers and customers (Terstriep & Lüthje, 2018). Horizontal relations refer to linkages among firms that operate at the same stage of the value chain (i.e. competitors). Finally, the lateral dimension includes relations with actors outside the cluster boundaries, such as public bodies, research organizations and universities.

Stakeholders' actions at the vertical, horizontal and lateral levels lead overtime to the establishment of norms and behaviours that form the institutional cluster dimension (Terstriep & Lüthje, 2018). As a result (i.e. potential outcomes, in the IAD jargon), participants form "contractual networks" as a way to coordinate their economic activities towards the achievement of a common objective (Swensson, 2012). A contractual network is a collaborative structure in which parties – that can even be competitors –aim to conduct one or more projects of common interest to achieve strategically significant goals (Cafaggi, 2008; Swensson, 2012). It constitutes a legal configuration of relationships characterized by strong economic interdependency among enterprises (Cafaggi, 2008).

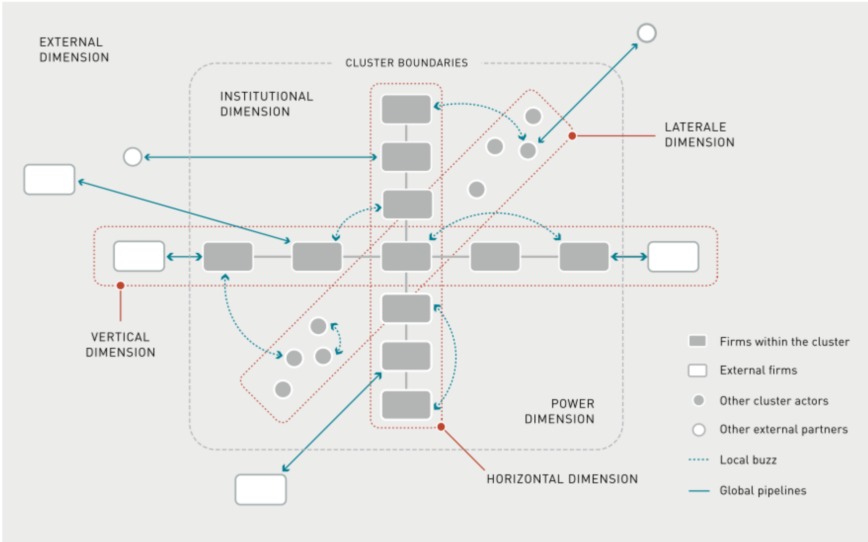


Figure 8. Multidimensional representation of cluster's relations (Terstriep & Lüthje, 2018)

Patterns of interaction

Depending on how actors agree on the distribution of costs and benefits of their collaboration, several forms of contractual networks can be identified. Such forms constitute the patterns of interaction, namely the structure resulting from the conduct of actors. In principle, there can be infinite structural forms of a contractual network: thus, the effort is to distinguish such forms in relation to existing conceptual devices in legal systems (Cafaggi, 2008). With this premise in mind, contractual networks can take mainly two legal forms (Cafaggi, 2008; Swensson, 2012):

1. **A set of interdependent, linked bilateral contracts**: the contractual network can assume several configurations based on how the exchanges among two contractual parties take place, on a horizontal or vertical network;

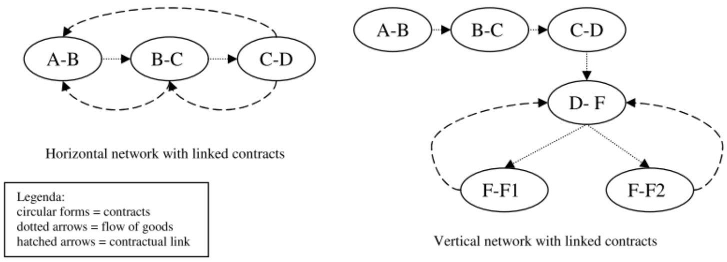


Figure 9. Example of contractual network governed by a set of bilateral contracts (Cafaggi, 2008)

2. **A multilateral contract:** this configuration allows the coordination of economic activities of more than two parties simultaneously. Typical examples of this legal form include the networks formed through contractual joint ventures and, most commonly, through consortia.

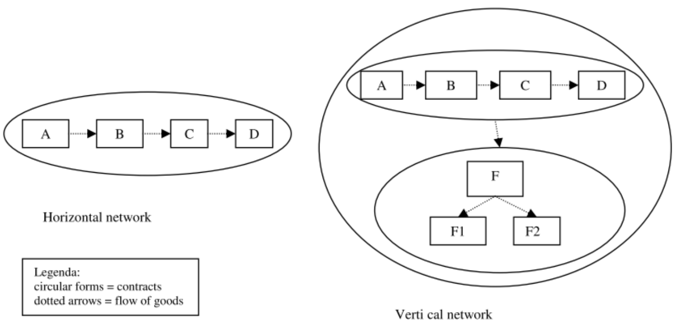


Figure 10. Example of contractual network governed by multilateral contracts (Cafaggi, 2008)

Final outcomes

The last element of the IAD framework to be discussed is the analysis of final outcomes, with the objective to draw conclusions on the performance of the institutional system (Ostrom & Polski, 1999). As anticipated, this insight is gained implementing an optimization model in Linny-R. The output of the model will provide the evaluative criteria to assess the implications of adopting different contractual structures on investment options.

2.4. Defining relevant contractual structures

The two main legal forms of contractual networks described above, together with the typical configurations they assume, deserve some further explanation.

2.4.1. Linked bilateral contracts

Bilateral contracts constitute a contractual network when there are two or more linked contracts among three or more contractual parties (heterogeneity) (Cafaggi, 2008). This implies that multiple linked contracts between the same two parties do not represent a contractual network (homogeneity).

The contracts are linked based on different interdependencies for different purposes. For instance, a contract may be valid conditional upon other contracts, or the setting of prices may depend on other contracts. Thus, the use of conditions is generally used to link bilateral contracts with each other, especially when sequential performances along the supply chain require the deployment of subsequent contracts (Cafaggi, 2011). Hence, we deduce that this kind of contractual network is normally used to coordinate product exchanges rather than focusing solely on the realization of investment decisions. The latter, however, constitute relevant aspects to be evaluated by parties entering the bilateral exchange, as contract prices will also be dependent on CAPEX and OPEX of investment decisions.

2.4.2. Multilateral contracts

A network of multilateral contracts is established when multiple actors cooperate towards a common objective by combining their resources (Swensson, 2012). Thus, this model of contractual network normally implies joint investment decisions and/or resource pooling (Cafaggi, 2008).

Multilateral contracts involve more than two parties, subject to the same standardized conditions (Cafaggi, 2008). As previously mentioned, typical examples of this legal form include contractual joint ventures and consortia, now addressed in more detail.

2.4.2.1. Joint Ventures (JVs)

A joint venture (JV) can be described as a collaboration agreement in which two or more enterprises cooperate on a project by coordinating the use of resources of individual participants and by distributing risks, costs and profits resulting from the investment (Cafaggi, 2008). JVs may take the form of contractual (i.e. unincorporated) JVs when the parties wish to rely solely on contractual agreements. On the other hand, parties can decide to create a new legal entity (organised as a corporation) to pursue their shared undertaking, thus forming an incorporated JV (UNIDROIT, 2019). In both cases, there will be a general agreement between the parties defining the basic terms of the JV (such as the object and duration of the JV and the contributions of each party). This general JV agreement is used in conjunction with various ancillary agreements between the JV and its shareholders specifying in detail the organisation and management, share in profits and losses, termination of the JV, etc. (Cotula, 2010; UNIDROIT, 2019).

In a JV, rules are specified for sharing costs and profits (Kogut, 1988). In this respect, it is necessary to clarify each party's contribution to the joint venture: in fact, the participation of each party in profits and losses is dependent on equity shares, which in turn are linked to the parties' contribution (Cotula, 2010).

Normally, the JV assumes all the costs: thus, due to the JV structure, the parties automatically share the costs. Parties then distribute the profit (or loss) consistently with their stake in the JV (Bouckaert, 2018). The offer price determining the revenue stream is established jointly (Bouckaert, 2018).

2.4.2.2. Consortium agreements

In commercial law, a consortium agreement is considered as a collaboration agreement which does not imply the creation of an independent legal entity (Cafaggi, 2008). It can be defined as a "contractual relationship of two or more business entities [...] formed for the purpose of executing, jointly and severally, a specific contract, usually involving complex civil engineering, for the supply of goods and/or services" (Milton, 1979).

Differently from a JV, a consortium requires a definite scope allocation between the partners from the start of the project. Jointly, they are responsible for the whole scope (Bouckaert, 2018). A consortium crucially differs from a JV in that consortia lack a right to share profits (Milton, 1979). Each partner's potential profit or loss depends on the relevant party's performance on its scope. The actual profit is not known by the other partners: one party can incur a loss, while the others making profit do not need to compensate (Bouckaert, 2018). Hence, profit calculations are independent from calculations of other members (Milton, 1979).

Regarding the financing of a consortium project, partners usually avoid sharing of costs, and allocate costs to specific parties within their own scope (Bouckaert, 2018; Milton, 1979). However, companies bidding on the project may jointly arrange some kind of long-term financing – for instance, via a subsidy (Milton, 1979).

2.5. Concluding remarks

This chapter has placed our research into perspective, by specifying the theoretical lenses through which contracts are analysed. We have defined behavioural assumptions of industrial players and framed investment decisions as multi-actor games, ultimately distinguishing competitive and cooperative strategies, based on key concepts of game theory. Subsequently, the literature review has allowed to provide an overview of existing contractual structures that shape inter-organizational collaborations. Main legal forms of contractual networks have been defined, together with typical configurations these contractual structures assume (such as consortia and JVs). In this way, we have provided an initial classification of contracts, partially answering SQ1. This is further addressed in the next chapter, by understanding how contractual networks are operationalized in practice.

3. Contractual structures in practice: investment projects

This Chapter presents examples of major investment projects in the Rotterdam cluster, showing how the contractual structures addressed in Chapter 2 are operationalized in reality. Section 3.1 discusses the current competitive position of the Port, together with the envisioned plans for its transformation. Decarbonization options are presented with special attention to the envisioned actor configuration realizing the investments. The resulting contractual network is analysed in Section 3.2: this allows for a more thorough categorization of contractual structures in the context of industrial cluster, ultimately answering SQ1. Additionally, this analysis serves as a starting point to identify possible impacts of different contracts on clusters' transformation (Section 3.3.), thus providing an answer to SQ2. The rest of the section provides guidance on the experimental setup to be adopted to test such effects on the transition of the Rotterdam cluster: as a result, hypotheses are formulated, hence answering SQ3.

3.1. The Port of Rotterdam under transition

In the previous chapter, we have shown that industries in a cluster form contractual networks in order to coordinate their economic activities towards the realization and operation of projects of common interest. To provide a deeper understanding of these concepts, we have selected a set of investment plans that are currently under evaluation in the Rotterdam cluster.

3.1.1. Current processes and operations

The Port of Rotterdam is regarded as a leader in fossil fuel production in North-West Europe, with fossil fuel resources constituting more than half of its total throughput (52%: coal, crude oil, mineral oil products, and LNG) and bringing two-thirds of the economic added value in industry (Notermans, van de Lindt, van der Have, van Raak, & Rotmans, 2020). Considering the fossil value chain as backbone, the port is well positioned with its petrochemical complex, where refineries in the Pernis, Botlek and Europoort areas convert crude oil into fuels and chemicals. Refinery off-gas, as well as natural gas, are currently used in Steam Methane Reforming (SMR) processes to produce grey hydrogen, whereas methanol and ammonia are imported (Port of Rotterdam, 2020b).

Its strong position in fossil value chains has enhanced Rotterdam's competitive position, but it has also created a significant challenge in abating CO_2 emissions. In order to maintain its dominant position in the long-run, the port needs to move beyond fossil production processes and look for alternative, sustainable technologies.

3.1.2. Options for decarbonization

The port is working towards climate neutrality and circularity through efficiency measures and infrastructure (3.1.2.1), and is attempting to transition to a new energy system (3.1.2.2), by switching from oil and gas to electricity, hydrogen and green hydrogen.

3.1.2.1. Efficiency measures

Efficiency measures are needed to ensure reutilization of outputs as feedstock for other processes or purposes. In fact, the industrial sector can save approximately 20% of energy through the optimization of production processes, by cooperating more efficiently with other parties (Port of Rotterdam, n.d.).

CO_2 capture, utilization and storage: PORTHOS

The capture of carbon dioxide for subsequent reuse or storage underground is one of the options that the energy-intensive industry can take into account for CO_2 emissions abatement in the short term: this goes under the name of Carbon Capture Utilization and Storage (CCUS). CCUS has considerable potential for the chemical sector, hydrogen producers and refineries to significantly reduce their production impacts in the short term, while working on more structural, CO_2 neutral, innovations (Porthos, 2020a).

Porthos, a joint venture between the Port of Rotterdam Authority, Gasunie and EBN, aims to contribute to CO_2 reduction with its CCUS project, in which CO_2 captured by various companies is transported and stored in depleted gas fields under the North Sea (Porthos, 2020a). At the moment, Porthos works together with four potential customers, with whom has signed a Joint Development Agreement (JDA): Air Liquide, Air Products, ExxonMobil and Shell. The JDA partners will be charged a fee for transporting and storing their carbon via Porthos. The precise amount of this fee is determined by the costs incurred by Porthos for the system's construction and exploitation (including the energy costs for the pressurised injection of CO_2 in the deeper substrate), thus there is still no clear estimate (Porthos, 2020b). In return, partners will not be required to pay EU ETS allowances for the stored CO_2. Ultimately, the Dutch government will cover the difference between the companies' total costs and savings with the SDE++ scheme (Porthos, 2020b).

3.1.2.2. New energy system

In order to change the energy system, industry needs to reduce its reliance on oil and gas and foster electrification from sustainable sources, as well as the use of hydrogen.

Due to its high interconnectedness, both nationally and internationally, the Port is well positioned to develop hydrogen production and trade, in coalitions with companies. Hydrogen can be produced in several ways, using different production technologies and energy sources, as summarized in the table below. Based on this categorization, hydrogen is distinguished in grey, blue and green hydrogen.

Table 2. Commercial hydrogen production options (Rijk & van Dinther, 2019)

Energy source	Production technology	CO_2 capture rate	Hydrogen purity level	Application
Green electricity	PEM electrolysis ALK electrolysis SOFC electrolysis (high temperature, TRL 4)	Not applicable	100%	Fuel cells Chemical processes Heating
Natural gas	SMR (with or without CCS) ATR (with or without CCS)	50-70% >90%	99% (with additional processes) 95%	Chemical processes Heating Heating

Hydrogen backbone

Key for the development of a hydrogen economy is the realization of a hydrogen backbone through the port area. Ideally, this infrastructure will be in place as early as 2025 and will supply industries with hydrogen produced in the port (Port of Rotterdam, 2020a). The backbone will be connected to the national infrastructure owned by Gasunie, repurposing the existing natural gas pipelines and integrating hydrogen storage in salt caverns –currently the only feasible option for long-term storage (Port of Rotterdam, 2020b; Rijk & van Dinther, 2019).

As an infrastructure company, Gasunie works with the Port of Rotterdam Authority on the development of the regional hydrogen backbone, in the port area. The parties intend to realise the new pipeline in a JV, both investing in the infrastructure (Port of Rotterdam, 2020c). In addition, the partners are discussing possibilities for support and contribution with government authorities (Gasunie, 2021). The backbone will be constructed between the areas of Maasvlakte and Pernis and will be an open access pipeline: as such, companies that intend to produce or consume hydrogen in this area can link up to it, establishing contracts with the JV (Gasunie, 2021).

Blue hydrogen: H-vision project

Several parties in Rotterdam have joined forces to develop installations to produce blue hydrogen on a large-scale, constituting the H-vision consortium. This partnership is planning to set up a central ATR plant to supply refineries and electric power companies with low-carbon hydrogen. The concept behind the partnership is to produce blue hydrogen from refineries' residual gases, supplemented with natural gas off-grid (H-vision, n.d.). H-vision transports these refinery gases to a central location where they are used to manufacture hydrogen. Almost all the CO_2 that is produced in this process is captured and stored in depleted gas fields in the North Sea. Thus, the H-vision project ties in very well with the CCUS infrastructure from Porthos. The blue hydrogen produced from the refinery gases is then reused as a fuel in the refining process, significantly reducing CO_2 emissions from the refineries affiliated to H-vision, as hydrogen combustion releases water.

H-vision's technology can be scaled up to industrial scale and deployed in the short-term. In the long-run, the required infrastructure and the installations of the H-vision project can also be used for the application of green hydrogen: in this way, investing in blue hydrogen paves the way for green hydrogen future, while contributing to a significant reduction of emissions in the short term.

The parties involved are: Deltalinqs, Air Liquide, BP, Gasunie, Port of Rotterdam, ONYX Power, Shell, Uniper, Royal Vopak, ExxonMobil, EBN and Equinor. Having positively concluded the feasibility study, H-vision's partners are conferring with the government about regulations and financial support (Port of Rotterdam, 2019a). Initially, H-vision will be investing in a regional network to connect production locations and consumers, including room for adding new users if needed. In the long run, H-vision plans to integrate into the Port's hydrogen backbone (H-vision, n.d.).

Green hydrogen: Shell, Nouryon/BP, Uniper

To integrate green hydrogen in the Port's value chain, the Port envisions the construction of a conversion park on the Maasvlakte. Here, hydrogen will be produced centrally by a concentration of electrolysers connected to high voltage cables from offshore wind farms, and transported to companies using the backbone (Port of Rotterdam, 2020a).The conversion park needs to reach a 2 GW capacity by 2030 (Port of Rotterdam, 2019b).

Shell has already announced its plans to operate a 150-250 MW electrolyser in the Maasvlakte's 2 GW conversion park in 2023, as a launching customer. From here, the produced hydrogen will be transported via the backbone to Shell's refinery in Pernis, to partially decarbonize fossil fuels' production (Port of Rotterdam, 2020c; Shell Netherlands, 2020). For this reason, Shell's electrolyser will be completed concurrently with the realization of the hydrogen backbone (Port of Rotterdam, 2020c). Moreover, Shell is awaiting for the realization of ongoing plans with Eneco: under the CrossWind joint venture, they are participating in the tender for the Hollandse Kust (Noord) offshore wind farm (Shell Netherlands, 2020).

Another project planned at this site is the H2-Fifty project, consisting in the construction of a 250 MW electrolyser for 2025 by BP and Nouryon as partners for the Port of Rotterdam (Port of Rotterdam, 2020a, 2020c). BP's refinery currently employs hydrogen from hydrocarbons for desulphurization of products, thus green hydrogen offers the possibility to substantially abate its emissions. Nouryon will build and operate the facility. Finally, the Port of Rotterdam will facilitate local infrastructure. The partners are looking into whether this will constitute a stand-alone project, or whether it will be integrated into the backbone in the Port and linked to the H-vision project (Port of Rotterdam, 2019b).

Similarly, Uniper and the Port of Rotterdam Authority are exploring options for large-scale production of green hydrogen, aiming to realise an electrolyser with a 100 MW capacity by 2025.

Subsequently, upscaling to 500 MW is envisioned (Port of Rotterdam, 2021). The project is still at an early stage, thus connections in the Port area are still being considered.

3.1.3. Multi-actor configuration

As a result of the investment analysis conducted in the previous paragraphs, we summarize interactions of actors and the resulting contractual network via a stakeholder map. The stakeholder map is further elaborated by the following elements:

i. *Investment projects:* investments are categorized based on the product they are related to. Each investment or block of investments referring to the same product is placed in a dashed, coloured rectangle with round edges, labelled with the name of the product;

ii. *Actor representation:* each actor is represented in a white rectangle. Rectangles with dashed perimeters are used for actors that are involved in the contractual structures but do not take part in the exchange of products: they refer, for instance, to parties that have a coordination role or an advisory role. They are still included in the stakeholder map because they may still obtain profits from the project.

iii. *Actors' relationships:* each investment project is further specified by a representation of the actors involved and the underlying contracts. Multilateral contracts, such as consortia and joint ventures, are represented by dark-grey rectangles around the actors included in the contract. Bilateral contracts are represented by two-headed arrows connecting actors contained in the same investment block.

iv. *Investments' relationships*: each relationship/linkage is graphically represented by an arrow (note that dotted arrows represent potential linkages among projects that might be possible in the future). Linkages are labelled via an alphanumeric code which is placed within square brackets. For example, [P1 | P2] describes the linkage between two investment projects, namely Project 1 and Project 2. Similarly, [P1 | EP1] describes the interconnection between Project 1 and Existing Process 1. Interfaces are defined in Table 3.

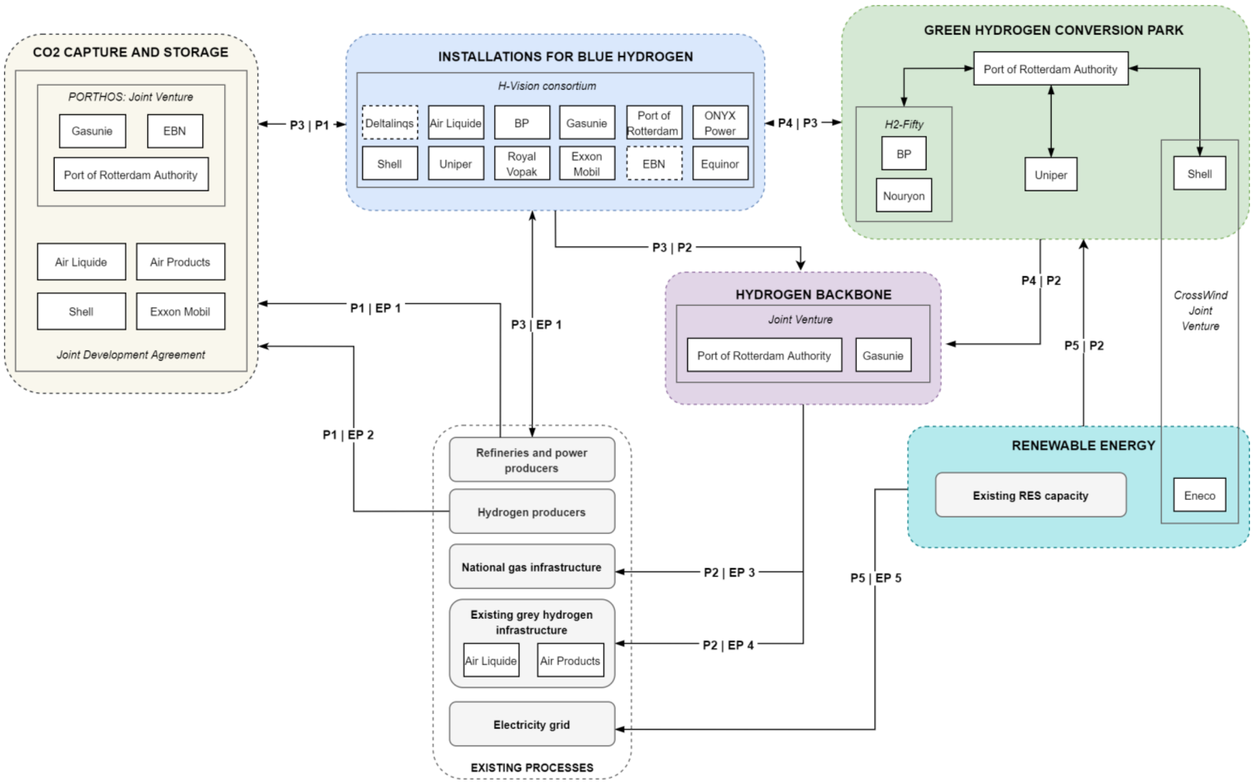


Figure 11. Stakeholder map Port of Rotterdam

Below, the alphanumeric codes used in Figure 11 to describe linkages are presented and explained.

Table 3. Overview of interfaces in the stakeholder map: Port of Rotterdam

[P1 | EP1] and [**P1 | EP2]:**	In addition to the JDA partners, other companies can join the project and connect to the pipeline to supply their CO_2 via additional JDA contracts
[P2 | EP3]:	The backbone will be connected to the national infrastructure owned by Gasunie, repurposing the existing natural gas pipelines and integrating hydrogen storage in salt caverns
[P2 | EP4]:	The port already features a hydrogen infrastructure which could be used to handle large volumes of hydrogen and related products. These networks are privately owned by Air Liquide and Air Products
[P3 | P2] and **[P4 | P2]:**	Several companies are envisioning the possibility of using the backbone pipeline [P2] to transport both blue and green hydrogen [P3 and P4]. Additional contracts with the JV will allow hydrogen transport
[P3 | EP1]:	H-vision transports refinery gases to a central location where they are used to manufacture hydrogen. The blue hydrogen produced from the refinery gases is then reused as a fuel in the refining process. The exchange of hydrogen is regulated via contractual agreements specifying the price and demand
[P3 | P1]:	Almost all the CO_2 that is produced this process is captured and stored in depleted gas fields in the North Sea. Thus, the H-vision project relies on the CCUS infrastructure from Porthos, via transport and storage contracts
[P4 | P3]:	The required infrastructure and the installations of the H-vision project can also be for the application of green hydrogen. Green hydrogen integration requires contractual agreements specifying the price and demand
[P5 | P2]:	Existing RES capacity and potential additional capacity resulting from investment projects [P6] are used to power electrolysis and produce green hydrogen
[P5 | EP5]:	Green electricity is transmitted using the electricity grid

3.2. Negotiating hydrogen contracts in practice

Figure 11 provides a basis to analyse contractual networks on two levels: (i)internal, regarding the relations among parties collaborating in a specific investment project, and (ii) external, related to the relationship between the members of each project and the rest of the cluster. Graphically, the former is represented by contractual agreements within an investment project, namely within the coloured, dashed rectangles labelled with the project's name. The latter is represented by the relations between the coloured rectangles, via the labelled arrows presented in Table 3.

Specifically, we observe that the former level of contractual networks regulates how to distribute costs and revenues among parties jointly realizing an investment project, consistently with the categorization provided in Chapter 2. We refer to these agreements as "investment-based contracts". Instead, the latter specifies how such investment projects are integrated with other cluster's processes, regulating how to exchange feedstock and/or products among cluster's members. This category of contracts goes under the name of "revenue contracts". By definition, a revenue contract is the agreement pursuant to which an off-taker buys all or a substantial portion of output from a facility, and provides the revenue stream supporting a project's financing (Ruiz, 2016).

Therefore, the analysis of contractual networks in practice allows for a further categorization of contracts: based on the incentives used to motivate the partners, contracts can be distinguished in (i) investment-based contracts and (ii) revenue contracts. Having provided an extensive literature review regarding investment-based contracts in Chapter 2, we now focus on describing the functioning of revenue contracts.

3.2.1. Revenue contracts

Sometimes the revenues produced by the project are the main, if not the sole source of payment for the loan. Consequently, a clear understanding is required of how the project's output will be sold, to which market will and what parties that will buy it (Ruiz, 2016).

Currently, there is an established hydrogen market, in which hydrogen is primarily produced through the reforming of natural gas. A limited number of producers is selling grey hydrogen to a limited number of consumers via bespoke bilateral contractual arrangements.

To ensure the analysed hydrogen investments are made, commercial frameworks need to be set up that are similar to those currently in practice: longer term bespoke bilateral contractual agreements (H-Vision Consortium, 2019). For long-term bespoke bilateral contracts, so-called offtake agreements have long been an investment vehicle of choice for renewable producers and LNG players, allowing producers to secure demand while hedging market participants from fluctuating commodity prices (Hydrogen Council, 2020).

For their similarities, it is informative to compare the nascent hydrogen market to LNG developments. LNG projects have identified two principal models of (offtake) revenue contracts, namely tolling agreements and sale-and- purchase agreements (Martin, 2021).

Under the LNG tolling model, an LNG facility provides natural gas liquefaction capacity to its customers. Each customer sources natural gas, delivers it to the liquefaction facility, and ships and markets the LNG produced with that natural gas. The customer pays the liquefaction facility to convert gas into LNG. Similarly, under a tolling model for blue hydrogen projects, the customer would buy the fossil fuel and pay the hydrogen plant to convert it into hydrogen (Dentons & OPERIS, 2021; Martin, 2021). For green hydrogen, the customer would purchase electricity to be used at the electrolyser and potentially supply the needed water. On top of that, the customer would pay a "conversion fee" to the owner of the electrolyser to convert water into hydrogen and oxygen.

On the other hand, under an LNG sale-and-purchase model, an LNG facility purchases (or produces) the upstream gas and is responsible for transportation to the liquefaction facility, liquefying the gas and then marketing it as LNG. Similarly, a blue hydrogen developer would procure natural gas and then produce and sell hydrogen made from it. Under a green hydrogen sale-and-purchase arrangement, a project developer would purchase electricity and water (Martin, 2021). This "integrated model" may allocate many risks to the hydrogen producer alone. Thus, several supply agreements may be advantageous. For instance, an electrolyser owner may buy electricity by entering into a Power Purchase Agreement (PPA) with a renewable power project: in this way, the electricity used is purchased in the spot market, but at a fixed price. Alternatively, the electrolyser owner may play a role in power production –for instance because the power and hydrogen producers have entered a joint venture agreement, as in the case of Shell and Eneco.

Such bilateral contracts may facilitate market penetration of blue and green hydrogen applications. However, once the market develops further and matures, it may be necessary to move to frameworks that are used for commodity wholesale trading, which make use of multilateral contracts where a standardized price is applied to all the parties involved in the transaction (H-Vision Consortium, 2019). In such multilateral perspective, the exchange could facilitate hydrogen with different characteristics (produced by different market participants), with the aim to market it as a single product (den Ouden, 2020). This requires a certain degree of standardisation. An in-between solution may be trading blue and green hydrogen as separate products, aggregating the hydrogen output from different producers to be sold at a standardized price per type of hydrogen.

An overview of the discussed contract classification is provided in the table below, ultimately providing an answer to SQ1.

Table 4. Overview table of contracts' classification

Type of contract	N° actors	Coordinated incentive				Contract form
		Investment-based contracts:		***Revenue contracts:***		
		Costs and revenue sharing		Price	Quantity	
Bilateral contract	*n=2*	Normally the investment is made by one actor with the counterparty's commitment to purchase the final product. Investment costs will enter price calculations for the exchanged material.		The customer purchases the feedstock and pays the producer to convert it to final product *Contract price = feedstock price + other fixed and variable costs + profit element (=conversion fee)*	Min-max production quantity	Bilateral contract: Tolling agreement
				The producer purchases the feedstock himself and sells product to customers at an agreed-upon price *Contract price = % of feedstock price + other fixed and variable costs + profit element*	Min- max production quantity	Bilateral contract: Sale-and-purchase agreement
Multilateral contract	*n>2*	*JV agreement* The participation of each party in gains and losses is dependent on equity shares: - Parties pool resources and share all the costs - Parties share the profit (or loss) consistently with their stake	*Consortium agreement* Partners usually avoid sharing of costs. Each partner's potential profit or loss depends on the relevant party's performance on its scope.	Generally partners decide the offer price jointly. Same standardized conditions apply to all the parties. *Contract price = single standardized price*	Min- max production quantity. Same standardized conditions apply to all the parties.	Multilateral contract: single standardized price
				Generally partners decide the offer price jointly. Same standardized conditions apply to all the parties. *Contract price = price standardization per commodity*		Multilateral contract: standardized price per commodity

3.3. Potential impacts on the transition of clusters

The hydrogen market must still largely grow in the coming years, in terms of both demand and supply. Thus, low-carbon hydrogen investors are beginning to consider key issues to be addressed via revenue contracts, but no measurable insight has yet been provided in their potential effects, being the market still in its infancy. Testing contracts' effects, given the specificities of low-carbon hydrogen breakthrough and the dynamic context of the energy transition, would amply reduce uncertainties. These issues are addressed in the following sub-questions:
SQ2: *"What are possible impacts of different types of contractual structures on clusters' transition, according to literature?"*
SQ3: *"How can the effects of contractual structures be tested in a structured manner?"*

To answer these questions, we first discuss foreseen effects of the classified contracts according to literature. Such elements are then used to formulate a set of testable hypotheses and to build the experimental set-up to obtain measurable insights.

3.3.1. Foreseen effects of contractual structures

Besides technical and financial uncertainties, it is crucial to consider how the commercial players can facilitate the integration and upscaling of the proposed investment projects.

Will it make sense for the same entity to purchase electricity, run the ATR facilities/electrolysers and sell to end-users, as in the case of sale-and-purchase agreements? This integrated model may leave the hydrogen producer managing a lot of risks (Dentons & OPERIS, 2021). On the other hand, such risks may be spread between the producer and the customer when adopting a tolling agreement: the customer would be responsible for procuring or supplying inputs, thus absorbing the risk of power supply and feedstock price. According to Martin (2021), customers that intend to use hydrogen for storage purposes, as a complement to electricity generation, may be more inclined to adopt a tolling model, as such customers have experience or portfolio benefits that may make them better suited to enter a PPA or other arrangement for feedstock supply. Users of hydrogen for other purposes may be less motivated to do so. Thus, given the investments selected in previous sections, we hypothesize that sale-and-purchase agreements are preferable to tolling models for hydrogen integration in industrial processes, as the former may create more incentives from the perspective of off-takers.

However, it should be noticed that end-users who are switching to hydrogen from another source of energy will not be used to buying energy on long-term contracts (Dentons & OPERIS, 2021). Hence, as previously stated, another possible approach for hydrogen integration in industrial applications is to move to frameworks similar to market conditions, which may make use of multilateral contracts. Although the aim would be to market blue and green hydrogen as a single product, a unique standardized hydrogen price may lead to a perceived lock-in of blue hydrogen, given no price incentives to switch to green (H-Vision, 2019). Thus, trading blue and green hydrogen as separate products with a standardized price per type of hydrogen may be a more attractive option.

The discussed positive (+) and negative (-) effects of contractual structures are summarized in the table below, distinguishing their implications for the considered categories of contractual parties. Besides answering SQ2, this offers useful guidance for the hypotheses formulation.

Table 5. Summary of effects of contractual structures according to literature

Contract form	Effects (+/-)	
	Producers	Off-takers
Bilateral tolling agreement	+: Reduced risk of price exposure and power supply	-: Increased risk of price exposure and power supply. Possibilities of risk mitigation only for customers using hydrogen for storage purposes, as better suited to enter PPAs.
Bilateral sale-and-purchase agreement	-: Increased risk of price exposure and power supply	+: Reduced risk of price exposure and power supply, no distinction for risk mitigation based on end-use of hydrogen
Multilateral contract: single standardized price	+: Reduced demand risk, by spreading it over a number of consumer	-: Perceived lock-in of blue hydrogen and fossil stigma
Multilateral contract: standardized price per commodity	+: Reduced demand risk, by spreading it over a number of consumer	+: More reliable prices, including value of CO_2 reduction / sustainable production

3.3.2. Hypotheses formulation and experimental set-up

Based on these insights, some hypotheses have been formulated. Specifically, hypotheses are constructed by varying contractual structures in the last column of Table 4, and suggesting possible effects on the cluster's cash-flow and on the optimal investment path. The qualitative effects summarized in Table 5 are used as guidance.

The hypotheses will be tested in Linny-R by running multiple model iterations, where the same system will be modelled under different contractual arrangements. The system boundaries are defined based on the stakeholder map presented in Section 3.1, under the envisioned investment-based contracts. Such system will be tested under different revenue contracts supporting the projects' financing, via the optimization model. This will enable a clear comparison of resulting (aggregated and individual) cash flows, as well as of investment timelines. An overview of the formulated hypothesis and the planned Linny-R simulations is provided in the table below, answering SQ3 on how to test the effects of contractual structures in a structured manner.

Table 6. Overview of hypotheses and experiments

Research Question	Hypothesis	Experiment	Expected result
1) *Which form of bilateral contract is best suited to stimulate scaling and integration of hydrogen production and supply in industrial clusters?*	Sale-and-purchase agreements are preferable to tolling models for hydrogen integration	<u>Set-up:</u> Each hydrogen consumer makes take-off agreements with specific hydrogen projects. Contract conditions are fine-tuned to the specific bilateral transaction. <u>Experiments:</u> 1. First model evaluates the system under tolling agreements 2. Second model evaluates the same system under sale-and-purchase agreements	Integration of hydrogen in the system will be slower in the model using tolling agreements compared to the case of sale-and-purchase agreements. This is reflected in lower cluster cash flow
2) *Which multilateral approach is best suited to stimulate scaling and integration of hydrogen production and supply in industrial clusters?*	Multilateral contracts with price standardization per commodity are preferable to multilateral contracts with a single, standardized price	<u>Set-up:</u> Multiple hydrogen producers sell on to multiple end-users via multilateral contracts. The same, standardized conditions apply to all parties involved in the multilateral exchange. <u>Experiments:</u> 1. First model evaluates the system under multilateral contracts in which green hydrogen (GH) producers pool their GH production and sell it at the same standardized price to multiple end-users. Same goes for blue hydrogen (BH) production and end-use. BH and GH have different prices. 2. Second model evaluates the same system under multilateral contracts in which GH and BH producers pool their hydrogen production and sell it at the same standardized price to multiple end-users	A single, standardized price causes lock-in of BH, which decreases the cluster cash-flow (due to lower CO_2 savings) compared to multilateral contracts with separate, standardized prices per commodity
Benchmarking (1) & (2): *Which contractual structure would support optimal investment decisions in hydrogen integration for the transition of industrial clusters?*	Multilateral contracts with separate, standardized prices per commodity yield the highest benefits	Compare results of previous experiments based on - Speed of transition (compare investment timelines) - Total cluster and individual cash flows	Hydrogen producers reduce their demand risk by spreading it over a number of consumer via multilateral contracts, causing more rapid investments and higher cash flows

3.4. Concluding remarks

This chapter has presented examples of major investment projects in the Rotterdam cluster. The actor configuration underlying the chosen decarbonization options has been discussed and visualized by means of a stakeholder map, showing the complexity of contractual networks. This analysis has provided a useful foundation for further categorization of contracts, thus answering SQ1. Additionally, insights in contracts' effects on the transition have been discussed and summarized in Table 5, answering SQ2 and ultimately providing guidance for the design of our experimental set-up. Table 6 provides an overview of the testing procedure that we intend to follow, providing an answer to SQ3.

In order to test the hypotheses, we aim to incorporate the discussed investment plans in the Linny-R optimization model, as examples of decarbonization options in a cluster setting. Thus, the choice of investment plans eventually provides useful guidance in identifying relevant building blocks to be integrated in the model, in which a stylized representation of the system will be provided. How to translate these investment projects with the respective contractual structures into options to be evaluated by an optimization model will be investigated in Chapter 4.

4. Modelling investment trajectories under diverse multi-actor configurations

This chapter proposes a conceptual representation of investment options and their integration in existing production processes via contractual agreements. Section 4.1. substantiates the choice of our modelling methodology by comparing different modelling techniques generally applied to study industrial ecosystems. We advance a solution based on Mixed Integer Linear Programming (MILP) that maximises the cluster's cash flow, while balancing the profit among the production units by means of contractual structures. After a thorough problem description, we specify typical relations to be modelled in mathematical programming terms. Subsequently, Section 4.2 offers insight in how to include investment-related constraints in Linny-R. The rest of the section discusses the conceptual implementation of investment-based contracts and revenue contracts in Linny-R. Lastly, the proposed representation is carefully verified by testing its functioning under extreme conditions and under different multi-actor configurations (Section 4.3). As a result, the chapter provides an answer to SQ4 and SQ5.

4.1. Modelling methodology

To identify optimal transition paths, suitable methods and tools are required that can represent industrial networks in a communicative manner, while affording an analysis of investment decisions and interdependencies between multiple companies. We found these characteristics in the Mixed Integer Linear Programming (MILP) modelling methodology, via the supporting tool Linny-R.

4.1.1. Assessment of modelling methods

MILP has been chosen as the preferred modelling methodology after performing a comparison with other "mainstream" modelling techniques to study industrial ecosystems.

Methods analysing industrial processes using flow-sheeters such as AspenPlus were excluded *a priori*, as the scope of AspenPlus simulations is often restricted to one production process: thus, using this approach for optimizing clusters is hardly possible. With this in mind, we compared MILP with two, widely adopted modelling techniques: Agent-Based Modelling (ABM) and System Dynamics (SD). Such techniques were selected based on literature reviews addressing approaches generally used for the study of industrial clusters from a system's perspective (Demartini, Tonelli, & Bertani, 2018).

ABM models is a class of computational models designed to simulate action and interaction between actors based on a set of rules, aiming to study effects at aggregate level (i.e. the emergent behaviour) on the system (Demartini et al., 2018; Raimbault et al., 2020). As such, it is able to analyse multi-actor perspectives, which may make this modelling technique suitable for our purpose. Moreover, it allows for hierarchical modelling via aggregations of specific processes. These advantages make ABM inherently suitable for modelling industrial clusters. It should be noted, however, that as a process simulation software ABM lacks the ability to perform model optimisation, focusing instead on the emergent behaviour using a bottom-up approach. According to Raimbault et al. (2020), parameter values determining a (near) optimal cluster performance can still be identified via heuristics, although with onerous computational resources. Finally, ABM's use of programming code as specification language makes it less user-friendly compared to models relying on a graphical specification language.

On the other hand, SD models provide a sound methodology to visualize and analyse complex dynamic systems (Groot, 2015). SD is a simulation method that identifies system changes by analysing the structural characteristics of the system, considering cause-and-effect relations among elements in subsystems and between subsystems (Demartini et al., 2018). When applied to industrial cluster's modelling, the system is normally first represented using a process flowchart, subsequently translated using SD models, via causal loop diagrams and stock-flow diagrams. The former allow for a conceptual understanding of the system via causal chains, the latter enables quantitative modelling (Cui, Liu, Côté, & Liu, 2018). However, contrarily to ABM, quantitative analysis is generally realized from a relatively high aggregation level, as SD is inherently a top-down methodology, meant to provide insights by analysing megatrends (Wirsch, 2014). For this reason, this approach may not be completely suitable for our research. Even adjusting the aggregation level, an SD software such as VenSim does not perform optimisation, just like ABM models.

These limitations are overcome by MILP models. Instead of relying on heuristics, optimization techniques help to identify the optimal transition strategy in a way that satisfies one or several objectives, subject to constraints. This offers enough flexibility to construct an optimization model that includes multi-actor goals and dependencies while optimizing the cluster's performance. Several types of cooperation at process level have been successfully modelled in MILP (Boix, Montastruc, Azzaro-Pantel, & Domenech, 2015). This signals opportunities to extend this approach by incorporating contract-related constraints that formalize such cooperation, allowing for an evaluation of consequences of hardware changes from a system's perspective. Although many MILP models are based on 'hard coded' models in the form of mathematical equations, some rely on intermediary tools (Boix et al., 2015). Of these tools, Linny-R offers interesting opportunities for our research, which be further substantiated in the next sections.

4.1.2. Applying MILP to industrial clusters: problem description

As part of this research, we aim to demonstrate the potential of an intra-cluster market established by means of contractual structures supporting the exchange and integration of new products resulting from (joint) investment projects.

An industrial cluster consists of a group of interconnected production units (PUs), whose connections identify potential flows of interchanged products (Jamal & Montemanni, 2018). The cluster PUs exchange products with the objective to maximize the total cluster cash flow, corresponding to the sum of the cash flows over the PUs of the cluster itself. Each PU's cash flow is determined by the amount of final product sold, times the difference between the selling price of final products and the costs of raw materials and inputs, the costs of production (i.e. fixed and variable operational costs, investment costs), and waste disposal costs –which may also include the costs associated with CO_2 emissions or with the CO_2 content of flue gases produced. It is important to point out that waste resulting from a production process may be efficiently integrated in other cluster's operations, being reused as input for other PUs. Examples could be reused water, steam, recovered energy or CO2 – such as for CCS purposes. In this chapter, we refer to these resources as by-products.

From a legal point of view, several bi- or multilateral contracts consolidate the exchange of (by)-products, thus reducing the risk of uncertainty of flows. This aspect is particularly relevant in the context of the energy transition, as contracts need to provide some certainty to investors that demand exists to make them willing to fund new projects. Thus, interdependencies between owners of PUs need to be carefully considered and regulated via contracts when evaluating investment decisions, as the revenues that are produced by exchanging the output of an investment option are often the main source of revenue for paying back capital investment costs. When a contract is established, a price is contractually agreed upon to perform the exchange of products, often under minimum and maximum contracted volumes. In addition, some initial costs are paid by the PUs exchanging materials: these may involve costs of constructing new connections or retrofitting production processes to integrate the new (sustainable) products. Thus, the multi-actor context might introduce additional changes both from a physical/technical and economic perspective. The presented problem is schematized in the figure below.

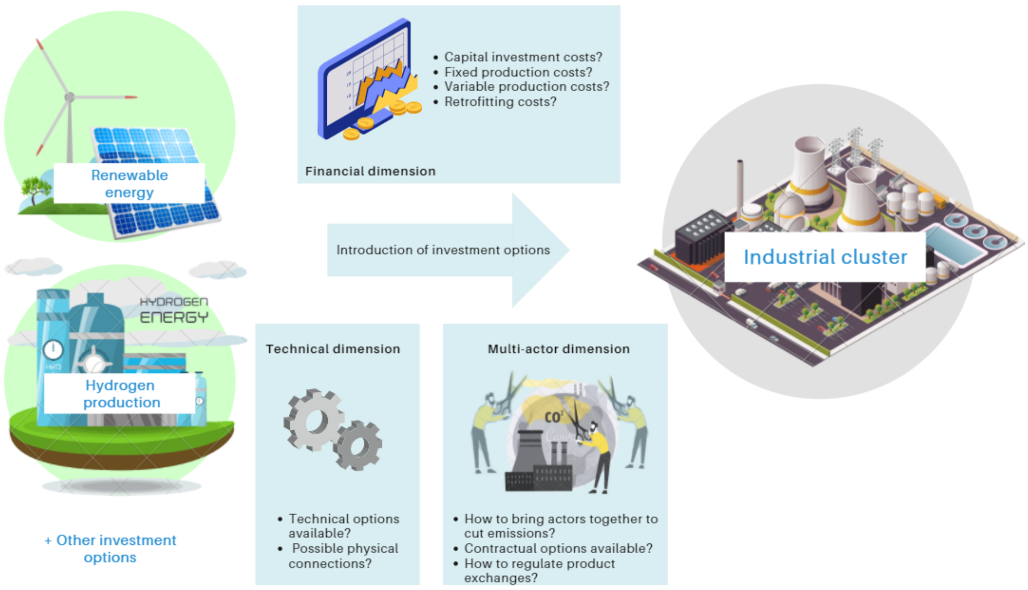


Figure 12. Problem representation

4.1.3. Mathematical formulation

The problem described above can be represented as a linear programming model. We begin by defining the variables of the model:

- P_{it}: the production level of product generated in production unit $i \in N$ in time step $t \in T$;
- $u_{it} \in \{0, 1\}$: binary variable indicating the operating status of production unit $i \in N$ in time step $t \in T$;
- $u_{ijt} \in \{0,1\}$: binary variable indicating the start of a contractual relationship between production unit $i \in N$ and production unit $j \in N$ (with $i \neq j$) in time step $t \in T$;

The constants of the model are the following:

- N: the set of production units, including possible investment options;
- K: the set of resources, including by-products;
- T: the total number of time-steps;
- c_{it}: variable production cost (=marginal cost of production) of production unit $i \in N$ in time step $t \in T$;
- f_{it}: fixed production cost for the product of production unit $i \in N$ in time step $t \in T$;
- i_{it} : investment cost for production unit $i \in N$ in time step $t \in T$;
- γ^M_{kit} : disposal cost (or emission cost)of by-product $k \in K$ in production unit $i \in N$ in time step $t \in T$. This cost arise when a by-product is not traded inside the cluster and needs to be disposed with a predetermined cost. Note that a trading by-products within the cluster would reduce the amount of waste that needs to be disposed and would potentially increase the overall profit of the production unit by selling the waste for another unit's production process.
- c^c_{ijkt}: contractual costs incurred by production unit $j \in N$ to be connected with unit $i \in N$ (with $i \neq j$) in time step $t \in T$, to enable utilization of by-product $k \in K$ / trade of product $k \in K$ produced by unit i; Note that when a product of a PU is used as an input for other processes, such product is indicated as a resource (k);
- p_{it}: market selling price for the product of production unit $i \in N$ in time step $t \in T$;

- p^C_{kt} : contract price for product or by-product $k \in K$ in time step $t \in T$ traded within the cluster;
- p^M_{kt} : market price (i.e. cost, from the PUs' perspective) for the resource $k \in K$ in time step $t \in T$;
- P^{max}_{it}: maximum quantity produced for the product of production unit $i \in N$ in time step $t \in T$;
- P^{min}_{it}: minimum quantity produced for the product of production unit $i \in N$ in time step $t \in T$;
- α_{ki}: amount of resource $k \in K$ per unit needed in production unit $i \in N$ (per unit of product);
- β_{ki}: amount of by-product $k \in K$ generated in production unit $i \in N$ (per unit of product);

Having defined the constants and variables of the model, the objective function can be specified as the sum of the total cash flows over all the production units of the cluster.

$$Max\ F(\boldsymbol{P}, \boldsymbol{u}) = \sum_{i=1}^{N} \sum_{t=1}^{T} (CF_{it} * u_{it})$$

To further specify the objective function, we define the elements that determine the cash flow CF_{it} of production unit $i \in N$ in time step $t \in T$. By definition, cash flows are the net amount of cash being transferred into and out of a business. Thus, CF_{it} corresponds to the difference of cash-in (CI_{it}) and cash-out (CO_{it}) , for each production unit $i \in N$ in time step $t \in T$. The cash-in CI_{it} is derived from revenues obtained via selling the product of production unit $i \in N$ in time step $t \in T$, as well as via by-product intra-cluster trading, if contractual relations with other production units (e.g. production unit $h \in N$) exist. As a result, CI_{it} can be defined as follows:

$$CI_{it} = p_{it} * P_{it} + \sum_{k=1}^{K} p_{kt}^{C} * \beta_{ki} * P_{it} * u_{iht}$$

The cash-out CO_{it} is determined by production costs, costs of raw materials and disposal costs of by-products (or emission costs), when a contract relation for intra-cluster trading for such by-product is not in place. Production costs consist of fixed operational costs, marginal costs of production and investment costs. The investment costs are calculated by taking into account both the current and previous time step. If the production unit being invested in is active in time step t, while the production unit was inactive in time step $t-1$, the formula equals the investment cost i_{it} of the production unit.

$$Costs\ of\ production = f_{it} + c_{it} * P_{it} + i_{it}, whereby$$
$$i_{it} = 0.5 * i_i * [(u_{it} - u_{i,t-1}) + (u_{it} - u_{i,t-1})^2] \quad \forall i \in N, t \in T$$

Costs of raw materials result from purchasing inputs from the market or via intra-cluster trading, from other production units (e.g. production unit $j \in N$) by means of contractual relations. With the same logic as for investment costs, contractual costs are calculated by taking into account both the current and previous time step. If the contract is active in time step t, but was inactive in time step $t - 1$, the formula equals the contractual cost c^C_{ijk} of connecting installations i and j for the exchange of by-product k. Therefore,

$$Costs\ of\ raw\ materials = \sum_{k=1}^{K} p_{kt}^{M} * \alpha_{ki} * P_{it} * (1 - u_{ijt}) + \sum_{k=1}^{K} p_{kt}^{C} * \alpha_{ki} * P_{it} * u_{ijt} + \sum_{k=1}^{K} c_{ijkt}^{C}$$
$$whereby\ c_{ijkt}^{C} = 0.5 * c_{ijk}^{C} * [(u_{ijt} - u_{ij,t-1}) + (u_{ijt} - u_{ij,t-1})^2] \quad \forall i \in N, t \in T$$

In case no contractual relations with other production units are present, PUs may have to face some disposal costs (or emission costs) for by-product $k \in K$ generated in production unit $i \in N$ (per unit of product). This translates into

$$Disposal\ (or\ emission) costs = \sum_{k=1}^{K} \gamma_{kit}^{M} * \beta_{ki} * P_{it} * (1 - u_{iht})\ \ \forall i \in N, t \in T$$

The algebraic sum of price and cost components gives the total cash-flow of production unit $i \in N$ in time step $t \in T$:

$$CF_{it} = [p_{it} * P_{it} + \sum_{k=1}^{K} p_{kt}^{C} * \beta_{ki} * P_{it} * u_{iht}] - \{[f_{it} + c_{it} * P_{it} + i_{it}] + [\sum_{k=1}^{K} p_{kt}^{M} * \alpha_{ki} * P_{it} * (1 - u_{ijt}) + \sum_{k=1}^{K} p_{kt}^{C} * \alpha_{ki} * P_{it} * u_{ijt} + \sum_{k=1}^{K} c_{ijkt}^{C}] + \sum_{k=1}^{K} \gamma_{kit}^{M} * \beta_{ki} * P_{it} * (1 - u_{iht})\}$$

Note that cash flow of production unit $i \in N$ in time step $t \in T$ only appears in the objective function of the MILP problem if its operating status is active, thus if $u_{it} = 1$. Thus, the objective function will be

$$Max\ F(\boldsymbol{P}, \boldsymbol{u}) = \sum_{i=1}^{N} \sum_{t=1}^{T} CF_{it} * u_{it}$$

The objective function is subject to several constraints. Since we aim to provide a generalized formulation of the problem, we present only some typical constraints that define the feasible area. General examples are:

- Capacity constraints: the production level of production unit $i \in N$ in time step $t \in T$ should always be within maximum and minimum production levels

  $$u_{it} * P_{it}^{min} \leq P_{it} \leq u_{it} * P_{it}^{max} \qquad \forall i \in N, t \in T$$

  This implies that the total amount of each by-product traded within the cluster cannot exceed the required amount of resources during production

  $$\alpha_{ki} * P_{it} \leq \alpha_{ki} * P_{it}^{max} \qquad \forall i \in N, k \in K, t \in T$$

  $$\beta_{ki} * P_{it} \leq \beta_{ki} * P_{it}^{max} \qquad \forall i \in N, k \in K, t \in T$$

- Equality constraints: a certain production level should be reached, denoted by P_{total}

  $$\sum_{i=1}^{N} P_{it} = P_{total} \qquad \forall t \in T$$

- Domains for the variables

The compact formulation appears as follows:

$$Max\ F(\boldsymbol{P}, \boldsymbol{u}) = \textstyle\sum_{i=1}^{N} \sum_{t=1}^{T} (CF_{it} * u_{it})$$

$$\begin{array}{lll} s.t. & u_{it} * P_{it}^{min} \leq P_{it} \leq u_{it} * P_{it}^{max} & \forall i \in N, t \in T \\ & \sum_{i=1}^{N} P_{it} = P_{total} & \forall t \in T \\ & P_{it} \in R^{+} & \forall i \in N, t \in T \\ & u_{it} \in \{0,1\} & \forall i \in N, t \in T \\ & u_{ijt} \in \{0,1\} & \forall i, j \in N, t \in T \end{array}$$

4.2. Conceptual representation in Linny-R

This research choses Linny-R as a software tool to simulate and optimise the operations of industrial clusters via MILP. Linny-R, developed by Dr. P.W.G. Bots, is an executable graphical specification language for MILP problems which relies on an external solver to optimize the scheduling of production processes, while maximizing the total cash flow. This program has used the LP_solve library version 5.5.2.0 developed by Michel Berkelaar, Kjell Eikland, and Peter Notebaert, since 2009. Since June 14th 2021, thanks to tailored updates by Dr. P.W.G. Bots, it was possible to switch to the (more powerful) solver Gurobi.

Besides providing a graphical specification language that is visually appealing, Linny-R is inherently suitable for this research. In fact, Linny-R allows to model production systems as a cluster of processes, and allows for nested modelling. Moreover, it can optimise cash flows for the total cluster or for selected companies, to analyse an actor's position in a cluster, and evaluate the impacts of different kinds of multi-actor strategies. This makes it an ideal tool for the evaluation of an (institutional) intervention on the cluster performance, both from a technical and economic perspective. Being based on MILP, Linny-R is inherently fit for optimisation, although when the number of binary variables in a model increases, solver times tend to become unfeasibly long. Specifically, this represented a significant barrier before introducing the Gurobi solver.

The Linny-R implementation aims to introduce a novel methodology to quantify the effects of different forms of contractual structures on the introduction of decarbonization options. To this end, conceptualization and formalization efforts need to be made to accurately represent investment-based and revenue contracts in Linny-R. The first logical step is to provide a representation of investment options in Linny-R. Subsequently, the investment representation is applied to a multi-actor context, where contractual agreements are used as an enforcement mechanism to ensure win-win situations for all the companies of the cluster.

4.2.1. Representing investments in Linny-R

It is worth noting that typical MILP optimisation problems in the context of industrial clusters seek to optimise existing production processes, rather than optimising investment decisions in new assets. The Linny-R tool itself is not meant for modelling investment decisions: therefore, we identify a methodology to include these elements in the model.

We start by formalizing a basic single-decision, single-actor model to explain the logic underlying investments' conceptualization. Figure 13 depicts a simple production process that converts Input A into Output B. To convert Input A into Output B, the production unit pays variable and fixed operating costs, for every time step in which the unit is operational (i.e. when its production level is $P_{it} > 0$). Such costs are modelled as non-physical products (i.e. "data products") denoted by a dashed perimeter. Data products consist of data and can be used to gain insight or add specifications, thus do not represent a physical flow of material. It is possible to select multipliers on the arrows linking a process to data products (i.e. "data links"): such multipliers allow to specify information to be extracted from the process. In this case, a multiplier was added to incorporate the fixed costs in the cash flow calculations. The selected multiplier, denoted by the symbol $\oplus$, allows a unitary flow through the link only when the process to which it is connected is operational, otherwise no flow is present. In this way, the owner of the production unit only pays a fixed amount of money f_{it} specified as a negative price (to represent a negative contribution to cash flow calculations), multiplied by 1 if $P_{it} > 0$, or 0 otherwise. Variable costs are modelled without selecting any multiplier, thus forcing the production unit to pay an amount of money equal to the specified quantity for every unit of product ($c_{it} * P_{it}$).

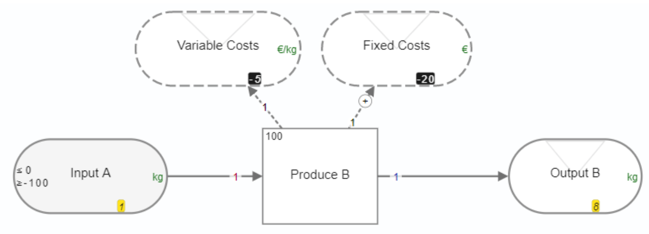


Figure 13. Linny-R representation of production process

Now, assume that an alternative process is introduced, that involves identical inputs and outputs and has lower variable costs, *ceteris paribus*. This alternative process depicted below represents an investment option that, if operational, would allow the production unit to increase its margin. Since its adoption is economically convenient for the actor owning the production unit, the new option is employed for the conversion of Input A into Output B when this simple model is executed.

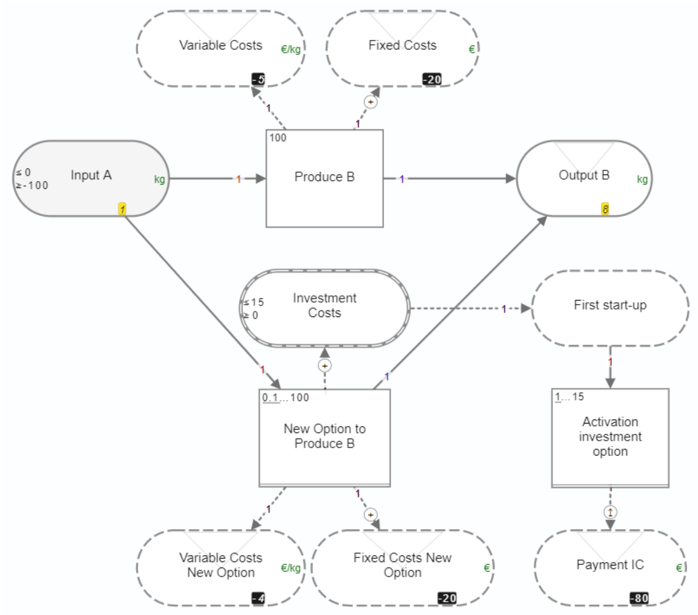


Figure 14. Single-decision, single-actor model for investments' conceptualization

A chain of data products and processes is included to incorporate investment costs immediately upon switching to the alternative process. This is done by considering the investment as a semi-continuous variable with a non-zero lower bound, associated to a binary variable to include start-up costs in the objective function. In the Linny-R notation, this is signalled by the double rim at the bottom of the alternative process, representing that the option can be *on* or *off*. Investment costs are then incorporated in the objective function by linking a semi-continuous process to a data product that specifies the capital investment costs as a negative price. The link between the process and the data product presents a "start-up multiplier", denoted by a circle with an upward arrow ↥: in this way, a data flow from the process to the data product will occur only at the time-step in which that *Option to Produce B* switches *on*.

Start-up costs typically represent the additional resources required by industrial processes when resuming production after being inactive – even for a short period. Evidently, this aspect becomes relevant when simulating operations with a smaller time step (for instance, in an hourly model). In this research, the 'start-up' feature of Linny-R is used to represent the binary decision to invest. Using a time-step of (say) 1 year, the MILP solver will start up an investment option only if the additional cumulative cash flow it generates (given the investment horizon) is able to at least recover the investment cost.

An in-depth explanation of the investment representation provided is presented in Appendix A. To sum up, an investment option switching on at time-step *t* implies several financial consequences, which are incorporated in the MILP by means of 'data products' and 'data links':

i. The investor pays fixed and variable costs for every time-step in which the unit is in operation;
ii. The investor pays capital investment costs immediately upon switching to the alternative process: when the investment option is switched on for the first time, a flow of 1 unit is added to the stock *Investment Costs* and reaches the process *Activation investment option*. Since the level of this process was 0 in time step *t-1* and 1 in time step *t*, the start-up multiplier allows a data flow of 1 into the product *Payment IC*, thus ensuring that the capital investment costs are only paid once, at the moment of the first start-up;
After switching on for the first time, the level of the process *Activation investment option* becomes positive and stays as such for the whole lifetime of the investment option. This makes the investment costs null in the objective function for every time-step *x>t*, consistently with the constraint
$$i_{ix} = 0.5 * i_i * [(u_{ix} - u_{i,x-1}) + (u_{ix} - u_{i,x-1})^2] \quad \forall i \in N, t \in T$$
iii. The level of the stock *Investment Costs* increases by 1 unit for every time-step in which the new process is operational, until it reaches its upper bound. At this point, the solver shuts down the production unit, having it exceeded its life span (in this example, 15 years as *t=1 year*).

Note that by representing investments with this configuration, the production unit can cease producing whenever it is economically disadvantageous, resuming production at a different time-step without having to pay the investment costs again. Various methods have been explored to solve this challenge, before choosing this representation as the most effective. Appendix A presents notes on the alternative investment representations.

The proposed investment representation can be extended to represent virtually any investment decision. For instance, it can be replicated to represent multiple independent investments, alternative investment decisions etc. Moreover, the same building blocks can be used to represent an investment decision made by multiple investors, in a shared perspective. An example of implementation is shown in Figure 15.

As shown below, it is possible to specify an actor as the owner of a specific process. This allows to distinguish the cash flows of each process owner that contributes to the total cash flow being maximized by the solver. In this example, the same building blocks for the single investor case are replicated for each actor contributing to the investment costs. Specifically, we modelled a shared investment in which each actor bears 50% of the initial costs, by means of a flow rate of 0.5 in the data links with start-up multipliers. The data product *Shared costs* then forces the investment costs to be paid by the two actors simultaneously. This is done by introducing an equality constraint of 0 on the data product, with two ingoing data links with a ⊕ multiplier, with opposite rates of +1 and -1. In this way, in order to comply with the equality constraint, the processes *Activation investment option* for Firm A and Firm B must either be both *off* or both *on*. In the latter situation, two flows of +1 and -1 units enter the *Shared costs* data product, still complying with the equality constraint.

Figure 15. Multiple actors, shared investment decision

This configuration can be extended to shared investments made by more than two actors, ensuring that the ingoing flows in the *Shared costs* data product always sum to zero. In addition, it should be noticed that the share of each actor's costs can be easily changed by correctly adjusting the flow rate in the data links with start-up multipliers, without significantly altering the investment representation.

4.2.2. Representing contractual structures

Having demonstrated that it is possible to use Linny-R to represent investments options, we now specifically focus on settings that involve multiple actors interested in investing in decarbonization options and/or integrating them in their processes as off-takers. Such decisions can be independently made by the actors, or multiple firms can choose their strategies collectively. In a real life setting, the latter situation requires contracts as an external enforcement mechanism.

Our representation of contracts in Linny-R relies on the categorization presented in Chapter 3, conceptualized and formalized in modelling terms in the subsequent sections.

4.2.2.1. Implementation of investment-based contracts

Investment-based contracts regulate the wealth distribution among contractual partners in relation to the realization of a joint investment decision. Such contractual coordination may involve the allocation of both costs and revenues of a joint investment, or may only regulate resource pooling.

Joint Venture agreements

Members of a joint venture participate in gains and losses proportionally to their equity shares: the parties pool resources and the JV assumes all the costs, in such a way that each actor bears a fraction of the investment costs equal to its equity share. Price setting of the investment's output is then addressed by revenue contracts (Section 4.2.2.2), in which generally the JV partners decide the offer price jointly and obtain a share of revenue proportional to their equity share.

We represent the JV agreement in Linny-R by focusing on the basic terms of this contractual arrangement, namely (i) the object of the agreement and (ii) the contributions of each party. The former refers to the investment being made; the latter specifies in which proportions the costs and revenues are allocated among parties. The proposed conceptual representation is illustrated in Figure 16 and builds upon the investment representation of the previous section, incorporating an additional set of (data) products and processes to represent revenue sharing between the participants.

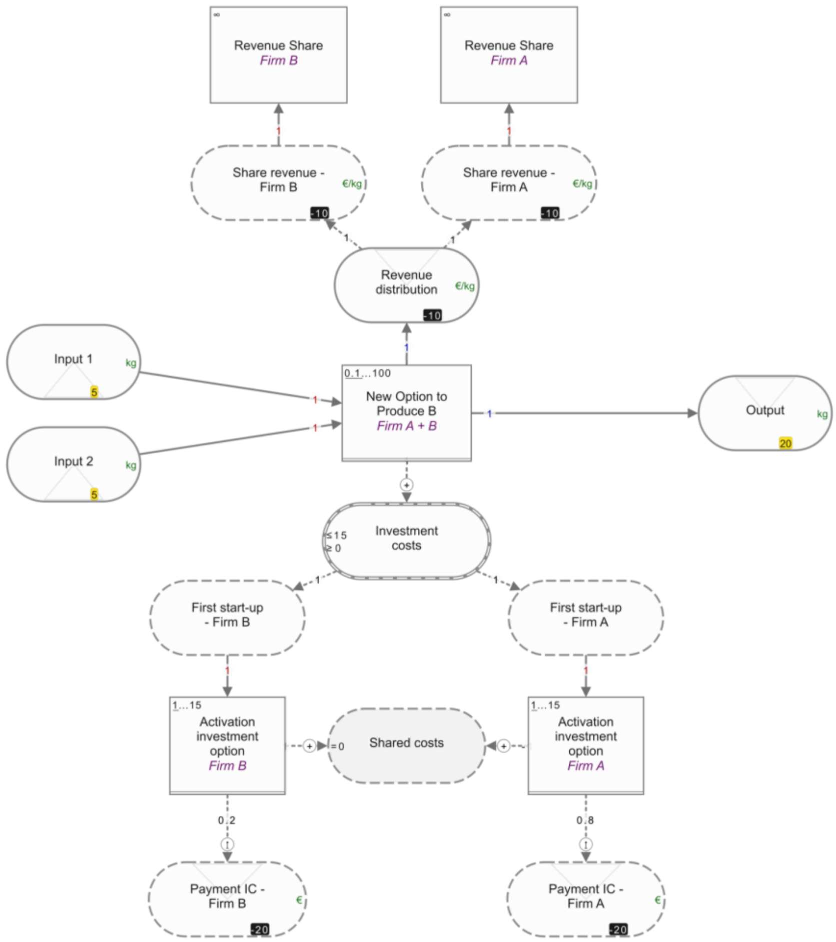


Figure 16. Conceptual representation of JV agreement

In this simple example, the joint venture invests in a process that converts two inputs into an output to be sold, which represents the only source of revenue. Besides sharing the investment costs proportionally to their equity shares (Firm A: 20%, Firm B: 80%), the partners divide the profits from the operation of the production process. This is done by creating the product *Revenue distribution*. Attached to it there is a negative price equal to the difference between the selling price of the end product and the cost of inputs (namely the profit to be distributed), to model that the joint venture itself does not retain profit, since it is entirely split between the JV participants. The negative price is then accounted for in the processes *Revenue share – Firm A* and *Revenue share – Firm B,* in the form of a payment. In this way, Firm A and Firm B receive a payment from the JV, equal to the total profit multiplied by their equity share, by setting ratios in the corresponding data links.

For reasons of clarity, the JV representation has intentionally been presented as an isolated process (i.e. not integrated with other processes). However, normally an investment realized by a JV is embedded in a system of interacting processes, involved in exchanges of products (or by-products).

To exemplify how an investment project realized under a JV agreement is integrated in the cluster dynamics, we present the hydrogen backbone as a typical example, jointly financed by the Port of Rotterdam Authority and Gasunie. Companies that intend to produce or consume hydrogen in the area between Maasvlakte and Pernis can link up to the pipeline, in exchange for a transport tariff.

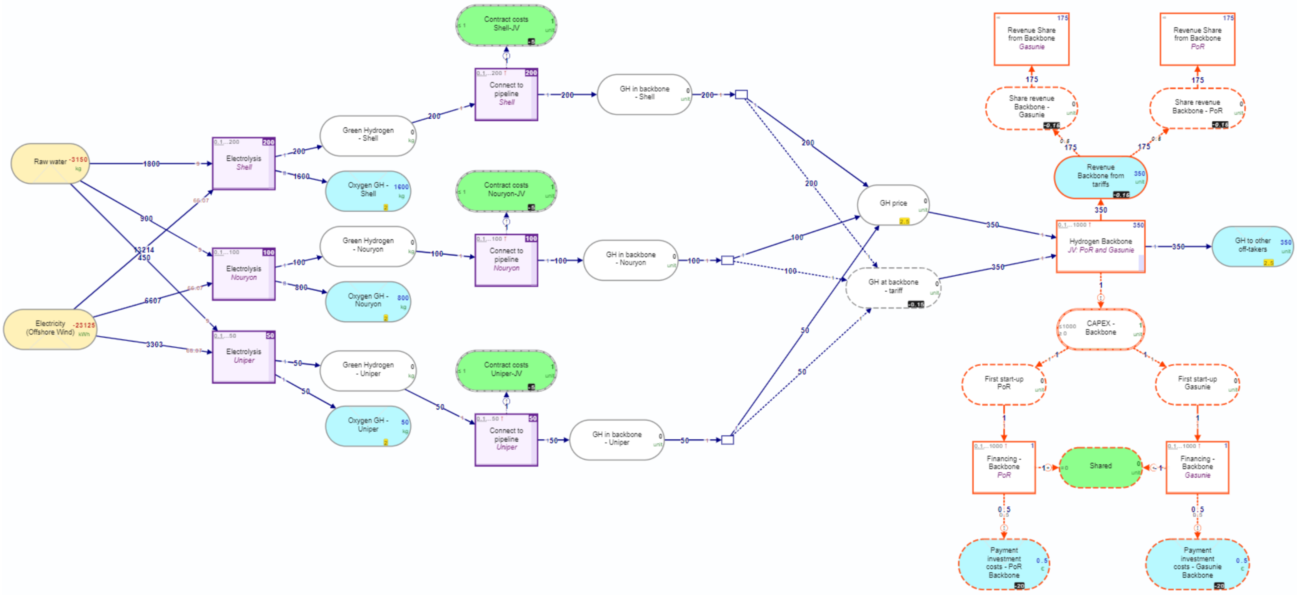


Figure 17. Example of investment decision under a JV agreement (executed)

As shown above, the investment in the backbone is integrated in a system in which three PUs produce green hydrogen via electrolysis, to be sold on to other hydrogen off-takers via the pipeline. The only costs incurred by the contractual partners are represented by the investment costs, while the only source of revenue is represented by the transport tariff. Note that the JV does not retain any additional profit from transporting the commodity, as operator of the transport pipeline infrastructure. Thus, to ensure a correct allocation of cash flows, we adopt the JV representation provided in Figure 16, adapted to the specific cash in and cash out to be distributed. Further explanation of this example is provided in Appendix A.

Consortium agreements

A consortium agreement crucially differs from a JV in that consortia lack a right to share profits (Milton, 1979): each partner's potential profit or loss depends on the relevant party's performance on its scope. Moreover, partners usually avoid sharing costs, and allocate them to specific parties within their own scope: each member pays its own expenses once the contract has been agreed upon. Despite the fact that neither costs nor revenues are normally shared, consortium partners can merge and combine other tangible resources, such as raw materials for the realization of end-products that can be smartly integrated in the production processes of the partners. A stylised representation of this situation is presented in Figure 18.

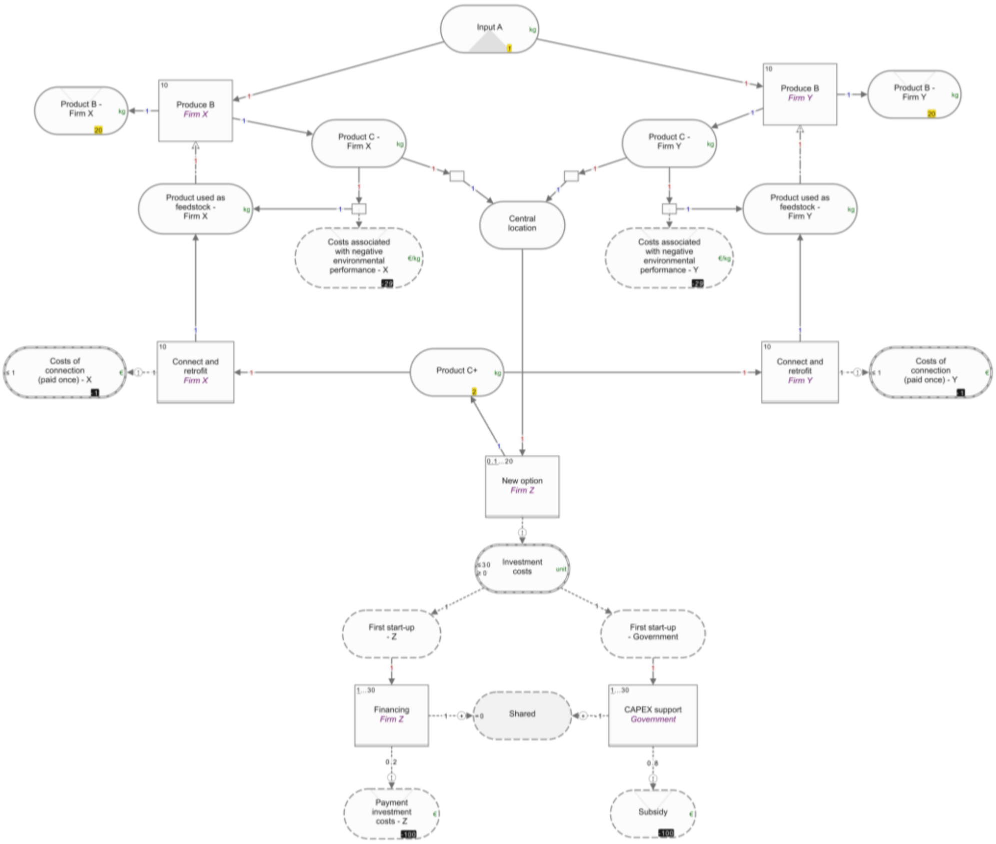


Figure 18. Conceptual representation of consortium agreement with resource pooling

The example above shows a hypothetical situation in which two firms, X and Y, are interested in substituting a by-product (*Product C*) which is normally reused as feedstock in their processes with a more sustainable raw material (*Product C+*). The latter can be produced by upgrading *Product C* via a new process, representing an investment option to be realized under a consortium agreement. *Firms X* and *Y* pool their by-products and transport them to a central location, in order to convert them into the upgraded product needed for their processes. A third contractual party, *Firm Z*, bears the costs of the new investment option, supported by governmental aid, and profits from selling the final product to the interested companies (with pricing mechanisms established via revenue contracts). Note that each contractual party pays its own expenses, and its profit or loss depends on performance on its scope (i.e. either delivering raw material or producing the end product), resulting in independent profit calculations. Such independence in profit distribution, however, is conditional upon resource pooling, which ensures the correct functioning of the envisioned process. Finally, the investment project may be co-financed by multiple consortium partners, or subsidized as in the example above.

A practical application of this type of contractual relation is found in the H-vision project. Here, the pooled product to be upgraded is represented by refinery gases, used to manufacture hydrogen to be reintegrated as a fuel in the refining processes. A simplified representation of the H-vision project is shown in the figure below.

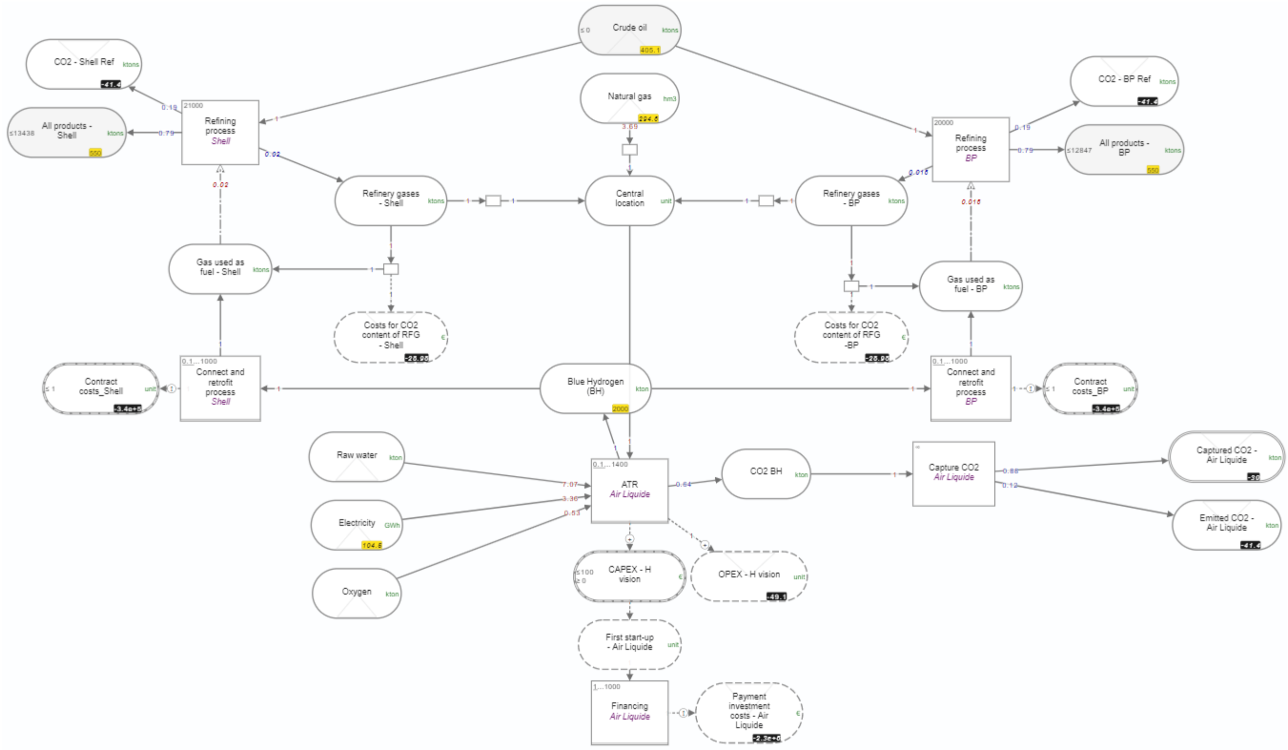


Figure 19. Example of investment decision under a consortium agreement

Following the same logic as in Figure 18, the refineries from Shell and BP pool their refinery fuel gases and transport them to a central location, where they are used for conversion to blue hydrogen. Air Liquide builds and operates the ATR facility, and profits from selling the final product to the interested refineries affiliated to H-vision (with pricing mechanisms established via revenue contracts).

Bilateral agreements

Bilateral investment-based contracts allow to establish the allocation of wealth deriving from a joint investment. However, far more common is a situation in which an investment is made by one of the actors involved, with the counterparty's commitment to purchase the final product. Investment costs then enter price calculations for the exchanged material. The bilateral agreements present in the stakeholder map in Chapter 3 are consistent with this definition.

A conceptual representation for this type of contractual agreement is provided in Figure 20.

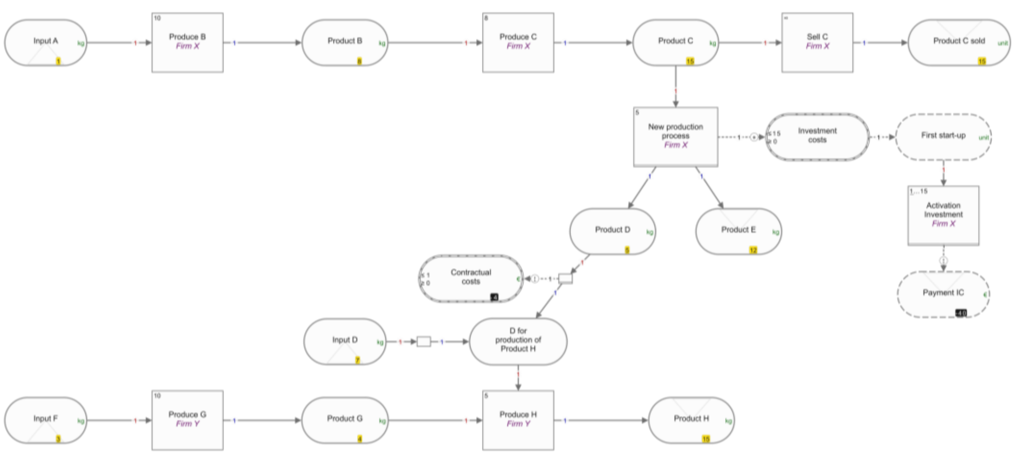


Figure 20. Conceptual representation of investment under a bilateral agreement

This representation is derived from the basic investment representation in Figure 14, extended to include a second production chain owned by the contractual counterparty. The second production chain is connected to the new investment option to purchase its output (at a price established via revenue contracts).

This situation has been widely adopted for the exchange of materials in the establishment of an intra-cluster market. In the context of the Rotterdam cluster, a typical example is represented by investment plans in green hydrogen integration in refinery processes (Figure 21).

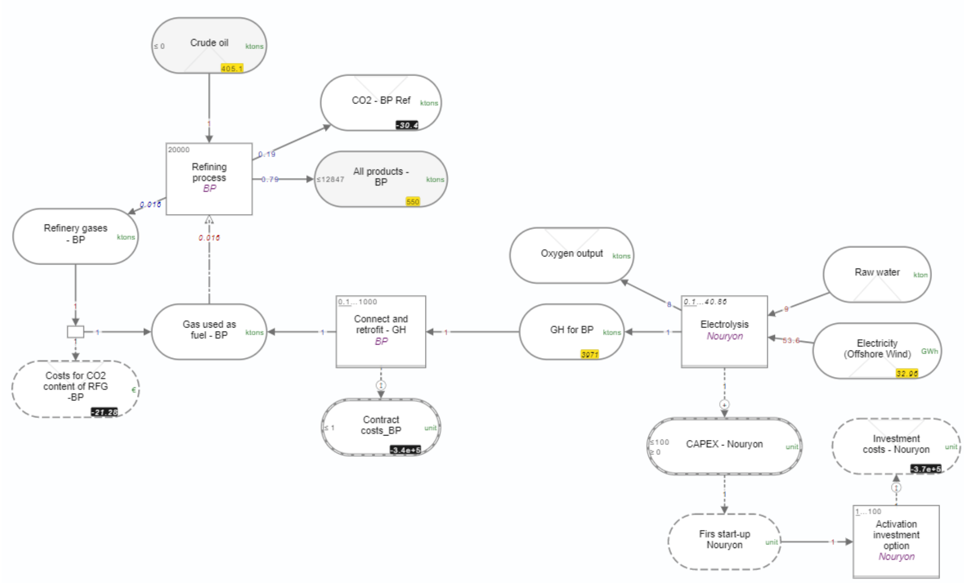


Figure 21. Example of an investment decision under a bilateral agreement

4.2.2.2. Implementation of revenue contracts

Revenue contracts establish how the revenue stream is provided to project partners once the investment decision is made and the new asset needs to be integrated with existing processes. These contracts regulate (i) the quantity of (by-)product to be delivered or purchased by each contractual entity and (ii) the price at which the exchange takes place (i.e. the contract price). In addition to these two key factors, a revenue contract needs to set out the correct incentives to motivate the partners to sustain the exchange: the underlying transaction can only take place when the integration of an investment's output is beneficial for all the contractual parties involved (Albino et al., 2015). Hence, our aim is to devise a methodology that allows to implement contracts with these characteristics.

According to Albino et al. (2015), a contractual relation does not occur or is broken (contract failure) under three conditions:

i. When the relationship is not economically convenient for firm *i*, even though it is convenient for firm *j*
ii. When the relationship is economically convenient for firm *i*, but not convenient for firm j
iii. When the relationship is not economically convenient for both firms involved

whereby economical convenience refers either to (i) the profitability of a given product exchange (i.e. whether the resulting cash flows constitute a positive or negative contribution to the actor's pre-existing cash flows) or to (ii) the selection of the least costly option to be purchased (hence reducing the actor's cash out as much as possible, simulating rational behaviour of agents, seeking cost minimization).

We strive to provide a conceptual representation of revenue contracts that complies with the above-mentioned conditions: our contract representation should push each actor to behave in a way that is desirable for all parties involved in a product exchange, guaranteeing the achievement of win-win situations while maximizing the total cluster welfare.

Various model iterations were performed to achieve this goal. The iterative process of gradually expanding the model and solving the issues detected along the way allowed us to gain insights on the functioning of the MILP solver, hence on how the needed conditions should be implemented.

It is worth recalling that the objective function of the optimization problem at hand is to maximize the sum of the cash flows over all the production units of the cluster. This implies that the Linny-R solver optimizes the transition process for the overall cluster, evaluating the attractiveness of investment options and the convenience of engaging in intra-cluster trading from a cluster perspective, rather than from the point of view of individual actors. Although this might seem a reasonable approach, it should be noticed that optimizing for the whole cluster can easily end up in situations where the chosen strategy is highly beneficial for some players, whose payoffs amply compensate for the negative payoffs of other actors. This situation, however, cannot materialize in a real cluster setting, where the interests of individual actors reshape the incentives at stake. This situation is stabilized by means of contracts, that push firms to behave in a way that is desirable for all parties.

To accurately model the state of affairs, clear conditions need to be set out that allow to evaluate the economic convenience of the single transactions for each actor. Explicitly implementing these conditions in Linny-R allows (i) to correctly simulate the establishment of a contractual relation and (ii) to ensure that the solver takes into account additional constraints to give relevance to the interests of individual actors, while maximizing the cluster welfare. This ensures that unrealistic situations in which the benefits of cooperation are highly rewarding to some parties but detrimental to others will not materialize, as they will not be included in the set of feasible solutions.

Below, we propose a methodology to model this situation in Linny-R. We refer to this general representation of revenue contracts as "contract module", displayed in Figure 22.

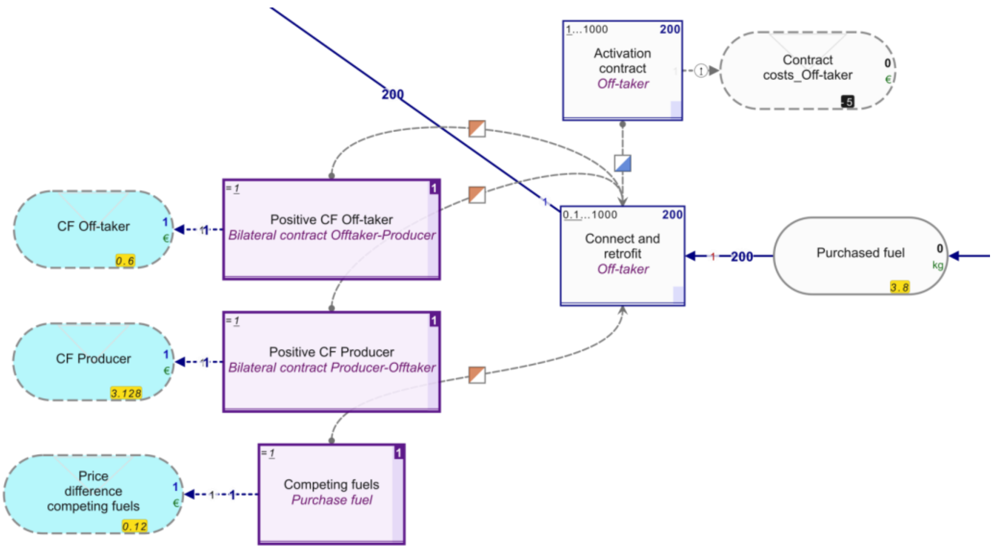


Figure 22. Contract module (executed) between a fuel producer and an off-taker

The figure above represents a contract used to regulate the integration of a specific fuel used as feedstock in the production unit of an off-taker. The contract itself is represented by a decision from the off-taker to connect its PU to the production process of the fuel producer, via the process *Connect and retrofit*. The contract is characterized by (i) a contract price attached to the product being exchanged (normally, the output of an investment option) and by (ii) a minimum and maximum quantity that must be purchased when the contract is activated. The former is specified in the product *Purchased fuel*, while the latter can be included by specifying an upper and lower bound in the process *Connect and retrofit.* The activation of this contract allows the exchange of the fuel to take place under the condition that the transaction is always economically convenient for both the producer and the off-taker. This is formalized via the three (purple) processes connected to data products on the left-hand side, each one representing a specific condition explained in the next paragraphs.

These conditions influence the decision of starting-up or shutting down the process *Connect and retrofit,* allowing or prohibiting the exchange of material at the contractually–agreed price. This is modelled using upper bound (UB) constraint lines (i.e. the dashed curved arrows containing a coloured square), which work under the logic illustrated in Figure 23.

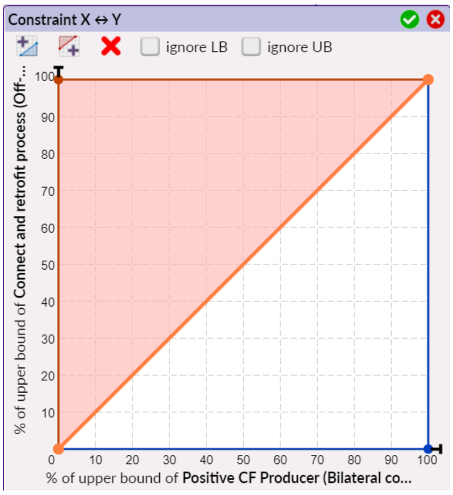


Figure 23. Upper bound constraint following a linear relation

The level of the process on the y-axis is linked to the level of the process on the x-axis (namely one of the explicit conditions to ensure the transaction's profitability). This relation is relative to both upper bounds, where the coloured area represents the unfeasible area. If the UB constraint follows the line *y*=*x*, the level of the process on the y-axis can be *n%* of the UB provided in that process, limited by the orange line (the UB). Therefore, whenever the level of the process on the x-axis is 0, the constraint line forces the process on the y-axis to shut down. Thus, referring to our representation in Figure 22, each process representing a condition of economic convenience of the contract acts as a switch on the processes representing the decision to engage in a transaction. Consequently, the contractually-bounded transaction will materialize if and only if all the conditions are satisfied.

The conditions that monitor the activation of the contract are constructed as follows:

i. The first two conditions allow to monitor the cash flows (CF) of the partners involved in the transaction. This is done via a data product *CF [name of actor]* connected to a process *Positive CF [name of actor]* that is allowed to switch on and shut down based on the value of the price of the data product. The price of the data product *CF [name of actor]* represents the cash flow of the actor to which it is referred. Note that it is not possible to incorporate an actual measure of the CF (computed by the solver) at each time step, since CFs are a result of the optimization and thus cannot be used as input data for the solver. Therefore, a proxy for the CFs of each actor is used to exogenously set the price of the data product: this is equal to the potential marginal profit that would be realised by the actor if the contract was activated. The potential marginal profit is calculated as the price of the product being sold (i.e. marginal revenue of the actor) minus the costs the amount of raw material needed for the production of a unit of product (i.e. marginal costs of the actor).

This is used as an expression, exogenously determining the price of *CF [name of actor]*. In this way, the values are known by the solver *ex ante*.
The process *Positive CF [name of actor]* switches on only when the data product connected to it has a positive price, indicating a positive (marginal) profit. To ensure that the process does not switch on when the price of the data product is still negative, an if-condition is implemented to characterize the upper and lower bounds of the process. The if-condition expresses that the upper and lower bound of the process should be zero when the cash flow of the actor to which it is referred is negative. Denoting the price of the data product *CF [name of actor]* of actor *i* as cf_i, the if-conditions are implemented as follows:

$$cf_i < 0 \Rightarrow UB_{\text{Positive CF [actor i]}} = 0, \text{ or else } UB_{\text{Positive CF [actor i]}} = 1 \qquad \forall t \in T$$
$$cf_i < 0 \Rightarrow LB_{\text{Positive CF [actor i]}} = 0, \text{ or else } LB_{\text{Positive CF [actor i]}} = 1 \qquad \forall t \in T$$

It is in fact sufficient that the process *Positive CF [name of actor]* reaches a level of 1 to allow the process representing the contract to switch on (when all the conditions are respected). If all the processes are switched on, it means that the exchange is profitable for all the parties and the contract is activated. Thus, for every time step, the model checks whether each actor has a positive or negative cash flow based on the explicit conditions: in case of negative cash flows, the actor would produce at a loss, so the contract is not activated because it would not lead to a win-win situation for all parties.

ii. The same logic is applied to the last condition, which compares the prices of fuel options in order to ensure that the most convenient fuel is integrated in the off-taker's process. In this case, the data product has a price equal to the price difference between the costs of two alternative fuels. For instance, a refinery may have the option to either reuse refinery fuel gases or integrate blue hydrogen in the refining process. When blue hydrogen is cheaper than reusing fuel gases, the price in the data product is positive, switching on the process to which it is connected. If the conditions that monitor cash-flows' positivity are also complied with, hydrogen is integrated in the refining process and substitutes the fuel gases. This condition has proved to be extremely relevant in modelling rational choices of individual actors, as we will discuss in Section 4.3.1. Note that, in case of multiple fuel options, this type of reasoning is still valid, applying more specific if-conditions to the price calculations controlling the economic convenience of fuels.

When the above-mentioned conditions are fulfilled, the transaction can take place. The solver can still chose the optimal allocation of material flows in the cluster, hence the activation of the three conditions does not force the solver to switch on the process *Connect and retrofit* and activate the contract. In this way an optimal path for the exchange of products can be found by the optimization.

When a contract is activated, start-up costs are paid at the first activation. The start-up costs are associated with the costs of retrofitting or repowering the off-takers' processes, and building the necessary connections (for instance, small pipelines) for the transport of material, when necessary. The start-up costs are modelled via the process *Activation contract* connected to a data product with a negative price attached to it, representing the costs of connections and retrofitting. The process *Activation contract* is switched on for the first time when the process *Connect and retrofit* is first started up. This is granted by the use of a constraint line representing a lower bound (LB) constraint, which functions as follows:

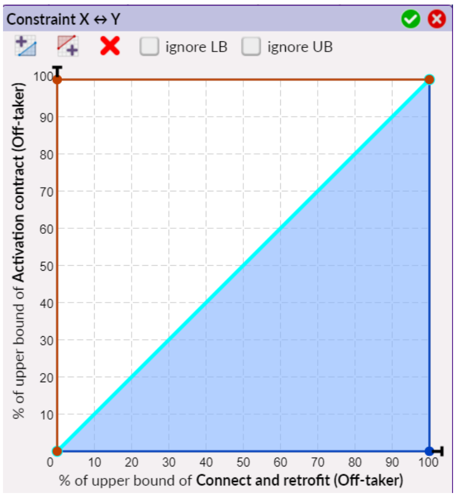


Figure 24. Lower bound constraint following a linear relation

Again, the coloured area represents the unfeasible area for the processes' levels. Thus, when the LB constraint follows the line *y=x*, the level of the process on the y-axis can be anywhere above the blue line (the LB). With this condition, we ensure that when the level of the process on the x-axis is positive, the constraint line forces the process on the y-axis to start-up. Thus, referring to our representation in Figure 22, the process *Connect and retrofit* is able to influence the level of the process representing the payment of costs of connections and retrofitting.

Note that the payment of contractual costs could have been modelled in the same fashion as for investment costs (Section 4.2.1) and the same model behaviour would have been obtained. However, we opted for this representation of contractual costs for two reasons: (a) to avoid confusion between investment costs and contractual costs and, most importantly, (b) to be able to use the same chain of process + data product to model costs of connections and retrofitting for other transactions involving the same asset that need the equal (or comparable) start-up costs. For instance, a refinery owner may want to integrate either blue hydrogen or green hydrogen in its process: for hydrogen integration, the refinery will bear retrofitting costs. To switch from one type of hydrogen to another, only small adaptations may be required due to similarities in the fuels and in the retrofitting process. Thus, retrofitting costs will need to be paid for only once, at the moment of integration of one type of hydrogen. We consider additional costs of future (small) adaptations as negligible and assume that, once the process has been repurposed for the integration of a fuel, no additional retrofitting costs are needed for integration of fuels with similar characteristics. Besides allowing a more compact representation of contract costs, this modelling choice allows to reduce the computation time compared to a situation in which each contract is associated to another binary variable to model contract costs for each new transaction.

The presented contract module can be used to model both bilateral contracts and multilateral contracts, with very slight differences in implementation.

Bilateral revenue contracts

Bilateral revenue contracts can be implemented in Linny-R by simply reproducing the contract module displayed in Figure 22. As the contract price may vary for each bilateral contract, the three external conditions need to be specified for each contractual relation. An example of application is shown in Figure 25, representing the use of a set of bilateral contracts to regulate the integration of blue hydrogen in two refining processes, as attempted by the H-vision project.

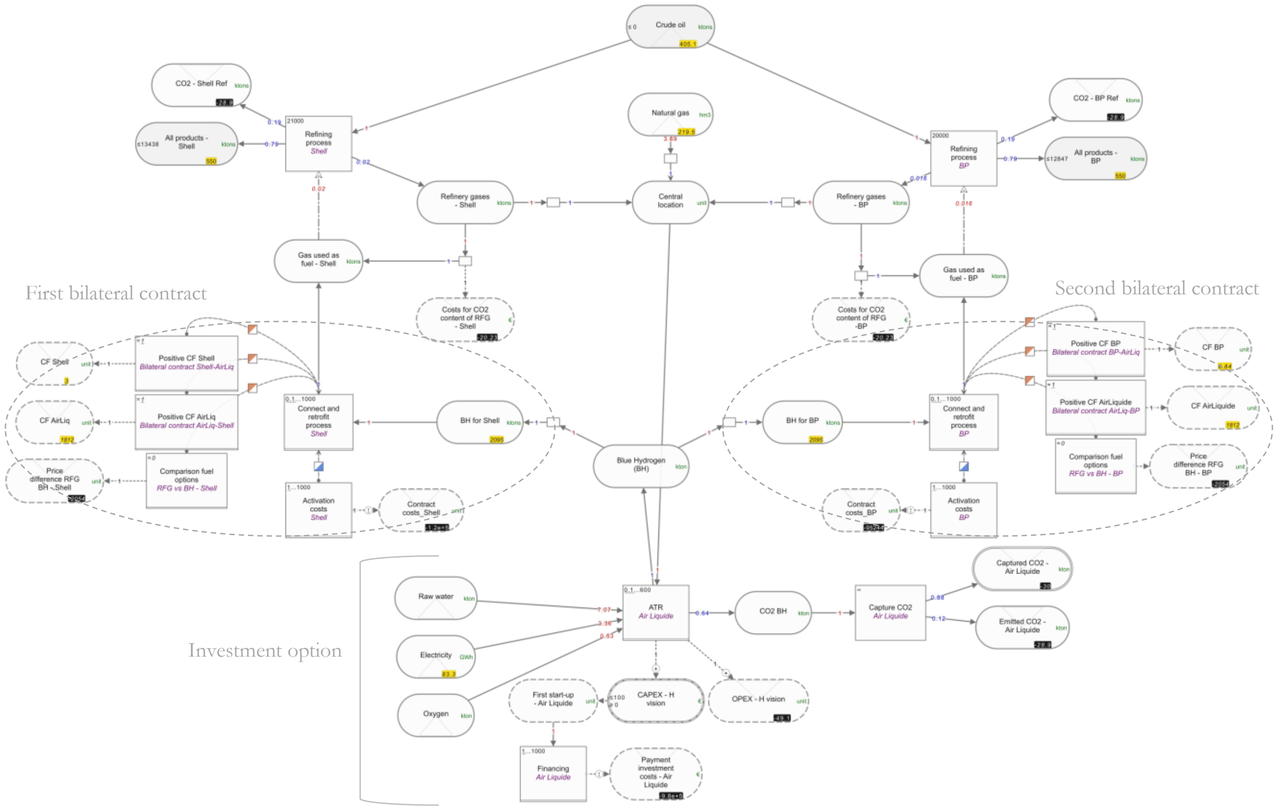


Figure 25. Application of contract module: set of bilateral contracts

A detailed explanation of how contract prices are set in hydrogen contracts is provided in the next Chapter. For now, suffice it to say that the representation in the figure above can be used to represent a system either under a tolling agreement or under a sale-and-purchase agreement, specifying the contract price in the product representing the exchanged material in the transaction (e.g. *BH for BP, BH for Shell*).

Multilateral contract

In a similar fashion, the implementation of multilateral contracts in Linny-R uses the contract module displayed in Figure 22 as a basis. In this case the contract module has to be applied to a situation in which the same, standardised conditions apply to all the parties involved in a transaction. Since a standardised price is applied to all actors involved in the multilateral contract, some of the contract conditions are common to all the transactions, and do not need to be replicated for each exchange with a different actor. Figure 26 presents an example of application, using the same system as in the previous paragraph to facilitate comparison.

This contract representation can be used to model a situation in which hydrogen with different characteristics is marketed as a single product, at the same standardised price. It may also be used to model an in-between situation in which blue and green hydrogen are sold as separate products, each one to be sold at a standardized price per type of hydrogen.

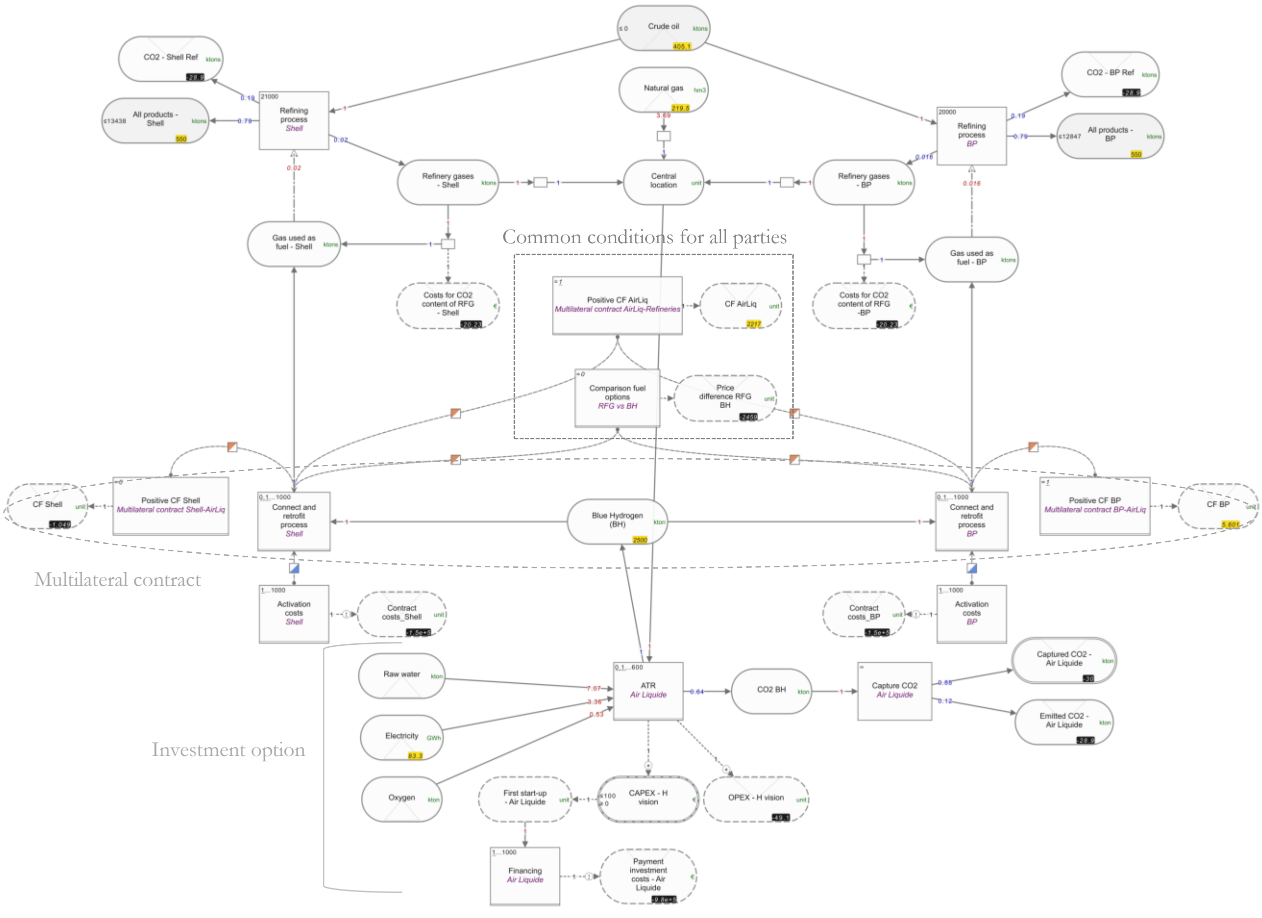


Figure 26. Application of contract module: multilateral contract

The examples above show how the contract module can be applied to situations in which one asset can be invested in, under a single or multiple contracts regulating its remuneration. Likewise, the contract module allows to model circumstances where multiple assets are invested in and operated under a single contract. For instance, this situation materializes when marketing hydrogen produced by different market participants under a single price. Figure 27 illustrates this example by considering two investments in electrolysers operated by different parties under the same contract.

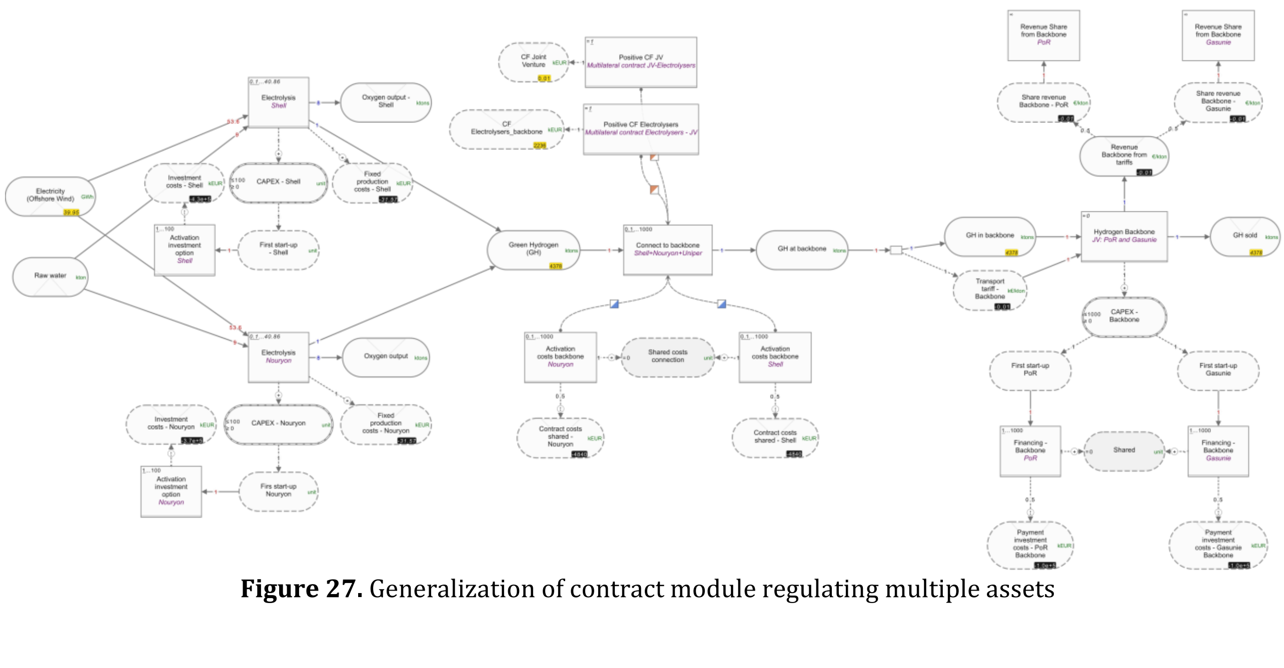


Figure 27. Generalization of contract module regulating multiple assets

The provided examples show that the implementation efforts discussed so far are flexible and suitable to model various multi-actor configurations that may materialize in the introduction of investment options.

4.3. Verification and preliminary insights

Having provided examples on the contract module's implementation, we now provide insight in its functioning. Specifically, we discuss results of simple verification models, constructed for the purpose of testing the robustness of our contract representation (i) under diverse multi-actor configurations and (ii) under extreme conditions, such as extremely high price spikes or negative prices.

Each of the models used for verification consist of a system of existing processes and investment options, whose output is exchanged among the cluster's actors when the investment is operated. The output of investment options is integrated in existing processes via revenue contracts, represented via the contract module, either bilaterally or multilaterally .

4.3.1. Proposed contract representation under diverse multi-actor configurations

First, we aim to show that the proposed contract module is the most suitable representation for contractual agreements in Linny-R, among different possible options. This is done by varying the representation of revenue-based contracts and evaluating the impact on the total cash flow of the cluster and on cash flows of individual actors. Specifically, with this verification experiment the following contract representations are tested:

a. *Contract module consisting of activation costs only*: no conditions to monitor profitability or economic convenience of the transaction are implemented;
b. *Contract module consisting of activation costs and conditions to monitor cash flows' positivity:* this representation ensures that no actor operates at loss when engaging in a transaction. However, no price comparisons of fuel options are explicitly modelled as an additional condition to evaluate the economic convenience of the transaction;
c. *Contract module consisting of activation costs and conditions to monitor cash flows and to perform fuel price comparisons:* this corresponds to the contract module discussed so far.

Configurations (a), (b) and (c) are tested with a simple model. Such experiment is repeated for multiple models in which more actors are gradually included in the system, in order to assess whether the proposed contract module behaves in the same way under different multi-actor configurations.

The first experiment was run using the most simple system configuration, consisting of one blue hydrogen producer and one refinery interested in using the product of the ATR facility (namely, the investment option) for desulphurization of its products. The integration of blue hydrogen takes place under a revenue contract, represented either under configurations (a), (b) or (c). A visualization of the three modelled configurations can be found in Appendix B. The resulting cash-flows over a thirty-year time span are summarized in the bar chart below, for each of the tested configurations.

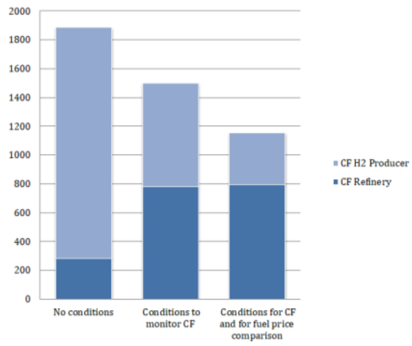


Figure 28. Contract between blue hydrogen producer and refinery

The first bar shows the cash flows resulting from contract configuration (a), in which no explicit conditions are modelled to monitor the profitability and economic convenience of the exchange. In this case, the transaction is basically unregulated, meaning that the transaction takes place if it maximizes the total cluster welfare, ignoring possible detrimental effects on cash flows of individual actors. As it can be clearly seen from the chart, although this situation generates the highest total cash flow (i.e. maximum cluster wealth), it does not represent a win-win situation for all actors as the distribution of the total cash flow among individual actors is extremely uneven. In fact, considering an increasing blue hydrogen price over time, the refinery is forced to purchase hydrogen even at a loss, as shown in the figure below.

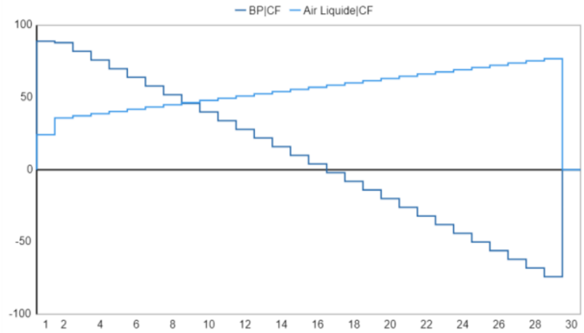


Figure 29. Actors' cash flows per time-step – contract representation with no conditions

As the gains of the hydrogen producer amply compensate the losses of the refinery, the solver returns this solution as optimal, since the total cash flow is maximized. The aim of contracts is precisely to avoid this kind of situations: in reality, the output of the investment option in the ATR facility would only be integrated in the refining process if actors reached an agreement on how to behave in desirable way for both. Therefore, this contract representation does not accurately model contractual agreements in a cluster setting.

The second bar represents the cash flows obtained when additional conditions monitoring the positivity of cash flows are explicitly modelled (configuration b). In this case no actor produces at a loss, thus the situation obtained in the previous configuration does not materialize. This comes at the cost of a lower total cluster welfare, which is justified however by a more even distribution of individual actors' profits.

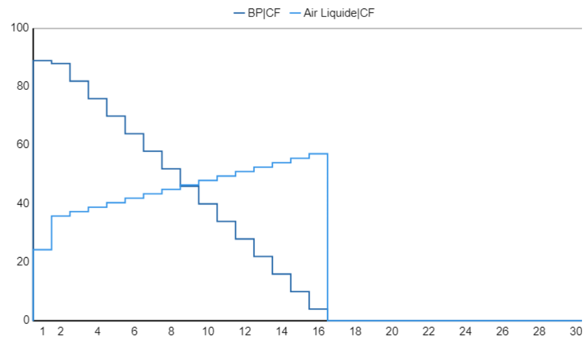


Figure 30. Actors' cash flows per time-step – contract representation monitoring cash flows

This contract representation seems more satisfactory compared to the previous configuration. Nevertheless, in this case the solver does not choose the fuel option that is the most convenient for the refinery entering the agreement. In fact, the solver integrates immediately the option with the highest price, since it creates higher gains for the producer of that option, which translates into a higher total cash flow. Therefore, this contract representation does not fully mimic rational choices of individual players, because the refineries would not engage in a transaction knowing that the option they are integrating in their processes will increase their expenditures.

The last representation, namely the contract module discussed in the previous sections, overcomes this limitation by explicitly implementing an additional condition that allows price comparison, for the integration of the most convenient option for the off-taker. This condition leads to decreased profits for the hydrogen producer, as the investment option in the ATR facility will occur later in time, but implies a slight increase in the off-taker cash flow.

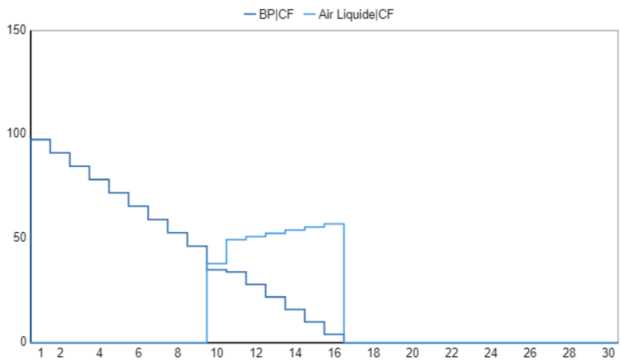


Figure 31. Actors' cash flows per time-step – contract module representation

Although the total cluster welfare is lower compared to the previous two configurations, we have shown that this representation better reproduces rational choices of individual actors. Thus, we consider the contract module as our best approximation of real cluster dynamics.

The experimental procedure adopted for this experiment is replicated for multiple models in which more actors are gradually included in the system. Figure 32 shows results for the performed verification experiments.

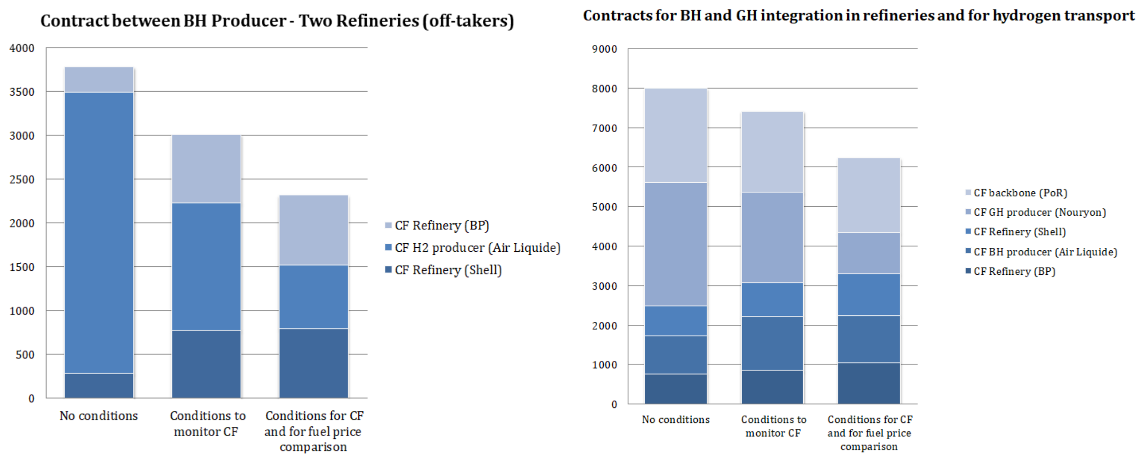


Figure 32. Results of other verification experiments simulating diverse multi-actor configurations

As more investment options and more actors are included in the modelled system, it becomes more visible that the contract module representation allows a more even distribution of the total cash flow. The last contract representation (i.e. the contract module) mirrors a desirable situation in a cluster compared to the other two representations, (a) and (b): in fact, also in these experiments, the former maximizes the cluster cash flow hampering the performance of individual actors, some of which keep producing at a loss just for the sake of increasing other actors' profits; the latter maximizes the total cash flow by forcing off-takers to integrate the most expensive fuel option for their processes, even when there are more convenient alternatives.

Therefore these verification experiments allow to conclude that, although coming at the expense of lower total cluster cash flow, the contract module enables a better representation of rational actors' behaviour, prohibiting transactions that would be detrimental to at least one of the players involved. As a result, the contract module provides the best approximation of a win-win situation, avoiding (i) the realization of negative cash flows and (ii) skewed distributions of cash flows.

4.3.2. Proposed contract representation under extreme scenarios

To illustrate the functioning of the contract module and how it behaves under various scenarios, we test the robustness of the contract representation under extreme conditions. We use a simple model consisting of a system where blue hydrogen (produced by one ATR facility) or green hydrogen (produced by one electrolyser) can be integrated in two refineries or can be sold to other end-users via the hydrogen backbone. The end-users interested in integrating hydrogen are not specified in our model, as this falls out of the scope of the research.

As we do not attempt to provide absolute answers on the attractiveness of investments or on optimal investment timelines in this section, data used for the verification experiments was not validated.

The verification experiments were performed by manipulating contract prices of the outputs of each investment option. This is because contract prices are the variables that most affect the economic convenience or profitability of a transaction, monitored by a revenue contract.

The results of the performed verification experiments are briefly presented in the table below: for each experiment, the contract price of one of the products on the columns was manipulated, leaving the rest unchanged. The price manipulations correspond to the rows of the table. Further details on experimental results can be found in Appendix B, including a description of the model's behaviour and a comparison of cash flows per time-step.

Table 7. Overview of results from contract module's verification experiments

Contract price	For blue hydrogen (BH) at refineries	For green hydrogen (GH) at refineries
High (p=100 €/kg H_2)	Integrating BH is never convenient for the off-takers: thus, the contract module allows the refineries to keep producing relying solely on reusing refinery fuel gases or integrating green hydrogen, when cost effective;	GH is never convenient for the refineries: thus, the contract module allows the off-takers to keep operating reusing refinery fuel gases until BH becomes cheaper, then stop operating when using BH becomes unprofitable;
Low (p=0.1 €/kg H_2)	Integrating BH in the refineries is never convenient for the producer: thus, the contract module allows the producers to only sell hydrogen at a price that allows to at least cover the costs of production;	Integrating GH in the refineries is never convenient for the producer, as it does not allow to cover its variable production costs: thus, the contract module allows the producers to only sell hydrogen at a price that allows to at least cover its costs;
Periodic price fluctuations	Whenever the price is not convenient (too high) for the refineries or not convenient for the producer (too low to cover costs of production), blue hydrogen is not integrated in refineries. This would have not been the case hadn't the contract module been implemented in the optimization model;	The contract module ensures that the solver picks the cheapest option to be integrated in refineries between reusing refinery fuel gases and incorporating BH or GH. When the price of GH is positive, interesting insights are obtained, discussed in the paragraph below;

In a nutshell, the verification experiments show that the contract module accurately models the behaviour of rational actors in a cluster setting. More precisely, we demonstrate that our contractual representation responds effectively to extreme model inputs, avoiding the selection of optimal solutions characterized by distorted allocations of cash flows. These solutions materialize in the case of unregulated transactions (i.e. no contractual relations). A typical output that proves this insight is displayed in Figure 33, which compares the obtained cash flows without and with the contract module for the case of extremely low blue hydrogen prices.

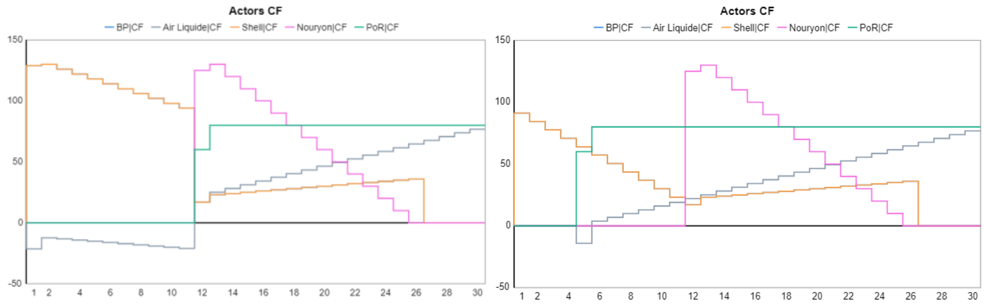


Figure 33. Actors' cash flows for low prices–without contract module (left); with contract module (right)

The example clearly shows that, without implementing the contract module, the solver allows blue hydrogen integration in the cluster even when it is detrimental to some actors (notice the negative cash flows of Air Liquide in the first 12 time-steps). Specifically, the solver selects an investment path that switches on and operates the investment in blue hydrogen even when the hydrogen producer (Air Liquide) is not able to cover its production costs, thus causing a loss for the producer. On the other hand, off-takers (BP and Shell) benefit from such low hydrogen prices, reducing their cash out and generating higher revenues. As their gains compensate for the producer's losses, this solution maximizes the total cluster cash flow at the expense of the hydrogen producer.

It is clearly visible that the contract module (right) prevents from obtaining optimal solutions that force some actors to keep producing at a loss. In fact, the only negative cash flow is represented by capital investment costs in the ATR facility of Air Liquide, whose activation is shifted in time to a moment that allows cost-recovery via an alternative transition path. In this way, the implementation of contracts optimizes the sequence of investments for all actors by identifying win-win situations and without skewing the cash flows' distribution.

Additional insights are obtained via verification experiments considering variable contract prices, as in Figure 34. Specifically, we demonstrate that the implementation of the contract module generates cash flows that are less sensitive to price fluctuations, as clearly visible in Figure 35. In fact, when the contract module is not implemented, the cash flows of the blue hydrogen producer evidently follow the same trends of the blue hydrogen contract price

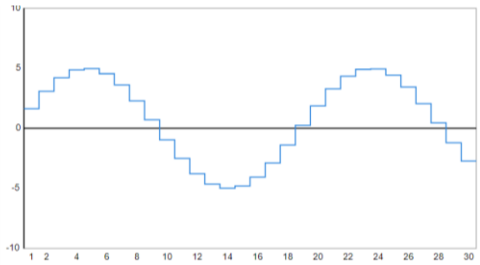


Figure 34. Periodic blue hydrogen for verification experiments

Specifically, the producer is forced to keep selling hydrogen even at a negative price, because of the resulting increase of refineries' cash flows. The contract module, on the other hand, ensures that hydrogen integration in refineries only takes place when their incentives are aligned with the ones of the producers.

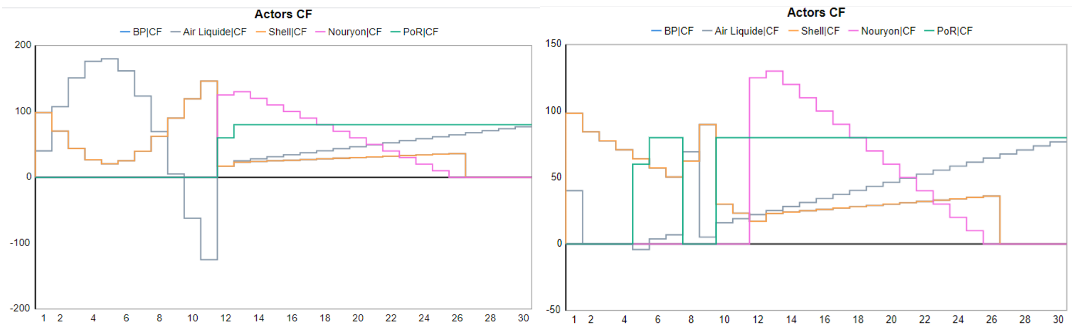


Figure 35. Actors' cash flows for periodic prices – without contract module (left); with contract module (right)

In addition, by scrutinizing the cash flows obtained when implementing contracts, interesting dependencies between investment options are observed. Specifically, the last verification experiment allowed to reflect on the general attractiveness of green hydrogen integration in refining processes. More specifically, the experiment revealed that green hydrogen is only integrated in the refineries if fuel gases are captured by the ATR facility, thus used for production of blue hydrogen to be sold to other end-users. This is because the process of electrolysis does not reform gases, so the CO_2 from the refinery fuel gases would still be emitted, and would have to be captured in some other way for green hydrogen to be competitive with blue hydrogen. Thus, we can already hypothesize that a development based on proven and cost-effective blue hydrogen technology will enable a much more rapid establishment of hydrogen infrastructure. As observed from our verification experiment, green hydrogen can then feed into this ready-made system. This preliminary insight is found to be consistent with findings from the H-vision feasibility study (H-Vision, 2019). Thus, the implementation of contracts already allows to make some interesting considerations, even with the simple model used for verification.

In conclusion, the contract module provides a robust methodology to model contractual relations in Linny-R. Our methodological efforts fundamentally provide added value in several aspects.

First, the provided methodology adds value to MILP-based approaches to model the transition of industrial cluster, as it allows the identification of optimal solutions that better reflect the behaviour of rational actors. Specifically, the implementation of contracts optimizes the sequence of investments for all actors by identifying win-win situations and avoiding skewed, distorted and highly price-sensitive cash flows' distributions. As shown in Figure 33 and 35, the contract module ensures that investment decisions and the resulting intra-cluster trading only take place when the incentives of contractual parties are aligned.

Secondly, our methodology generates insights in investment's analysis from a system perspective, adding value to traditional investment evaluation methods. In fact, our method allows to identify transition paths that optimally takes advantage of potential synergies between investment options, while considering the alignment of incentives of individual participants. This would hardly be possible by computing Net Present Values (NPVs) and other economic indicators for each investment alternative. In fact, traditional methods require timing and cash flows of investments as exogenous variables for financial analysis: however, besides being dependent on pricing and exogenous factors, cash flows are also fundamentally determined by the availability of other investment options which may strengthen or jeopardize each other, as proven by the example in Figure 35. For traditional investment evaluation methods, it would be possible to factor in potential externalities produced by interactions of investments by iterating analyses in which the timing of each investment's activation is gradually shifted to account for multiple combinations of investments overtime. It is trivial to note that such procedure would be inefficient and time-consuming, especially when considering large systems. Our methodology offers an agile approach to the problem, allowing for a dynamic analysis of investments that, via optimization, intrinsically takes into account synergetic effects in the activation of new assets and prevents situations in which different investment options would be mutually damaging. This creates important insights for decision-makers which would hardly emerge from other methods, enabling greater coordination of multi-actor decisions and providing direction via the identification of an optimal investment timeline. Such synchronicity of investments becomes extremely relevant in a context where every actor strives to transform its production processes in a sustainable direction.

4.4. Concluding remarks

This chapter has extensively discussed a conceptual representation of investments and contractual agreements in Linny-R. Having introduced the methodology underlying MILP for the optimization of production processes in industrial clusters, we have provided insight in how to include investment-related constraints into the solver formulation. In this way, we have provided an answer to SQ4:
How can investment decisions be effectively represented in Linny-R?

The same was done for the inclusion of constraints representing contractual relations underlying the exchange of products, answering SQ5:
How can contractual structures be effectively represented in Linny-R?

Results from verification experiments have proved the robustness of the proposed methodology. Such experiments have also shown that contractual relations have a fundamental role in the analysis of investment opportunities for the energy transition, and allow a simultaneous optimization of both individual actors' cash flows and of the total cluster wealth. Ultimately, we have provided a solid method that allows to represent investment-based and revenue-based contracts in a way that is functionally correct, simulating rational behaviour of actors.

In the next Chapter we propose a practical application of our conceptual effort. Specifically, a Linny-R representation of the Rotterdam cluster is formalized, together with the procedure that we follow to structure the model outputs in a way that allows (i) to evaluate the system's investment trajectories and (ii) to quantify the effects of contractual structures on investment decisions.

5. Implementation

This chapter aims to provide an example of application of the proposed methodology to incorporate contractual agreements in MILP via Linny-R. Investment-based contracts and revenue contracts are modelled in the setting of the Rotterdam cluster as a means to provide a proof of concept on how to assess the effects of different forms of contracts on the transition. The chapter begins with a description of the Linny-R model and its intended use. Section 5.2 specifies modelling choices by providing an overview of the modelled industrial system, underlying assumptions and rationale. Subsequently, our modelling approach is presented in Section 5.3, clarifying our experimental set-up and scenario approach to assess the effects of each contractual structure on the system. Finally, the chapter verifies and validates the model.

5.1. Functionality of testing tool and testing procedure

In this Chapter, we devise a procedure that allows (i) to evaluate the system's investment trajectories and (ii) to quantify the effects of contractual structures on investment decisions, via Linny-R models. It should be reminded that we do not aim to build a complete model of the existing cluster, evaluating all possible options for decarbonization. We rather intend to exemplify a method to obtain measurable insights on the effects of different forms of contractual structures. In this perspective, the Linny-R model is used as a testing tool rather than for its predictive value.

The use of the testing tool is explained via the model workflow in Figure 36. This schematic overview briefly describes which data is necessary for the model's operation and which inputs are required to perform the desired experiments, the outline of the process and the relevant outputs. Subsequently, we show how to structure the model outputs in more compact and communicative manner.

5.1.1. Model workflow

The first dashed box in Figure 36 contains an overview of the input data required for the model's proper operation. This consists of data necessary for an accurate system's representation, including process properties and their respective financial parameters.

Additional user input is represented by contract prices, which are inserted as a parameter in the contract module representation. Contract prices are distinguished from the market price. Process outputs, in fact, are normally sold in mature markets at a market price responding to demand and supply dynamics. On the other hand, there are outputs for which a spot price does not yet exist due to thin markets, where the actors are few and scattered. Such outputs are sold at a contract price, negotiated by the parties involved in the transaction. In our model, this distinction applies specifically to hydrogen prices. The current hydrogen market relies bespoke bilateral contracts (H-Vision Consortium, 2019; Martin, 2021), where contract prices for grey hydrogen are based on the actual price of feedstock plus other fixed and variable costs and a profit element. Until a benchmark price for hydrogen is adopted in the market, green and blue hydrogen contract prices may follow a similar formula based on fixed costs plus variable costs actually paid (Martin, 2021). This pricing procedure has also been confirmed by S&P Platts, active in the pricing of commodity markets (den Ouden, 2020; Martin, 2021). Consistently with literature and current practices, we adopt the same methodology as a starting point to derive contract prices, as we explain in Section 5.3. For this reason, the components of hydrogen prices are included in the input data box in Figure 36. By varying the contract prices, together with the bilateral and multilateral contract representation discussed in Chapter 4, experiments to test the effect of different contracts on the system can be performed.

Finally, scenario parameters are defined as a separate category of input data. These parameters are varied in several model iterations to conduct a final evaluation on the model results: in this way, the model's robustness to changes in input variables is tested, and the credibility of conclusions is increased.

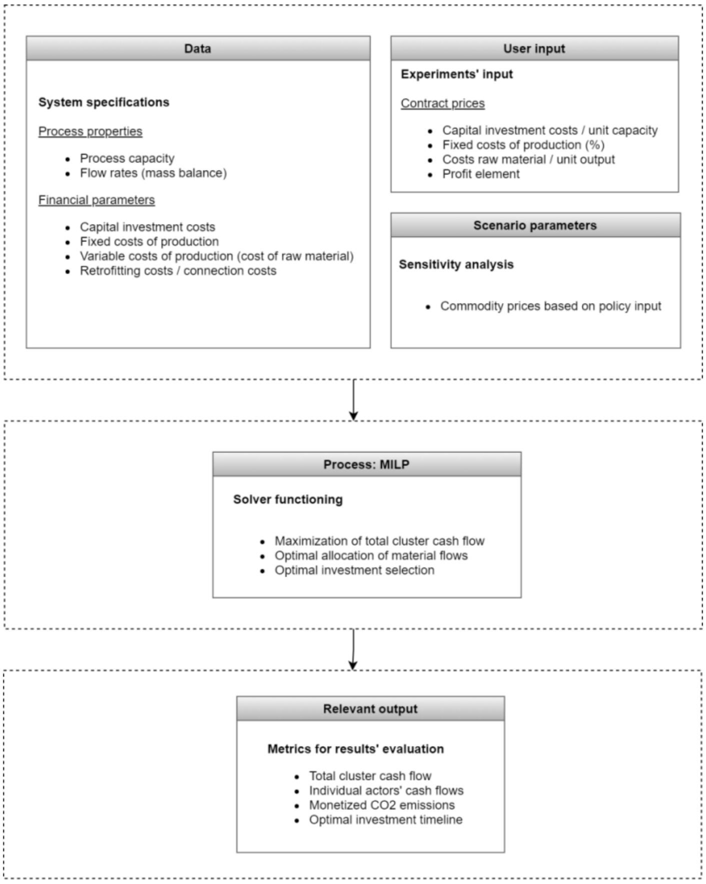


Figure 36. Model workflow

The input data is used by the MILP solver to maximize the total cluster cash flow, determining an optimal allocation material flows together with the optimal combination of investment options that maximize the profitability of the cluster's operations. This results in an optimal transition path under a given contractual structure. Different metrics are extracted from the results of the optimization to assess the effect of contractual structures on the adoption of decarbonization options, as explained below.

5.1.2. Envisioned testing procedure and expected results

In order to quantify the effect of different contractual forms on the transition of clusters, we envision a testing procedure that makes use of two distinct models, consistently with the overview table of experiments (Table 6) provided in Chapter 3.

The first model allows to gain insight in which form of bilateral contract (tolling model vs. sale-and-purchase agreement) is best suited to stimulate a fast integration and scale-up of hydrogen production, relying on the contract representation provided in the previous chapter (Figure 25). A specific hydrogen price per bilateral transaction is established based on the production pathway, as explained above.

The second model serves the same purpose, but is adapted to the case of multilateral contractual agreements, as shown earlier in Figure 26. The effect of multilateral contracts are quantified by (i) marketing green hydrogen and blue hydrogen as a single commodity, using the same standardised price or (ii) marketing green hydrogen and blue hydrogen as separate products, but using a standardized price per commodity. In both cases, the multilateral contract price is derived by aggregating hydrogen prices calculated consistently with Section 5.1.1.

For both models, the same system of processes and investment options is implemented. In this way we ensure that models differ only in the representation of the contractual structure used to regulate the hydrogen exchange.

5.1.2.1. Envisioned testing procedure

We now exemplify our experimental setup by performing the envisioned experiments on two simplified versions of Models I&II. The objective is to make the reader familiar with the logic behind our experimental procedure, before moving on to the (more complex) simulations that will answer the main research question. Given this premise and the purpose of these experiments, the data used was not validated, but was reasonably established based on known trends and estimates from multiple reports.

In these simplified experiments, the modelled system consists of two existing refining processes owned by Shell and BP, which seek to decarbonize their operations by integrating blue hydrogen or green hydrogen as alternative fuel options to refinery fuel gases. The former is produced by one, large-scale, ATR facility owned by Air Liquide. Green hydrogen, on the other hand, is supplied by two, smaller scale electrolysers owned by Shell and Nouryon. Integration of green hydrogen and blue hydrogen is enabled by revenue contracts, which stipulated either bilaterally or multilaterally: the former are tested in Model I, the latter in Model II. Appendix C further elaborates on how the models are constructed and distinguished.

For each model, based on the fuel that guarantees the most profitable integration from a cluster perspective and from the standpoint of individual actors, specific contracts are activated that maximize the cash flows. As a result, each model will return a specific optimal investment path, given the modelled contractual structure that regulates hydrogen integration: using a set of bilateral contracts for hydrogen trade will most likely result in a specific investment timeline, differing from the one obtained if multilateral contracts are employed.

5.1.2.2. Expected model results

The results obtained from Model I and II presented below, to provide the reader with an approximate idea of the kind of insights that the Linny-R testing tool is able to generate. The cash flows per time-step are visualized in a more compact manner, by means of bar charts with stacked columns. This visualization is chosen to allow a comparison of the contributions of the individual actors' cash flows to the total cluster wealth, across categories of contracts.

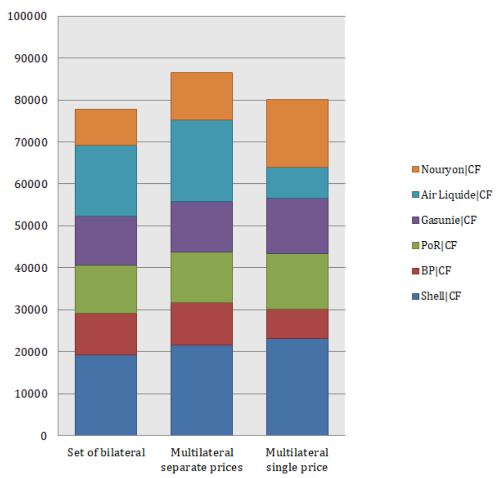


Figure 37. Cluster cash flows under distinct contractual structures (simplified models)

As expected, varying the contractual structures that facilitate hydrogen integration results in visible differences in cash flows of the individual actors, impacting the level of the total cluster cash flows. The variation across contractual structures can be traced back to several factors. Firstly and most certainly, the most direct effect on each actor's cash flow is related to different contract prices (bilateral vs standardized), being the main determinant of the producer's marginal revenue and a relevant cost source for off-takers. Moreover, based on how contract prices compare to other commodity prices, hydrogen integration may (not) be an interesting option for existing cluster processes: this implies that varying the form contractual structures affects the optimal investment timeline extracted from each of the models. As a result, for a given contractual structure, specific capital investment costs may or may not materialize: thus, the total and individual cash flows of actors will be substantially influenced. Finally, based on the optimal investment selection performed by the solver, the level of (monetized) CO_2 emissions will also vary across test cases (Figure 38), ultimately impacting the cash flows.

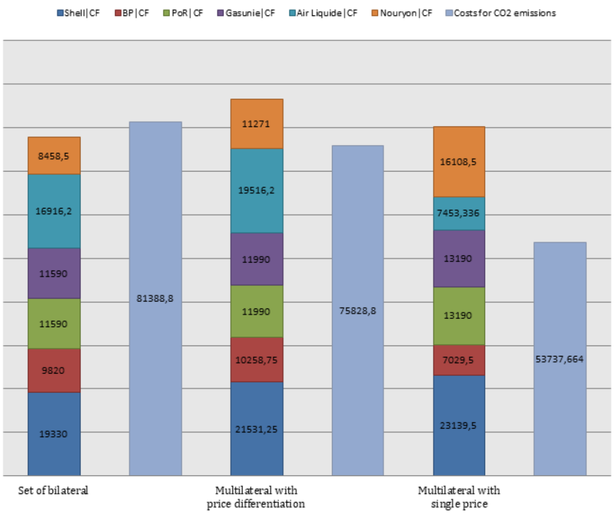


Figure 38. Cluster cash flows and monetized CO2 emissions (simplified models)

With these premises, interesting relations between contractual structures, investment decisions and CO_2 abatement can be identified and unravelled by applying the proposed methodology.

5.2. Linny-R representation: case study

Having elaborated on the functionality of the testing tool and the testing procedure, we now move to the (more complex) case study representation that will be the subject of our analysis.

5.2.1. System's structure and preliminary simplifications

Modelling entails a certain degree of simplification of real world dynamics. In this research, we follow the cycle of enquiry in scientific modelling (Figure 39) to translate complex phenomena into a simplified set of relations between relevant variables (Bryden, 2007).

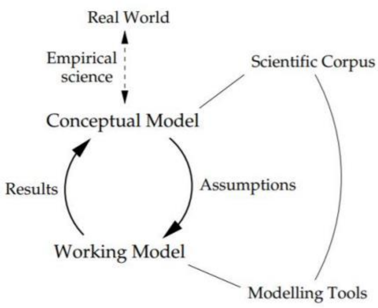


Figure 39. Empirical cycle and modelling (Bryden, 2007)

The first steps towards the model conceptualization have been performed in Chapters 2, 3 and 4, in which literature has been scanned to gain insight in the characteristics of contractual structures, how they are operationalized in reality and how they can be represented in a model. We now aim to perform the subsequent step of the research cycle, namely generating a working model using a set of assumptions. The main assumptions and simplifications are presented below.

The investment selection performed in Chapter 3 was conducted to ensure that the full variety of investment-based contractual structures (i.e. bilateral agreements, consortium agreements and joint venture agreements) could be included in the system. In this way, the effect of different revenue contracts can be assessed on a heterogeneous system, as it would happen in reality. Given the investment projects selected in Chapter 3, the following simplifications are made:

i. Blue hydrogen production (H-vision consortium)
As different development concepts are still under evaluation, we chose to model the H-vision project based on the Reference Scope. According to the H-vision feasibility study, hydrogen will be made from natural gas and/or refinery fuel gases through a single ATR reformer plant at a single location at the Maasvlakte. The foreseen hydrogen production capacity in the Reference scenario is intended to be used for:
- Firing the 2x140 MW gas turbines of the Engie Maasvlakte and Uniper Maasvlakte power plants, fully integrated with the existing boiler (topping cycle +heat integration) and steam integration (2x805 MW)
- Replacing of natural gas of the Pergen CHP plant (286 MW)
- Replacing of refinery fuel gas of the BP (520 MW) and Shell Pernis refineries (650 MW)

Given the complexity of the system, we choose to model only three representative processes, namely the refining processes owned by Shell and BP, and one electric power plant owned by Uniper. This choice was made because of these actors' plans to explore opportunities for green hydrogen integration, next to the H-vision project. Thus, the Linny-R model could offer insights in which would be the no regret option and/or which contractual structure could optimally support the afore-mentioned investments;

ii. CO_2 capture and storage
Given the purpose of this research, a choice was made to focus on CO_2 capture for hydrogen production solely. Specifically, we do not aim to evaluate the attractiveness of the whole Porthos project as an investment option: we rather make a simplification and consider it in relation to the H-vision project. This makes Porthos a prerequisite for enabling blue hydrogen production via H-vision. Such choice is made consistently with the H-vision Reference Scope, which assumes that Porthos will provide the network connection for the CO_2 captured by the large-scale ATR reformer (H-Vision, 2019).
We realize that blue hydrogen may displace other fuels in the industrial area or modify investment decisions in future capture operations, potentially reducing the supply of CO_2 to Porthos. Such analyses are outside the scope of this report, being Porthos evaluated with reference to the H-vision project.

iii. Green hydrogen production (conversion park)
Consistently with the Port's plans, in our model green hydrogen is produced centrally by a concentration of electrolysers located in the Maasvlakte. We model the three largest green hydrogen projects being mentioned in several roadmaps for the Port's transition: projects by BP/Nouryon, Shell and Uniper. Contractual agreements are being set up to supply the

produced green hydrogen to refineries by Shell and BP, and to Uniper's power plant. Being these companies H-vision partners, and given the geographical proximity to the ATR reformer, green hydrogen produced at the Maasvlakte can be transported using the H-vision distribution network to gradually replace blue hydrogen in the furnaces and power plants that have been upgraded (H-Vision, 2019). At the same time, green hydrogen and blue hydrogen can be transported to other (potential) end-users using the backbone (Port of Rotterdam, 2020a).

iv. Hydrogen backbone:
Given the focus of this research on the Rotterdam cluster, we leave the investment in the nation-wide hydrogen backbone out of the scope. Only the regional pipeline between the areas of Maasvlakte and Pernis is modelled, considering the above mentioned hydrogen projects as the only contributors to hydrogen supply.

5.2.2. Assumptions and rationale

5.2.2.1. H-vision project

Having made the choice of modelling three representative processes connected to a central ATR reformer as a way to simplify the H-vision Reference Scenario, we now elucidate how these are represented in Linny-R.

Refining processes: Shell and BP

A refinery site is a complex system composed of different physical separation processes (distillation, extraction, etc), catalytic conversion processes (reforming, hydrotreating, hydrocracking, etc) and thermal conversion processes (thermal cracking, visbreaking, delayed coking, etc) (Oliveira & Schure, 2020). Each refining site differs in its configuration and in the levels of integration. However, using different process schemes for each site and calculating the respective mass balances for all the process units would have been extremely time consuming, with the added value being solely a more detailed representation of the cash flows obtained from refineries' operations.

Hence, overcomplicating the model with a complex representation of refineries is clearly unnecessary. As a result, we opted for a simplified representation of refineries that could be applied both to Shell and BP, with sufficient adjustments based on differences in material flows. Appendix D contains the Linny-R representation of such processes.

Specifically, refineries were modelled as a single process using crude oil as input, from which refinery products are produced, together with CO_2 emissions and refinery fuel gases as by-products. Fuel gases are then captured and used as a fuel in the refining processes at a cost that represents the additional CO_2 emissions released when these gases are burnt. Integrating hydrogen would allow the refineries to avoid these additional costs, since water is generated from its combustion.

Refinery products are aggregated and represented as a single output. This decision was made based on the available data to perform the mass balance of each refining site. As no information was available on the share of each refinery product, such aggregation offered a solution that could guarantee the most agile way to perform mass balance calculations. The pricing of such aggregate product was then established based on crude oil price, in such a way to ensure at least 10% profit for each refinery.

Mass balance calculations for the Shell refinery are summarized in the table below. A more detailed overview of the performed calculations is presented in Appendix D.

Table 8. Mass balance calculations: Shell refinery

Shell refinery	*Formula*	*2016*	*2017*	*2018*	*2019*	*Average*
Emissions based on nameplate capacity *(%)*	$\frac{Direct\ CO2\ emissions\ in\ year\ Y^{(1)}}{Crude\ oil\ nameplate\ capacity^{(1)}}$	0.160	0.151	0.152	0.164	*0.157*
Actual CO_2 emissions *(%)*	$\left(\frac{Direct\ CO2\ emissions\ in\ year\ Y}{Crude\ oil\ intake}\right)^{(1)}$	0.197	0.189	0.185	0.194	*0.191*
Capacity utilization *(%)*	$\frac{Emissions\ based\ on\ capacity}{Actual\ CO2\ emissions}$	0.811	0.800	0.821	0.846	*0.820*
Total crude oil intake Shell *(ktons/y)*	$Crude\ oil\ nameplate\ capacity\ Shell^{(1)} * Capacity\ utilization$	17020.648	16809.189	17245.475	17773.339	*17212.163*
Total intake RFG Shell *(ktons/y)*	$\frac{Demand\ RFG\ (MW)^{(2)} * \frac{8760\ h}{year}}{0.00977 \frac{m3}{MWh} * 0{,}554 \frac{kg}{m3} * \frac{10^{-6} ktons}{kg}}$	-	-	-	-	*322.892*
Ratio RFG	$\frac{Total\ intake\ RFG\ Shell}{Total\ crude\ oil\ intake\ Shell}$	-	-	-	-	*0.019*
Ratio CO_2	$Actual\ CO2\ emissions$	-	-	-	-	*0.191*
Ratio end products	$1 - (Ratio\ RFG + Ratio\ CO2)$	-	-	-	-	*0.790*

1) Data source: Table D.1. Dutch refineries nameplate capacities and CO_2 emissions (Oliveira & Schure, 2020)
2) Data source: Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)

The same calculations are performed for the BP refinery, obtaining the results in Table 9.

Table 9. Mass balance calculations: BP refinery

BP refinery	*Formula*	*2016*	*2017*	*2018*	*2019*	*Average*
Emissions based on nameplate capacity *(%)*	$\frac{Direct\ CO2\ emissions\ in\ year\ Y^{(1)}}{Crude\ oil\ nameplate\ capacity^{(1)}}$	0.160	0.151	0.152	0.164	*0.157*
Actual CO_2 emissions *(%)*	$\left(\frac{Direct\ CO2\ emissions\ in\ year\ Y}{Crude\ oil\ intake}\right)^{(1)}$	0.197	0.189	0.185	0.194	*0.191*
Capacity utilization *(%)*	$\frac{Emissions\ based\ on\ capacity}{Actual\ CO2\ emissions}$	0.811	0.800	0.821	0.846	*0.820*
Total crude oil intake BP *(ktons/y)*	$Crude\ oil\ nameplate\ capacity\ BP^{(1)} * Capacity\ utilization$	16210,141	16008.752	16424.262	16926.990	*16329.536*
Total intake RFG BP *(ktons/y)*	$\frac{Demand\ RFG\ (MW)^{(2)} * \frac{8760\ h}{year}}{0.00977 \frac{m3}{MWh} * 0{,}554 \frac{kg}{m3} * \frac{10^{-6} ktons}{kg}}$	-	-	-	-	*258.214*
Ratio RFG	$\frac{Total\ intake\ RFG\ BP}{Total\ crude\ oil\ intake\ BP}$	-	-	-	-	*0.016*
Ratio CO_2	$Actual\ CO2\ emissions$	-	-	-	-	*0.191*
Ratio end products	$1 - (Ratio\ RFG + Ratio\ CO2)$	-	-	-	-	*0.793*

1) Data source: Table D.1. Dutch refineries nameplate capacities and CO_2 emissions (Oliveira & Schure, 2020)
2) Data source: Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)

An observation on the potential of hydrogen integration can be already made based on the calculations above. In fact, given the low flow rate of refinery fuel gas intake, it is very probable that the decision to invest in blue hydrogen replacing fuel gases will only minimally contribute to the cash flows of refineries. However, it might still be of interest to explore its consequences for the cash flows of producer. Moreover, the investment might be of interest from a cluster perspective, as it may contribute to CO_2 abatement in the Rotterdam industrial area, in turn increasing the total cluster cash flow due to lower (monetized) CO_2 emissions.

This perspective is consistent with the focus of the H-vision feasibility study, which is carried out from a 100% project perspective without taking into account the project internal commodity and cash flows between the separate H-vision participants (H-Vision, 2019). In this research, we attempt to combine the two perspectives.

Power generation: Uniper

While the H-vision concept envisions limited modifications of refining processes for high temperature heating, major modifications are required for power generation, combined with a challenging transition to biomass as an alternative for coal (H-Vision, 2019). Application in power plants appears as a technically feasible option by either co-firing (next to biomass) or installing additional new hydrogen turbines, to be connected to the existing plant. In this research, we model the conversion of Uniper MPP3 power plant into a combined biomass and hydrogen power plant, consistently with the H-vision Reference Scope. In this configuration, the plant uses biomass as primary fuel and hydrogen as a secondary fuel source, as illustrated in Figure 40 (Perner & Van Der Poel, 2019).

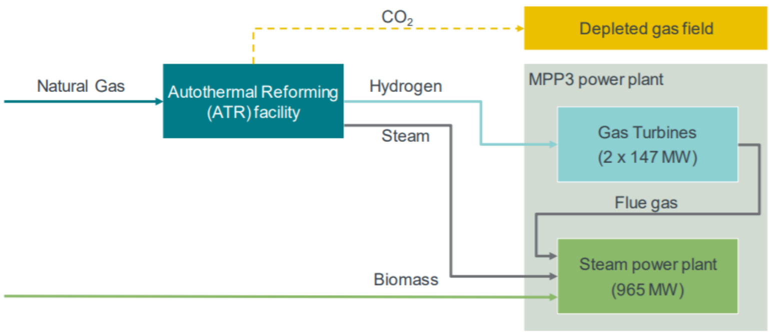


Figure 40. Illustration of the modelled repowering option for MPP3 (Perner & Van Der Poel, 2019)

To compensate for the lower heating value and heat input from biomass, two gas turbines fired with blue hydrogen from the H-vision ATR reformer are integrated into the existing plant. The resulting hot flue gases are subsequently integrated in the steam cycle of the power plant, allowing the MPP3 plant to work in a more efficient state than with biomass alone.

Similarly to what was done for refineries, we avoided overcomplicating the model with a complex representation of the MPP3 power plant. Instead, we opted for a simplified representation based on the scheme provided in Figure 40, for which we calculated the flow rates using Table D.6. (Appendix D) as input data. An overview of the performed calculations for the flow rates is displayed in Table 10, and Appendix D further elaborates on the followed procedure.

Table 10. Mass balance calculations: MPP3 power plant

MPP3 power plant	***Input data***	***Input units***	***Calculated ratio***	***Ratio***
Repowered plant parameters				
Heat input hydrogen	805	MW(th)	$\frac{Heat\ input\ hydrogen}{Power\ output\ GT} = \frac{1}{GT\ efficiency}$	2.73
Power output GT	294	MW(e)	-	1
Efficiency GT	0.365	-	-	-
Heat input biomass	1395	MW(th)	$\frac{Heat\ input\ biomass}{Total\ power\ output}$	1.11
Heat input steam turbine	227	MW(th)	$\frac{Heat\ input\ steam\ turbine}{Total\ power\ output}$	0.18
Power output steam turbine	965	MW(e)	-	-
Total power output	1259	MW(e)	-	1
Coal power plant parameters				
Heat input coal	2174	MW(th)	$\frac{Heat\ input\ coal}{Power\ output\ steam\ turbine}$	2.17
Power output steam turbine	1000	MW(e)		1

Data source: Table D.6. Model results for a repowered 1000 MW coal-fired power plant (H-Vision Consortium, 2019)

Auto thermal reformer: Air Liquide

In this research we model a single large-scale central production site, dimensioned based on the hydrogen demand from the modelled off-takers. Data reporting the input-output ratios was available, thus no additional mass balance calculations were performed –only unit conversions were needed. Our Linny-R representation of the ATR process in displayed in Appendix D, including the input data sources for the flow rates used in this representation and the conversions performed.

Differently from the case of refineries and the MPP3 power plant, this PU is modelled as an investment option, producing blue hydrogen to be integrated in the refineries and in the electric power plant. The investment is evaluated in combination with CO_2 capture and storage via the Porthos project, as envisioned in the Reference Scope of the H-vision feasibility study. The financial parameters in Table 11 are used as input in the model to correctly evaluate the attractiveness of this investment option and its integration with other cluster processes. Details on the derivation of these parameters and data sources are presented in Appendix D.

Table 11. Overview of financial parameters associated with investment in ATR

Parameter	*Reference value*	*Unit*
Capital investment costs reformer	981.6	M€
Annual fixed costs reformer (% capital costs/capacity)	49.1	€/ton
Capital retrofitting costs Shell refinery	119	M€
Capital retrofitting costs BP refinery	95.2	M€
Capital retrofitting costs Uniper power plant	162.5	M€
Default WACC	8.00	%

Blue hydrogen produced in the ATR investment option is integrated in existing cluster processes, which in turn require technical adaptations to their installations. For this reason, retrofitting costs derived from the H-vision feasibility study are taken into account. Using the same assumptions as in the feasibility study, no additional O&M is assumed.

Besides the needed technical modifications to furnaces, capital retrofitting costs of refineries also include the costs of connections to the existing natural gas grid. Furthermore, refinery fuel gases need to be transported to the blue hydrogen production facility. These costs are also incorporated in the refinery retrofitting costs.

Regarding the retrofitting costs of power plants, two main cost items are reflected, namely (i) the installation of new gas turbines and (ii) modifications to enable hydrogen firing in the preheat section. The costs for conversion of the coal power plants to biomass are not included in the study.

5.2.2.2. Green hydrogen production: conversion park (Shell, BP/Nouryon and Uniper)

The Port of Rotterdam plans to achieve its targets for green hydrogen production investing in multiple electrolysers over the course of the coming 30 years. We model this strategy by focusing on the existing plans of Shell, Nouryon and Uniper. More specifically, the three electrolysers are modelled in Linny-R replicating the same representation for each actor (see Appendix D), differing only for the capacity of each process.

Projects by BP/Nouryon and Shell will create 0.5 GW of capacity before 2025, to be supplied to their respective refining processes. Similarly, Uniper aims to realise a hydrogen plant by 2025 with a 100 MW capacity, to be subsequently up-scaled to 500 MW. However, no additional information on expansion plans is publicly available. For this reason, assumptions were made for the timing and dimensioning of subsequent capacity expansions for each of the electrolyser projects considered. Investments in additional capacity were assumed to be made approximately every 10 years, with the ambition to meet hydrogen demand for the considered off-takers. An overview of the assumptions is displayed in Table 12. The rationale of such assumptions is further explained in Appendix D.

Table 12. Overview of assumptions for capacity expansions of electrolysers

Required capacity	*Shell*	*Nouryon*	*Uniper*
Required capacity to meet refineries'/power plant's hydrogen demand (ktons H_2)	170.8	136.7	211.6
Required capacity to meet refineries'/power plant's hydrogen demand (GW electricity input)	1.04	0.84	1.29
Decision			
Initial capacity	40.86	40.86	40.86
Capacity 2025 (ktons)	40.86	40.86	81.72
Capacity 2030 (ktons)	81.72	81.72	211.6
Capacity 2040 (ktons)	171	137	211.6

Capacity expansions can be modelled in Linny-R via additional investment options whose capacities gradually add up to the required level of output. For each of the envisioned expansions, therefore, an additional binary variable needs to be introduced, exponentially increasing the solver's computing time. Given the size of the model, representing expansions with this procedure made the solver time infeasibly long, thus an alternative modelling choice was made.

Specifically, instead of considering capacity expansions as separate investment options, we made the decision to model an investment in a system of electrolysers for the coming 30 years. This means that, for every green hydrogen producer, we decide to model the investment in an electrolyser *strategy* over the whole model time horizon, rather than single investment decisions in electrolysers of different capacities, to be repeated every 10 years –namely and the end of an electrolyser's lifetime. This is done by modelling each of the three electrolyser strategies (by Shell, Nouryon and BP) as three electrolysis processes with an increasing upper bound overtime, to simulate upscaling of the technology. The capacity of each electrolysis process increases based on the values displayed in Table 12. Capital investment costs are calculated accordingly, by adding together all the capital investment costs of subsequent expansions. Expansions take into account future cost reductions, influenced by technological innovations (for instance, the development of less costly materials for electrodes and membranes), and by economies of scale. Therefore, each capacity expansion is associated to a specific CAPEX estimate decreasing overtime, added together with the other capital investment costs, as shown in Table 13.

Table 13. Overview of financial parameters for electrolyser strategies

Electrolysis Parameter	***Formula***		***Today***	***2030***	***2040***	***Unit***
CAPEX	$\dfrac{CAPEX\ per\ capacity\ \left[\frac{\$}{kW}\right]^{(1)} * 10^3 \left[\frac{kW}{MW}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(2)} * Discount\ factor^{(3)})}{8760\ \left[\frac{h}{y}\right] * Efficiency^{(1)} * \frac{1}{33.33\ \left[\frac{MWh}{tons}\right]}}$		2104.7	1518.34	1203.60	€/ton
Fixed production costs	$1{,}5\%^{(1)} * CAPEX\ [\frac{€}{ton}]$		31.57	22.77	18.05	€/ton
Total CAPEX	***Formula***	***Initial investment***	***Expansion 2025***	***Expansion 2030***	***Expansion 2040***	***Total CAPEX***
Shell	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2104.7*40.9	-	1518.3*81.7	1203.6*171	415.8 M€
Nouryon	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2104.7*40.9	-	1518.3*81.7	1203.6*137	374.9 M€
Uniper	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2104.7*16.3	1829.5*(81.7-16.3)	1518.3*215	1203.6*215	738 M€

1) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
2) Assumed 0.85 €/$
3) Assumed 10 years lifetime and discount rate of 8%

It should be noted that this modelling choice was made when Linny-R still relied on the LP_solve solver. Since June 14th 2021, thanks to tailored updates by Dr. P.W.G. Bots, it was possible to switch to the (more powerful) solver Gurobi. The computing times using Gurobi are reduced by approximately a factor 10 compared to the open source LP_solver, thus potentially allowing to implement capacity expansions as separate investment options without significantly hampering the model's running time.

5.2.2.3. Hydrogen backbone: Gasunie and Port of Rotterdam

As an infrastructure company, Gasunie works with the Port of Rotterdam Authority on the development of the regional hydrogen backbone, in the port area. The parties intend to realise the new pipeline in a joint venture, whose representation in Linny-R has already been discussed in the previous chapter. In our model, the representation provided in Chapter 4 is implemented with slight adjustments (see Appendix D) and specific assumptions, summarized below.

According to the projections of the JV partners, the regional backbone throughout the port area will be available in 2025. After this year, a start will be made on connecting the regional pipelines with each other and with foreign countries, so that they are integrated in the national (and future European) hydrogen backbone (Gasunie, n.d.). Based on the expected time of operation, we model the hydrogen backbone as an investment option that can only be brought into operation after 2025. This is done by limiting the upper bound of the backbone process to 0 before 2025. Subsequently, the hydrogen backbone can be evaluated as an investment option with a non-zero upper and lower bounds. As information on the stakes of Gasunie and the Port of Rotterdam in the Joint Venture was not publicly available, we assumed the two JV partners to have equal equity shares of 50%-50%. An overview of the financial parameters used to evaluate the investment in the pipeline is provided in Appendix D.

5.3. Modelling approach

The system described in Section 5.2. is used to perform our research experiments, following the procedure elucidated in Section 5.1. The effects of contracts on actors' cash flows will be quantified across three different macro-economic scenarios, in order to draw robust conclusions on the obtained results.

5.3.1. Key uncertainties and scenarios

Three scenarios have been drawn up due to the uncertainty regarding future macro-economic developments influencing commodity prices. It is important to quantify the effects of contractual structures across multiple commodity price scenarios, as they represent a critical variable that may swing the choice of the contract form that is best suited to support specific investments. These uncertainties are summarized in the uncertainty table in Appendix E, which is used as a basis for the scenarios' definition. The resulting scenarios were considered:

1. **As Usual World:** this scenario assumes no ground-breaking new policies or developments; prices follow the current trend and there is no accelerated CO_2 reduction. As a result, CO_2 prices are not expected to increase much further and gas prices follow a similar trend;
2. **Economical World:** in this scenario, persistent ambitions to achieve climate goals and strong economic growth result in resource constraints, giving rise to price increases both for commodities and CO_2 certificates. Importantly, high CO_2 prices do not lead to lower demand for natural gas, allowing for price hikes of the commodity;
3. **Sustainable World:** the last scenario assumes that the implementation of ground-breaking climate policies provokes shortage on the CO_2 market, pushing up CO_2 emission prices so as to enable the investments needed to limit global temperature rise to 2°C. This creates economic distress and low demand for fossil-based resources, leading to low natural gas prices.

The described scenarios are predominantly based on the IEA's "Current Policies", "New Policies" and "Sustainable Development" scenarios (International Energy Agency, 2018), as well as on scenarios from the H-vision feasibility study (H-Vision, 2019). Such scenarios served as a basis to derive future trends of commodity prices, in combination with electricity and biomass price forecasts from CE Delft, Frontier Economics and more recent reports from the International Energy Agency (Afman, Hers, & Scholten, 2020; IEA, 2020; Perner & Van Der Poel, 2019). An overview of the range of considered future outcomes is presented in the aforementioned uncertainty table (Appendix E), and summarized in Table 15.

As the focus of our research is on sensitivities versus determinants of hydrogen contract prices, scenarios focused mainly on variations of CO_2, natural gas and electricity prices. For coal and crude oil, prices of the IEA Current Policies scenario are applied. Biomass prices are assumed to remain constant in real terms at the level of today's forward prices (32.6 €/MWh). This assumption was made consistently with the Frontier Economics feasibility study on coal-fired power plants' conversion into biomass power plants (Perner & Van Der Poel, 2019). Appendix E further elaborates on such choices.

Below, an overview of the considered price ranges across scenarios is provided. Commodity prices are expressed in the units required by the model, and the ranges present the lowest and highest price values from today until 2050. The performed conversions are shown in Appendix E.

Table 14. Overview of the As Usual World, Economical World and Sustainable World scenarios

Commodity prices	Required unit	Scenarios		
		As Usual World	***Economical World***	***Sustainable World***
Gas market price[(1)]	k€/hm^3	MED *219-295 k€/hm^3* *(7.3-9.8 $/MBtu)*	HIGH *219-313 k€/hm^3* *(7.3-10.4 $/MBtu)*	LOW *219-235 k€/hm^3* *(7.3-7.8 $/MBtu)*
CO_2 certificates[(2)]	k€/kton	MED *30-42 k€/kton*	HIGH *30-160 k€/kton*	HIGH *30-160 k€/kton*
CO_2 transport and storage tariff[(3)]	k€/kton	MED *30 k€/kton*	HIGH *80 k€/kton*	LOW *22.5 k€/kton*
Electricity price[(4)]	k€/GWh	MED RES penetration *83-105 k€/GWh*	MED RES penetration *83-105 k€/GWh*	HIGH RES penetration *83-66 k€/GWh*

1) Data source: International Energy Agency. (2018). *World Energy Outlook 2018.* LOW, MED and HIGH estimates derived from the Sustainable Development, New Policies and Current Policies scenarios' price projections, respectively
2) Data source: International Energy Agency. (2018). *World Energy Outlook 2018.* MED and HIGH estimates derived from the New Policies and Sustainable Development scenarios' price projections, respectively
3) Data source: H-Vision Consortium. (2019). *Annexes to the H-vision Main Report* . LOW, MED and HIGH estimates derived from H-vision scenarios
4) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*

5.3.2. Experimental setup and contract price determination

As previously discussed, this research makes use of two models to test the effects of contractual structures. The system described in Section 5.2. is represented in both models, the only difference being the contract representation that facilitates the integration of hydrogen, as discussed in 5.1.2.

Given the objective to analyse the transition of the system on a 30-year time horizon, combined with the availability of future price estimates and trends on an annual basis, we decided to run the two models using a time-step of *t=1 year*. This choice also resulted from the fact that a smaller time-step would have increased the model's computation time, already undermined by the high number of binary variables used to include investment options and the respective revenue contracts for their integration. A reflection on the implications of such choice is included in Chapter 6.

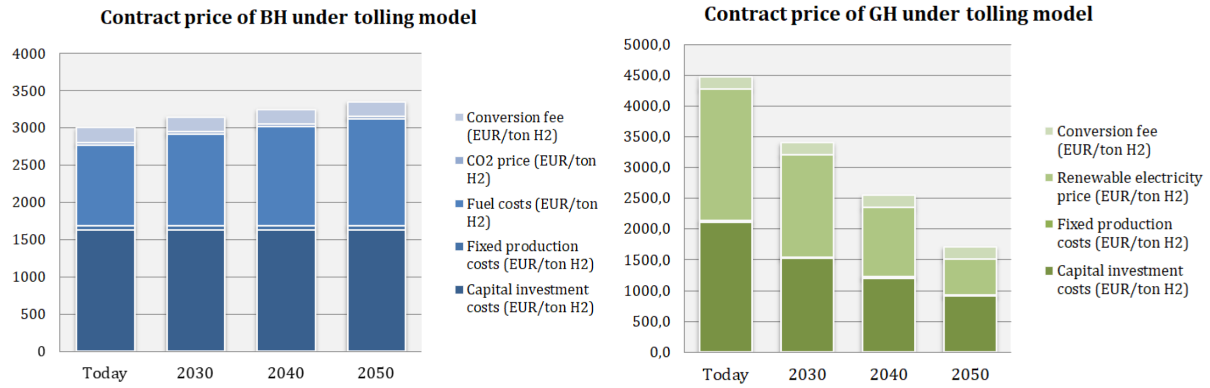
By implementing the models, two objectives are achieved: (i) providing a proof of concept of the devised methodology for contracts' representation in MILP models and (ii) providing insights in the kind of dynamics that may materialize in the realisation of investment projects when different contracts are implemented.

5.3.2.1. Bilateral contracts

As explained in Table 6 in Chapter 3, two separate simulations are run using the first model, as a result of which the effects of tolling agreements and sale-and-purchase agreements are quantified and compared.

Tolling model: characteristics and contract price determination

A tolling model for hydrogen projects works as follows: the hydrogen off-taker is responsible for procuring the required feedstock for hydrogen production and, on top of that, pays the hydrogen plant operator a fee to convert it into hydrogen (Dentons & OPERIS, 2021; Martin, 2021). In accordance with the logic underlying a tolling agreement, hydrogen contract prices under a tolling model are determined by (i) capital investment costs and fixed production costs –which need to be covered by any type of contract, (ii) variable production costs, represented by the feedstock price and (iii) a profit element, constituted by the conversion fee. Based on this pricing procedure, the following hydrogen contract prices (in €/ton) under a tolling agreement are derived:



Notes: Assumed WACC = 8%. Natural gas price of 7.3-9.8 $/MMBtu. CO_2 price of 35-40 €/tCO_2. Electricity price (grid) of 88-105 €/MWh. Renewable electricity price = 40-20 €/MWh; CAPEX and OPEX discounted over a 25y lifetime for ATR and 10y for electrolysers; More information on the underlying assumptions is available in Appendix F

Figure 41. Hydrogen contract prices under tolling model

Appendix F elaborates on the calculations performed to obtain the contract prices in Figure 41.

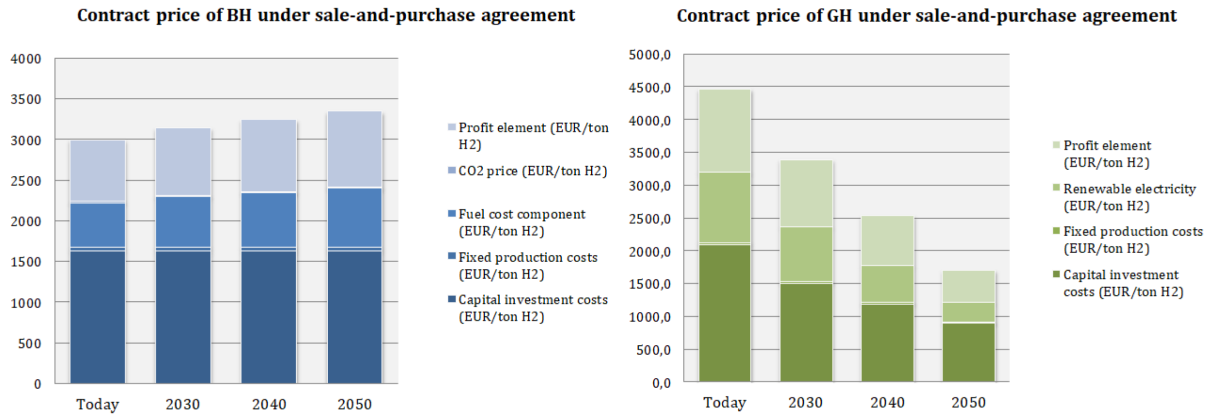
Sale-and-purchase agreement: characteristics and contract price determination

Under a hydrogen sale-and-purchase model, a hydrogen developer procures the feedstock fuel and then produces and sells hydrogen. This contracting model may leave the hydrogen producers managing a lot of risks, hence contract pricing mechanisms need to be set in a way that allows the producer to still cover the variable costs of production in some other way (Dentons & OPERIS, 2021).

This can be done by simply setting a higher profit element on top of the usual cost components described in the previous section. It is also possible that the hydrogen producer procures electricity/feedstock materials in ways that reduce risks of price exposure or power supply: this is possible via power purchase agreements (PPAs) or by playing a role in electricity production. These situations fall outside the scope of the research, which focuses on hydrogen contracts rather than on its combination with other cost-reduction strategies and/or agreements. Thus, we find an alternative way to set contract prices in a way that reflects lower price exposure from the side of the consumer compared to a tolling model.

Specifically, we assume that only a percentage of the total costs of raw material is passed on to the end-user via the contract price. The remaining variable costs of production are covered by the profit element. In order to make the effects of the two contracts comparable, we ensure that the total contract prices for a tolling model and a sale-and-purchase agreement are equal by setting the value of the profit element accordingly.

Based on the aforementioned considerations, hydrogen contract prices under a sale-and-purchase agreement are determined by (i) capital investment costs and fixed production costs, (ii) a share of variable production costs and (iii) a profit element. The following hydrogen contract prices (in €/ton) under a sale-and-purchase agreement are obtained:



Notes: Assumed WACC = 8%. Natural gas price of 7.3-9.8 \$/MMBtu. CO_2 price of 35-40 €/tCO_2. Electricity price (grid) of 88-105 €/MWh. Renewable electricity price = 40-20 €/MWh; Assumed 50% of raw material costs is incorporated in the contract price. CAPEX and OPEX discounted over a 25y lifetime for ATR and 10y for electrolysers; More information on the underlying assumptions is available in Appendix F

Figure 42. Hydrogen contract prices under sale-and-purchase agreement

By comparing the effects of a tolling model or a sale-and-purchase agreement for bilateral transactions, we aim to understand whether different pricing mechanisms for bilateral contracts influence the cluster's investment timeline. In case no significant difference is found, we can still draw conclusions on the effects of bilateral contracts in general, disregarding the (more detailed) effects of price exposure.

5.3.2.2. Multilateral contracts

The second model is used for experiments concerning the effect of multilateral contracts on investment decisions. Two rounds of experiments are performed, each one adopting a specific multilateral contract form that requires a different degree of standardisation. Specifically, the two experiments test the effects of multilateral contracts that (i) market green hydrogen and blue hydrogen as separate products, but using a standardized price per commodity or that (ii) market green hydrogen and blue hydrogen as a single commodity, using the same standardised price.

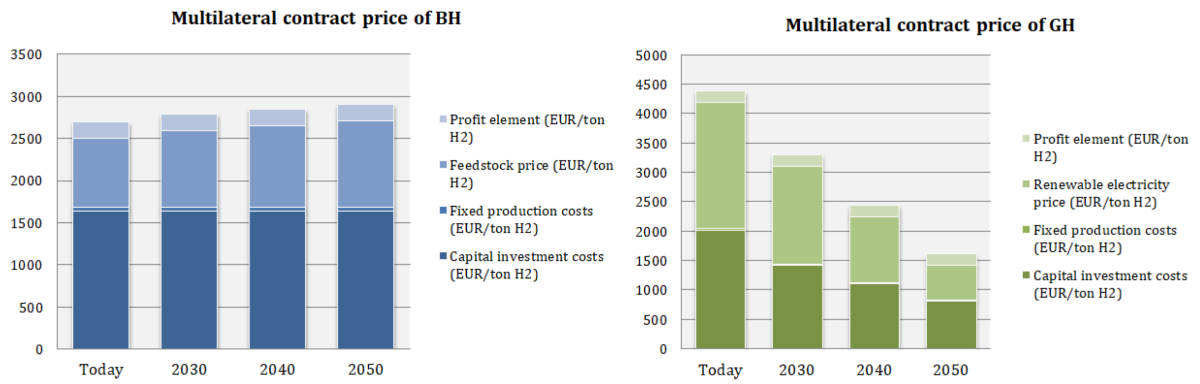
<u>Multilateral contract with separate, standardized commodity prices</u>

Under the first multilateral contract form considered, a single standardized price for blue hydrogen is established and applied to all the customers, and the same procedure is performed for green hydrogen pricing. Blue hydrogen and green hydrogen are therefore marketed as a separate products with distinct prices.

This differs from bilateral price-setting dynamics. In fact, under bilateral contracting, tailored prices for each bilateral exchange between producer and off-taker can be established based on the costs that a given producer bears to supply its hydrogen to the contract counter-party (see Appendix F, Section F.3). On the other hand, multilateral contracting seeks to reduce the transaction costs of formulating contract terms that are specifically adapted to the rights and obligations of each contracting party (Scott, 2020). This comes at the cost of fitting individual deals less perfectly than situation-specific tailored agreements (Scott, 2020).

It should be noted that there are currently no spot prices for hydrogen that could be used as a reference to establish a standardized contract price (den Ouden, 2020; Martin, 2021). Therefore, it is important to identify a multilateral pricing procedure, in order to guarantee that the standardized price per commodity is set at a level that is sufficient to make the project economically viable and capable of repaying the debt.

In this research we derive multilateral contract prices by aggregating hydrogen prices calculated in the previous section, resulting in the standardized multilateral prices displayed below. Further details on the contract price calculations are presented in Appendix F.



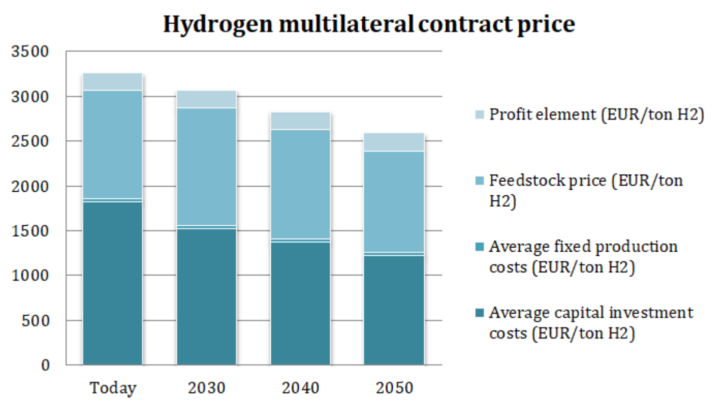
Notes: Assumed WACC = 8%. Natural gas price of 7.3-9.8 $/MMBtu. CO_2 price of 35-40 €/tCO_2. Electricity price (grid) of 88-105 €/MWh. Renewable electricity price = 40-20 €/MWh; CAPEX and OPEX discounted over a 25y lifetime for ATR and 10y for electrolysers; More information on the underlying assumptions is available in Appendix F

Figure 43. Hydrogen contract prices under multilateral contract with price differentiation per commodity

<u>Multilateral contract single, standardized hydrogen price</u>

Another possible approach for multilateral contracts' implementation is to move to frameworks that facilitate the exchange of hydrogen with different characteristics, but with the aim to market it as a single product (den Ouden, 2020). This results in a single hydrogen price, that is not differentiated based on the production pathway and that could be considered as a trading price applied to all market participants.

To derive an estimate of such single standardized price, we use the same pricing procedure applied in the previous sub-sections to derive a standardized price per commodity. However, in the case of a single standardized price for hydrogen, such method is applied by comparing and aggregating all prices of hydrogen of different varieties together. Appendix F further elaborates on the devised procedure. As a result, the hydrogen price in Figure 44 is obtained.



Notes: Assumed WACC = 8%. Natural gas price of 7.3-9.8 $/MMBtu. CO_2 price of 35-40 €/tCO_2. Electricity price (grid) of 88-105 €/MWh. Renewable electricity price = 40-20 €/MWh; CAPEX and OPEX discounted over a 25y lifetime for ATR and 10y for electrolysers; More information on the underlying assumptions is available in Appendix F

Figure 44. Hydrogen contract prices under multilateral contract without price differentiation

5.4. Model verification

Sections 5.2 and 5.3 have described a considerable number of implementation steps. As with any model, implementation comes with significant possibilities of human error. Hence, it is crucial to verify the testing tool to ensure correct implementation.

Model verification concerns building the model right, thus ensuring that a model implementation accurately performs as intended by the developer (Cook & Skinner, 2005). Since our testing tool cannot be compared to any known benchmark (as far as known no similar models have been developed on this subject with this same scope), it is verified in parts. To perform verification in parts, distinct model components with given relations between in- and outputs are isolated and examined. Once this procedure is systematically conducted for all components of a model, it can be considered verified. This is accomplished by deploying the following methods:

i. Structured walkthroughs
   A careful inspection of each model is performed, by double checking all input parameters through all calculation steps to the resulting outcomes;
ii. Balance checks
   Isolated calculations of different model parameters are performed and benchmarked against the model values
iii. Testing of extreme inputs
   The models' performance and robustness is assessed by evaluating outputs for extreme inputs and by benchmarking them with the expected model's behaviour

5.4.1. Structured walkthroughs

During the structured walkthroughs, different model parameters are inspected by following all calculation steps. Particular attention has been given to the examination of mass balances of the modelled processes, checking for consistency between the inputs, the performed calculations and the values inserted as flow rates in the Linny-R models. Special consideration has been taken when reviewing hydrogen price calculations, making sure that all cost components and profit elements had been correctly plugged into the model, in the right proportions. Finally, the expressions determining the fulfilment of contract conditions in the contract modules have been carefully inspected to ensure that the positivity of cash flows are correctly monitored, as well as for price comparisons between alternative fuel options. The correct functioning of these elements is then tested via balance checks (Section 5.4.2.). For all the examined model components, walkthroughs did not generate any surprises.

5.4.2. Balance checks

Throughout the balance checks, simple isolated calculations are performed with model parameters and compared with the model outputs. An overview of the performed balance checks is provided in Table 16.

Table 15. Balance checks of calculated values

Balance Check	Description	Verified	Conclusion
Computation of investment costs	Investment costs and contract costs are charged only at the moment of the first start-up and correctly discounted according to the discount factor	✓	Correct implementation of investment costs and contract costs are
Revenues of H_2 producers	Hydrogen producers receive a revenue stream that allows to cover the (fixed) costs of the production facilities and the (variable) market price of inputs at every time step	✓	Correct implementation of pricing formulas establishing the contract price of hydrogen
Monitoring of CFs	Contract conditions to monitor cash flows' positivity accurately simulate the revenue trends	✓	Correct implementation of contract conditions for CF positivity
Comparison of fuel prices	Contract conditions that monitor the integration of the most convenient fuel accurately perform pairwise price comparisons	✓	Correct implementation of contract conditions for fuel convenience

5.4.3. Extreme conditions

By testing the models under extreme conditions, their robustness is verified. In this section, we perform price manipulations similarly to Section 4.3.2. However, these verification experiments crucially differ from the ones in previous chapters in that pricing formulas are adopted as expressions for the specification of hydrogen contract prices. Therefore, to achieve the desired variations in contract prices, their underlying cost components (such as natural gas price, electricity price, CAPEX and OPEX) are manipulated by increasing and decreasing their value by ±99%. Under all above-mentioned conditions, the models perform as expected. The table below displays the manipulated parameters, the lower and upper bounds and expected results for the extreme cases (i.e. combined increase or reduction of the selected manipulated parameters). This is done to allow a more straight-forward prediction of the model behaviour and identification of expected results.

Table 16. Model verification under extreme conditions

Test parameters	Manipulated parameters	LB/UB	Expected results	Verified
Low green hydrogen price; Blue hydrogen price at default value	Electricity (RES) price CAPEX OPEX	-99%	Favourable conditions for green hydrogen integration in refineries and power plants. Price very low but allows to pay back investment costs	✓
Low blue hydrogen price; Green hydrogen price at default value	Natural gas price Electricity price CO2 price CAPEX OPEX	-99%	Favourable conditions for blue hydrogen integration in refineries and power plants. Price very low but allows to pay back investment costs	✓
Low blue hydrogen and green hydrogen price	Natural gas price Electricity price CO2 price Electricity (RES) price CAPEX OPEX	-99%	Favourable conditions for the integration of both types of hydrogen in refineries and power plants, switching from one fuel to the other based on price. Price very low but allows to pay back investment costs	✓
High green hydrogen price; Blue hydrogen price at default value	Electricity (RES) price CAPEX OPEX	+99%	Prohibitive costs for green hydrogen integration for refineries and power plants, which make transactions unprofitable for the off-takers. Only investments in blue hydrogen are made. When the price of green hydrogen decreases below an acceptable threshold (simulating the maximum willingness to pay of end-users), green hydrogen is sold via the backbone to external off-takers (end-use not specified, out of scope)	✓
High blue hydrogen price; green hydrogen price at default value	Natural gas price Electricity price CO2 price CAPEX OPEX	+99%	Prohibitive costs for blue hydrogen integration, which make transactions unprofitable. Only investments in green hydrogen are made. When the price of blue hydrogen decreases below an acceptable threshold (simulating the maximum willingness to pay of end-users), blue hydrogen is sold via the backbone to external off-takers (end-use not specified, out of scope)	✓
High blue hydrogen and green hydrogen price	Natural gas price Electricity price CO2 price Electricity (RES) price CAPEX OPEX	+99%	No investments are made until the contract price drops below an acceptable threshold. Then hydrogen is sold via the backbone but not integrated in the processes because its price is still too high for the specified end-use.	✓

5.5. Model validation

Model validation refers to assessing the degree to which a model and its associated data constitute an accurate representation of real world dynamics (Cook & Skinner, 2005). Due to the longer-term orientation of this research, model outputs cannot be compared to real life results. However, input validation can still be performed as a way to measure the accuracy of inputs. To this end, the following elements are evaluated:

i. Inputs' complexity
ii. Sources' reliability
iii. The degree of manual manipulation of inputs from source to model

Generally speaking, the greater the complexity of model inputs and assumptions, the greater the risk of errors. For instance, by aggregating multiple input data to generate one model input, the model will be inherently more subject to risks of inaccuracies. In our model, the inputs requiring this kind of aggregation are contract prices. Such inputs are validated by comparing partial outputs of aggregation to the corresponding expected values according to literature or reports. Specifically, the value obtained from the aggregation of hydrogen cost components is benchmarked against projections and estimates from different sources (such as IEA, IRENA, Hydrogen Council) that provide expert analytical insights into the potential of hydrogen for decarbonization. In this way we ensure that the calculated hydrogen contract price is consistent with future estimates. This kind of validation has been performed in Appendix F.

In addition to that, the degree of manual manipulation of inputs from source to model increases the risk of inaccurate results. An example of manual manipulation concerning our model is the conversion of source data units of measurement to fit the needed model input units. Although this task does not involve significant complexity, it increases the potential of errors compared to a situation involving simply copy-pasting data in the correct input entries. The simplest method to validate manual operations is to individually repeat manual operations from source to model input to identify any possible inaccuracy. The same validation procedure is employed to validate calculations of used trends derived by linear extrapolation from yearly data, obtained from the above-mentioned sources.

Finally, it is important to distinguish between inputs with significant impact on model outputs, and inputs with minimal effect. For the former case, a scenario analysis can be performed. This is done by comparing the model results across the presented scenarios, in which inputs with significant impact on model outputs are varied to test the robustness of results (Section 4.6).

Notwithstanding the fact that input validation does not correspond to a successfully validated model, it does significantly lower the risk of inaccuracies and distorted outputs. Thus we can conclude that our model has successfully been validated by the method of input validation. The next chapter presents the results of the experiments performed with the verified and validated models.

6. Results and discussion

This chapter discusses the results of the experiments of the Linny-R models proposed in Chapter 5. Section 6.1. presents the results obtained from model iterations by quantifying the effects of each contractual structure on the cash flows of the total cluster and of individual actors, namely the main metrics for results evaluation. Results are described in relation to the underlying determinants of cash flows (i.e. CO_2 emissions and optimal investment curves), in order to provide an overview of these factors' contribution to the generated cash flows. In this way, we answers the last research sub-question. Section 6.2. subsequently provides an interpretation of the model results, accompanied by a critical reflection on the developed methodology, on its implementation and on the proposed model. Next, societal, managerial and theoretical relevance are discussed, together with research limitations.

6.1. Model results

This section provides an overview of the results obtained from the Linny-R experiments. The effect of the examined contractual structures is quantified based on actors' cash-flows over the considered time horizon of 30 years. For each category of contract, the total cash-flows are compared performing a scenario analysis, to allow for a robust interpretation of results. In this way, we aim to answer the last research sub-question, *"What is the effect of adopting different contractual structures on investment decisions for the transition of the Rotterdam cluster?"*.

6.1.1. Effects of bilateral contracts

Two model simulations are run to test the impact of tolling agreements compared to sale-and-purchase agreements on optimal investment decisions. Such model iterations allow to achieve two main objectives: (i) to quantify the effects of bilateral contracts as a category and (ii) to understand to what extent do different pricing mechanisms for bilateral contracts influence the cluster's investment timeline. If no significant influence of pricing mechanisms is detected, the performed experiments still allow to draw conclusions on the impact of bilateral contracts, to be compared with the effects of multilateral agreements.

The simulations return the actors' cash flows resulting from the optimal investment path identified by the solver, under the specified contractual structure. A typical output is displayed in Figure 45. Multiple model iterations are performed to obtain such results for tolling agreements and sale-and-purchase agreements, across the scenarios presented in Chapter 5.

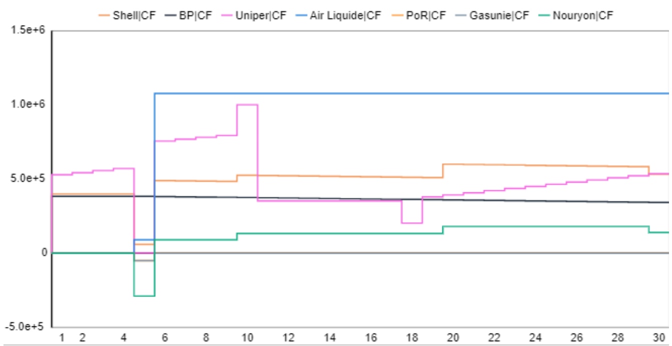


Figure 45. Actors' cash flows per time-step - Tolling model, As Usual scenario

This kind of results allow to visualize the effects of the activation of different investment options on the cash-flows of individual actors per time-step. This provides insight in the financial consequences of single or combined (hardware) changes in the system, as supported by a given set of contracts. In the context of the energy transition, capital investment costs and CO_2 levels are relevant factors that need to be monitored. Note that the effects of these factors are already accounted for in the obtained cash flows. These cash flows' determinants can be isolated and quantified, showing how they relate to the total cluster cash flows: hence, the model outputs allow to gain insights both in the financial and environmental performance of the cluster.

By aggregating the model outputs displayed in Figure 45, a more compact representation of results is provided. This is repeated for all model iterations across the As Usual World, Economical World and Sustainable World scenarios, and for both contractual forms: results are summarized in Figure 46, which compares the effects of adopting tolling agreements versus sale-and-purchase agreements to support bilateral exchanges in the Rotterdam cluster.

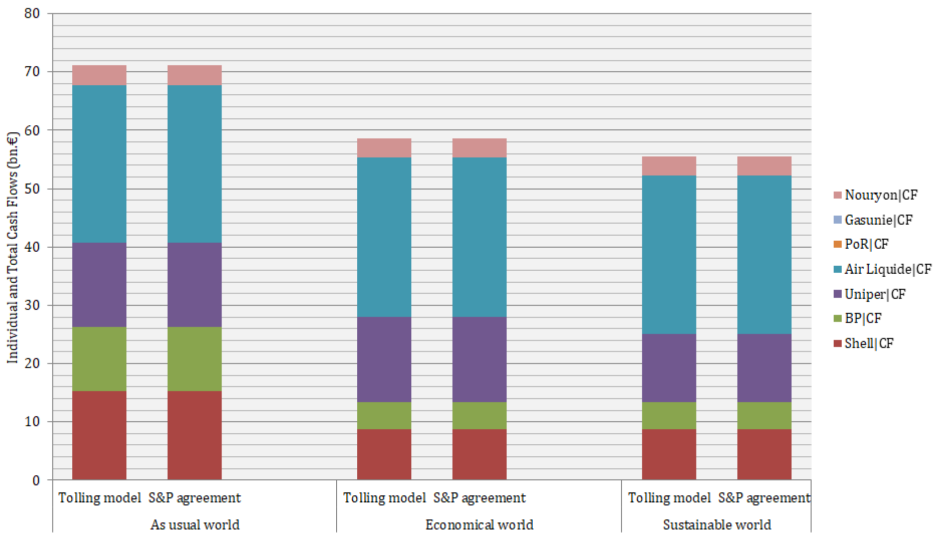


Figure 46. Model results: cluster cash flows under bilateral contractual agreements

Tolling agreements and sale-and-purchase agreements yield the same total and individual cash flows under each of the considered scenarios. Thus, adopting different pricing mechanisms to determine bilateral contract prices does not seem to affect the cash flow distribution within the cluster.

This result can be traced back to the optimal investment selection performed by the solver when optimizing the total cluster cash flow. Based on the selected investments, CO_2 emission levels vary accordingly, as some processes that are more or less carbon-intensive are activated or shut-down.

The graphs below represent the optimal investment curves obtained running the experiments under each scenario. The curves plot the level of cumulative investment costs in bn.€ over time. The graphs below clearly show that there is a complete overlap in investment curves resulting from the two experiments. Hence, the same investment decisions are taken.

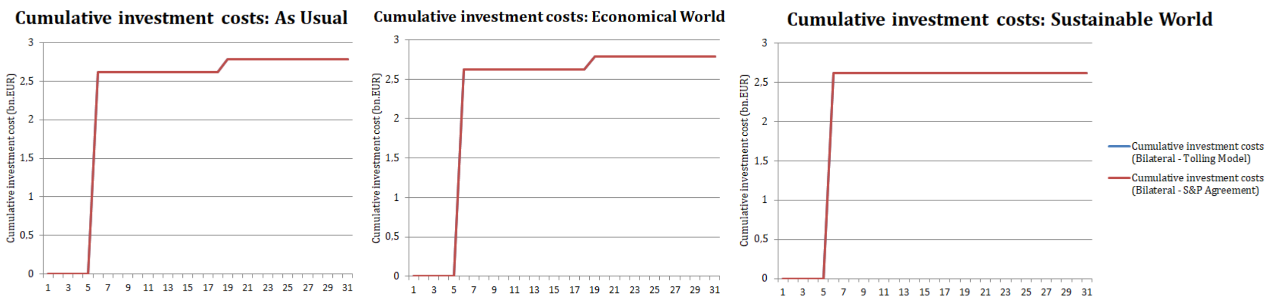


Figure 47. Optimal investment curves under bilateral contracts

More specifically, once the backbone becomes operational in 2025 (*t=5*), a steep increase in cumulative investment costs is observed. This behaviour is due to the fact that investment options in blue and green hydrogen automatically become attractive as their end-products can be sold via the backbone. However, no additional integration of hydrogen in refining processes nor in power plants takes place until time-step 18. Specifically, under the As Usual World and Economical Scenarios, only green hydrogen is integrated in the electric power plant from Uniper as a secondary fuel source, together with biomass. The decision of repowering the MPP3 power plant is not made in the last scenario. Blue and green hydrogen integration does not constitute an attractive option for refineries in any of the scenarios, as refineries gain a higher margin by continuing to rely on fuel gas reutilization.

Such overlap in investment decisions is reflected in identical levels of CO_2 emissions for both contractual structures, under all scenarios.

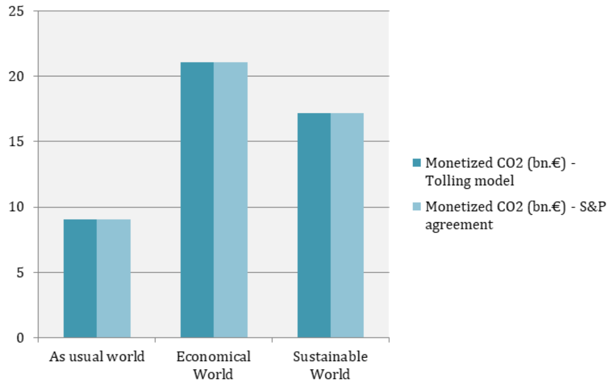


Figure 48. Monetized CO2 emissions per scenario under bilateral contracts

Being the relevant determinants of cash flows identical, total and individual cash flows calculated under tolling agreements and sale-and-purchase agreements amount to the same value under each of the considered scenarios.

The decrease in cash flows under each scenario is mainly due to differences in commodity prices. Based on how contract prices compare to other commodity prices, hydrogen integration may (not) be an interesting option for existing cluster processes. This eventually shifts investment decisions overtime, influencing the optimal investment path (thus the level of associated CO_2 emissions) across scenarios.

6.1.2. Effects of multilateral contracts

A second round of experiments is run to test the impact of two multilateral contract forms requiring different degrees of price standardization. Such simulations allow (i) to quantify the effects of multilateral contracts and (ii) to assess to what extent does price standardization influence the cluster's optimal investment timeline.

As previously explained, actors' cash flows in the form displayed in Figure 45 are obtained from simulations. Results are aggregated over the whole time horizon and compared in Figure 49, across the three considered scenarios.

Contrarily to the previous set of experiments, differences in the total and individual cash flows under distinct multilateral contractual agreements are detected. Thus, the degree of price standardization in multilateral contract prices is an additional factor that contributes to differentiate cluster cash flows – although with a minimal effect. Again, these differences can be traced back to the optimal investment path, and the resulting CO_2 emission costs.

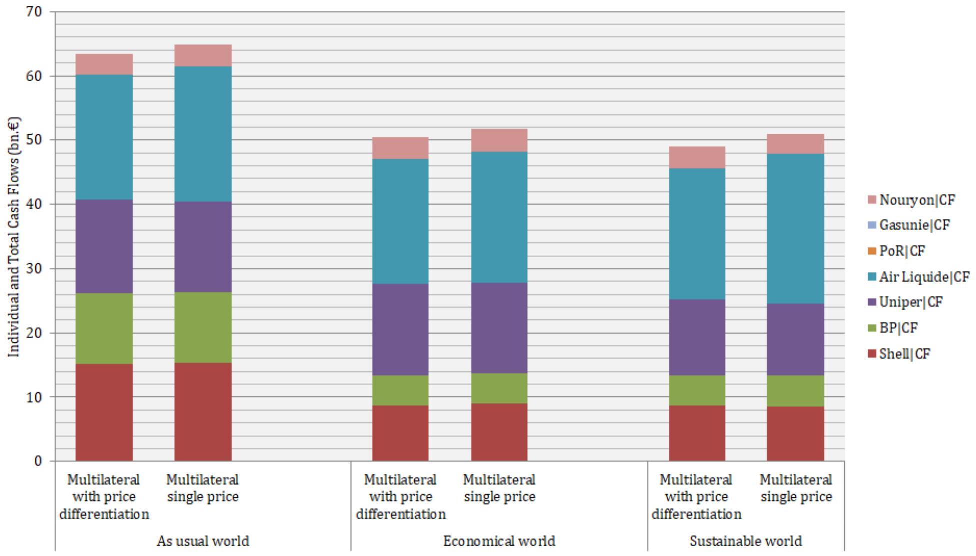


Figure 49. Model results: cluster cash flows under multilateral contractual agreements

Specifically, the adoption of multilateral contracts with a single standardized hydrogen price shifts investment decisions for hydrogen integration to a different moment in time, compared to the multilateral agreement with price differentiation. The optimal investment curves in Figure 50 show that, although most of the investment decisions overlap under different contractual structures, some assets are activated later in time. More precisely, cumulative investment costs rocket after 2025 due to the hydrogen backbone becoming operational, following the same trend under all scenarios for both types of contracts. Subsequently, hydrogen is integrated in Uniper's electric power plant at different moments in time, based on the contractual structure adopted. Similarly to the bilateral case, blue and green hydrogen integration does not constitute an attractive option for refineries. On the other hand, the integration in power plants is anticipated compared to the system that relies on bilateral agreements.

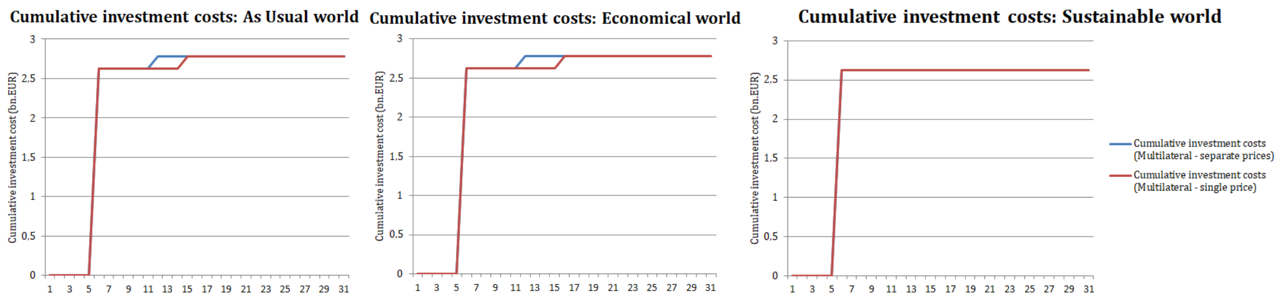


Figure 50. Optimal investment curves under multilateral contracts

It should be noted that, in this case, both blue and green hydrogen are integrated in the electric power plant from Uniper as a fuel source. The adoption of distinct multilateral contracts influences the sequence of hydrogen integration in the modelled industrial processes. In fact, when multilateral contracts with separate hydrogen prices per commodity are adopted, blue hydrogen is initially integrated in Uniper's MPP3 power plant, gradually supplemented with green hydrogen –once this option becomes more price competitive. The second contractual form, instead, allows for a simultaneous integration of green and blue hydrogen for Uniper, as both hydrogen types are marketed at the same price and no additional cost reductions are associated with choosing one option over the other. This difference slightly stretches the individual cash flows of hydrogen producers (Air Liquide, Nouryon, Shell and Uniper).

In this research, we have assumed that only small adaptations are required when a process is switching from blue hydrogen to green hydrogen as a fuel source, due to similarities in the types of fuels and in the retrofitting process: thus, for the second integration, we did not consider any additional retrofitting costs. For this reason, the switching time from blue to green hydrogen integration in the power plant is not visible from the investment curves above. Had we considered additional retrofitting costs, a more pronounced difference would have been visible in the last part of the curves.

The low variability in investment decisions for decarbonization is reflected in (minimal) changes in the level of CO_2 emissions for both multilateral contractual structures, as shown below.

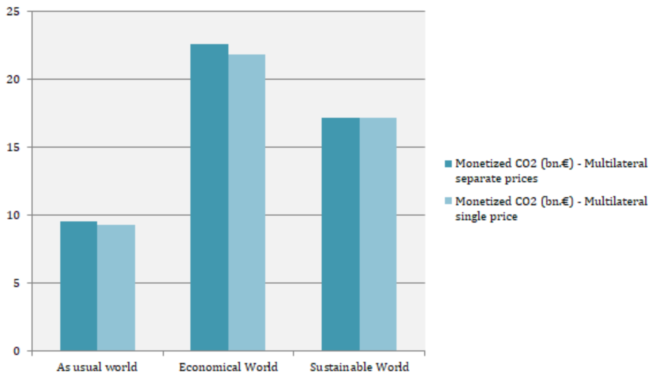


Figure 51. Monetized CO2 emissions per scenario under multilateral contracts

Again, the decrease in cash flows under each scenario is mainly due to differences in commodity prices. As a result, investment decisions are shifted in time, in turn impacting the level of CO_2 emissions. Notwithstanding the differences in total cash flows across scenarios, multilateral contracts using a single, standardized price generate the highest cash flows under all scenarios.

6.1.3. Comparison of effects of contractual structures

Figure 52 compares the obtained cash flows under each contractual structure across scenarios. This provides measurable insights on the effects of contractual agreements on the transition, from a financial (and, indirectly, environmental) perspective.

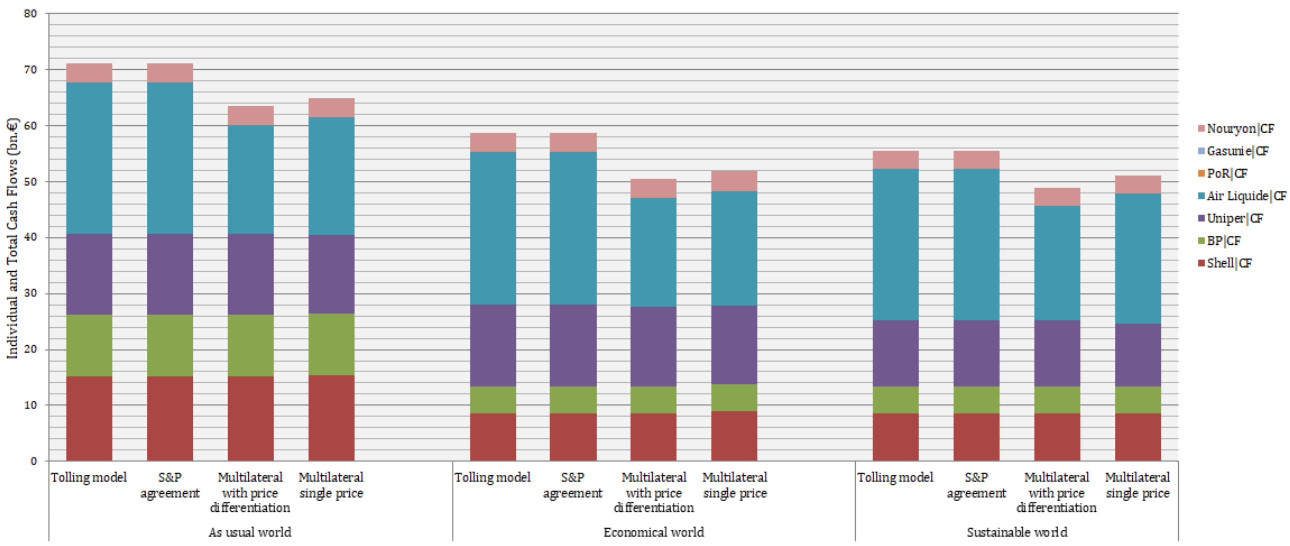


Figure 52. Model results: overview of cluster cash flows under tested contractual structures

Interestingly, bilateral contracts generate the highest cluster cash flows, reaching 71.13 bn.€, 58.62 bn.€ and 55.29 bn.€ under the As Usual World, Economical World and Sustainable World scenarios, respectively. Multilateral agreements with standardized prices per commodity, on the other hand, are the least convenient contractual structure from an economic standpoint, producing 63.46 bn.€, 50.43 bn.€ and 48.94 bn.€ under the same scenarios. Such effects are analysed in the next section, while providing an interpretation of the presented results.

6.2. Discussion

6.2.1. Interpretation and discussion of model results

Having presented the model results quantitatively, we now provide a higher-level assessment of the results, with a specific focus on the underlying sensitive parameters. This allows to confirm or reject our hypotheses and to provide an answer to SQ6.

6.2.1.1. Interpretation and discussion of effects of bilateral contracts

The performed experiments have shown that adopting tolling agreements versus sale-and-purchase agreements yields the same total and individual cash flows under all scenarios. As a result, no significant effects of adopting different pricing mechanisms are detected, thus rejecting our first hypothesis. This is due to several factors.

Firstly, the reader should be reminded that a modelling choice was made to set the same contract price under tolling agreements and sale-and-purchase agreements, while only varying the proportions of the underlying components. This decision was made (i) to make the effects of the two contracts comparable and (ii) to model different risk exposure of contractual parties, based on the type of agreement. However we were aware of the high chance that, by setting the contract prices the same, the Linny-R solver would allocate the same material flows, hence the same cash-flows, to the cluster actors in both the experiments. In fact, this effect did materialize, leading to a complete overlap in investment curves, as shown in Figure 47. As the same investment decisions are taken, the same CO_2 reduction trends are obtained under both contracts. Thus, from an economic and environmental standpoint, tolling agreements and sale-and-purchase agreements lead to identical results in the modelled system and show no incentive to choose any of the two contractual forms over the other.

This makes us reflect on the fact that some additional modelling choices could have been made to further capture the different risk exposure of contract partners, thus potentially differentiating their effects and stretching the models' results.

For instance, our model currently does not include any sudden fluctuations in commodity prices, as our datasets are mostly constituted by trends derived from expert analytical projections over a 30-year timespan (IEA, 2020; International Energy Agency, 2018; Perner & Van Der Poel, 2019; Renewable Energy Agency, 2020). Covering such a long time-span, and having chosen a time-step of *t=1 year* in our model, such trends are mostly linear and do not present relevant fluctuations, as each time-step captures the average commodity price over the considered year. The presence of unpredicted price peaks, however, could have allowed us to gain insights in what kind of situations would materialize under each form of contractual structure: what is the reaction of actors to such peaks? Who absorbs the risk of fluctuations? What is the impact on the cluster cash flow?

In addition to that, contract prices could have been differentiated by construction, incorporating the effects of establishing additional supply agreements to neutralize or shift the risk of power supply and price volatility. Modelling such situations would have differentiated sale-and-purchase contract prices from the ones derived from a tolling model, most certainly stretching the end results.

To conclude, under the modelling choices and assumptions specified in the previous chapter, adopting different pricing mechanisms for each form of bilateral contract will produce the same effects on cluster cash flows. This behaviour will materialize as long as the contract prices are kept the same for tolling and sale-and-purchase agreements. Although these assumptions do not allow to detect visible differences between the effects of the two types of bilateral contracts, it is still possible to quantify the effects of bilateral agreements as an overarching category, to be compared with the effects of multilateral contracts. This comparison is performed in Section 6.2.1.4.

Differences between bilateral contractual forms would be stretched under conditions that create a (temporary) contract price distinction between the two contract models. For instance, the contract prices could be differentiated by construction, considering different market prices of feedstock based on PPAs or alternative supply agreements, which are currently out of scope. Similarly, using datasets that capture more price volatility (for instance, by considering a smaller time-step) would temporarily distinguish the contract prices, whenever a peak in feedstock prices materializes: in fact, while the tolling price would absorb the full cost of such fluctuation, a sale-and-purchase agreement would hedge the consumer from such risk, as only part of the cost is incorporated in the contract price's components.

6.2.1.2. Interpretation of effects of multilateral contracts

Contrarily to the previous set of experiments, testing the effects of multilateral contracts has shown that different forms of multilateral agreements have an impact on the total and individual cash flows. Thus, the degree of price standardization in multilateral contract prices constitutes a factor that differentiates the economic performance of the cluster – although with a minimal effect, as shown in Figure 49. As a result, our second hypothesis is also rejected. This happens because, when multilateral contracts with separate hydrogen prices per commodity are adopted, blue hydrogen is initially integrated in Uniper's MPP3 power plant, gradually supplemented with green hydrogen –once this option becomes more price competitive. The second contractual form, instead, allows for a simultaneous integration of green and blue hydrogen for Uniper, as both hydrogen types are marketed at the same price. This produces a slight increase in individual cash flows of hydrogen producers (Air Liquide, Nouryon, Shell and Uniper), reflected in higher total cash flows.

Although the different degree of price standardization determines a shift in some of the investments to different moments in time (Figure 50), the same investment decisions are made under different contractual structures. Differences in timing do not matter much on the (aggregate) level of cash flows. The low variability in investment decisions for decarbonization is also reflected in minimal changes in the level of CO_2 emissions for both multilateral contractual structures.

This allows to reflect on the fact that the modelled system has low flexibility to test the effects of multilateral contracts. In fact, the actual advantage of multilateral contracts lies in its application in thick markets, where standardization of contract terms are enabled by economies of scale and network externalities (Scott, 2020). Had the system included more actors for which hydrogen integration is convenient, much more visible differences in the end results would have been identified. For example, investment decisions would have been shifted or modified for a higher number of actors, altering material flows overtime, thus further differentiating the revenue generation under each form of contract. As a result, more pronounced differences in cash flows would have been detected.

6.2.1.3. Remarks on investment projects

Generally speaking, there is low variability in the optimal investment paths selected by the optimization under each contractual agreement. Therefore, some considerations can be made on the general attractiveness of investments for the actors of the cluster, regardless of the adopted contractual structures.

Some observations on the potential of hydrogen integration in refineries were already made in the previous chapters, based on the contract module's verification experiments and on the calculations for refineries' mass balances. Specifically, verification experiments highlighted a dependency of investments in green hydrogen on blue hydrogen, as green hydrogen's integration in refineries only took place when fuel gases were captured by the ATR facility, thus generating a cost reduction for refineries. This observation highlights an important aspect regarding green hydrogen competitiveness, with specific respect to its integration in refining processes: green hydrogen cannot decarbonize refinery fuel gases, thus it cannot significantly affect the environmental performance of refining processes, as the CO_2 from the refinery fuel gases would still be emitted. Producing blue hydrogen, on the other hand, allows to reform refinery fuel gases: in this sense, green hydrogen cannot compete with blue hydrogen integration. Such observation is also supported by other relevant studies (H-Vision, 2019; Joint Research Centre, 2018).

A second observation was made in the subsequent chapter as, given the low flow rate of refinery fuel gas intake, we anticipated that the decision to integrate blue hydrogen would only minimally contribute to the cash flows of refineries.

Both the observations were confirmed by the performed experiments, in which hydrogen integration does not constitute an attractive option for refineries. Specifically, blue hydrogen is not integrated in refineries as its costs are considerably higher than the ones they would need to undergo by using refinery fuel gases. Thus, in our system, there is no economic incentive to switch to hydrogen as a fuel. From an environmental standpoint, the incentive to switch to hydrogen is also low, since the resulting CO_2 savings would not justify the investments in retrofitting the process, nor would cover the costs to buy blue hydrogen. Hence, the model results allow to identify barriers to the introduction of the analysed decarbonization options.

It should be noted that an unsubsidized analysis was carried out for this research. As a consequence, our results diverge from findings of other studies that conclude on the feasibility of blue hydrogen integration in refineries. For instance, the H-vision feasibility study assumes a blue hydrogen price cheaper than the price of natural gas based on subsidies, thus obtaining much more optimistic results.

As blue hydrogen is not integrated in refineries, refinery fuel gases cannot be captured in the modelled system, thus making green hydrogen integration inherently unattractive for these off-takers – as the CO_2 from fuel gases would still be emitted. Although the validity of these results is circumscribed to the modelled system, this observation fundamentally proves the ability of the model to signal dependencies among investment options, as well as opportunities for the introduction of additional assets that would add value to the given set of investments, exploiting synergetic effects. Generally speaking, it is plausible that green hydrogen integration alone will not be sufficient to contribute to the CO_2 abatement of refineries if not complemented with additional investment options that capture and eventually reuse their flue gases. This raises questions on the general profitability of green hydrogen integration for refineries, as the costs of potential options that capture refinery fuel gases would come on top of the (already high) capital investment costs of electrolysis.

Such dependencies are not detected in the case of hydrogen integration in power plants. With specific respect to coal-fired power plants, the incentive to switch to hydrogen as a secondary fuel source is inherently higher compared to the case of refineries: this observation results from the fact that, due to the imminent coal ban in 2030, the alternative to hydrogen integration would be shutting down the power plant itself. This results in much greater interest for coal power plants' owners in switching to hydrogen and biomass. The choice between blue hydrogen and green hydrogen then depends on the local economics –such as the availability of storage capacity for CCS or cheap renewable electricity for green hydrogen production.

As a final remark, the model results show that investments in hydrogen production are per se attractive options, as the modelled contract prices allow a relatively quick payback. However, the attractiveness of hydrogen integration in industrial processes has to be carefully evaluated depending on the potential for decarbonization of off-takers' processes, coupled with an analysis of the economic benefits from the perspective of end-users.

6.2.1.4. Remarks on contractual structures

Based on the effects of contractual structures displayed in Figure 52, some general observations can be made, wrapping up on the considerations made in the previous sub-sections.

First of all, the models show that contracts do have an effect on the transition of the industrial sector. Figures 50 and 51 highlight that adopting different contractual structures shift investment decisions overtime, affecting the timescale of investments and the associated CO_2 reduction. For each of the resulting transition paths, it is possible to identify barriers and opportunities for the introduction of decarbonization options, as discussed above. Relevant examples are the need for increased CO_2 savings and/or the need to complement green hydrogen with additional measures to capture refinery fuel gases to improve the business case of such investment projects from the perspective of end-users. It should be noted that such insights would hardly emerge without implementing contracts in Linny-R, as the solver would allocate material flows to maximize the total cluster welfare, without giving relevance to the incentives of individual actors. Hence, a more accurate understanding of the dynamic behaviour of actors is provided with our methodology.

Different cash flows are generated depending on the contractual agreements supporting investments' remuneration. Based on Figure 52, bilateral contracts seem to yield the highest benefits for the modelled system, both from an economic and environmental perspective. This result is supported by all model iterations across scenarios. However, given the fact that differences in cash flows resulting from different contractual structures are not very pronounced, it is not possible to provide an absolute answer on which type of agreement would better support the considered investment decisions.

Specifically, bilateral contracts generate the highest cluster cash-flows in the modelled system because contract terms are tailored to the specific needs of the contractual parties. This makes off-takers less constrained than with multilateral conditions, since the contract terms do not need to take into account the needs of multiple partners.

Note that, in practice, the current hydrogen market also relies on bespoke bilateral contracts, hinting at the fact that introducing bilateral agreements for blue and green hydrogen might be easier compared to shifting immediately to a multilateral framework, as actors of the cluster are already quite used to this form of contracting. The current market is thin, with a few, scattered participants. Only in a thick market, the advantages of multilateral contracts can be fully observed. As a result, it is possible that the model points at bilateral contracts as the structure that generates the highest cluster cash-flows only because the dynamics of a thin market are simulated. In such context, it is convenient to adopt bilateral contracts as compared to multilateral ones, as the latter would not fully capture the advantages of standardization if a thin market is modelled.

The results show that cash flows resulting from multilateral contracts do not differ too much from the ones obtained with multilateral agreements. The similarity in the level of cash flows across contractual structures in every scenario might signal that adopting both contractual structures could be beneficial for the cluster: for instance, the adoption of a specific contractual structure to support investments may shift overtime. It could well happen that, initially, commercial frameworks similar to those currently used (i.e. based on bilateral contracts) are needed to ensure a successful integration of blue and green hydrogen. Subsequently, once the market matures and more actors are included, frameworks that are used for commodity wholesale trading may be more efficient. Such (thick) market, in fact, would create network externalities that improve standardization of contract terms. As hydrogen would be priced by a higher number of market participants, the multilateral price would become more accurate and reliable compared to bilateral contract prices.

As a result, there may not be a universal, one-size-fits-all approach in establishing a set of contracts that is best suited to support hydrogen projects. The choice of the optimal contractual structure may be dependent on the specific context of the industrial cluster and, most importantly, on the stage of development of the hydrogen market.

6.2.2. Reflection on the methodology

To the best of our knowledge, contractual structures had never been implemented in Linny-R before this research. This significant challenge was overcome providing a methodology to incorporate contracts in MILP and to assess their effects. This adds an appreciable element of novelty to the research, showing that it is possible to introduce institutional elements in optimization models and to assess the transition in an integrated manner, thus addressing an important knowledge gap discussed in Chapter 1.

In addition, our methodology proves additional insights in the identification of optimal investment paths that respond to the incentives of the cluster members, providing a more accurate representation of the behaviour of rational actors. In fact, we have shown that the implementation of contracts optimizes the sequence of investments for all actors by identifying win-win situations and avoiding skewed, distorted and highly price-sensitive cash flow distributions (see Figure 33 and Figure 35). In this way, investment decisions and the resulting intra-cluster trading only take place when the incentives of contractual parties are aligned. These insights are coupled with inherent advantages of optimization of investment portfolios, namely the evaluation of potential externalities produced by the interaction of assets and the identification of transition paths that enhance their synergies (see Figures 47 and 50). Hence, this method enables a dynamic analysis of the system's behaviour, which proves to be of fundamental importance in a context where every actor strives to transform its production processes and/or to introduce new assets, enabling greater coordination of multi-actor decisions.

The methodology has been tested in a stylised model, showing that contracts do have an effect on the transition as highlighted in Figure 52. Specific insights on the attractiveness of decarbonization options for certain end-users, and the resulting timescale of investments, were unravelled in the previous sections: although the results' validity is relative to the stylised system (provided the methodological orientation of this study), general lessons are learned on the potential of our method to identify barriers and opportunities for the introduction of decarbonization options. Implications are further discussed in Section 6.2.5. Although the methodology has been tested on the particular case of hydrogen integration, the method can be applied to a broader set of systems, eventually requiring slight modifications on the contract implementation. Minor adaptations would be, for instance, the adopted pricing mechanisms or boundaries on exchanged quantities. However, having included the most general set of building blocks in the contract representation, additions of more specific contract conditions might be required to incorporate detailed contract clauses. The same logic used in the contract module (Chapter 4) to incorporate explicit conditions should hold for additional contract clauses, making the methodology scalable to a different system.

6.2.3. Reflection on contracts' implementation

Overall, we are confident and pleased with the proposed contract implementation in MILP. Specifically, we have implemented a methodology that, besides allowing to perform the envisioned experiments, is also flexible and replicable, thus suitable for various research applications. As proved in Chapter 4 (Figures 25, 26 and 27), the contract module can be applied to situations in which one asset can be invested in, under a single or multiple contracts regulating its remuneration. Likewise, the contract module allows to model circumstances where multiple assets are invested in and operated under a single contract. Thus, our implementation efforts are flexible and suitable to model various multi-actor configurations.

Additionally, the flexibility of the proposed contract implementation lies in the use of the explicit conditions defining the contract module. These allow for a relatively straightforward interpretation of results, as the conditions that determine a contract's failure or activation are visualized as active on inactive processes, constraining the contract's activation. Besides easing results' interpretation, the conditions confer flexibility to the testing procedure, as it is always possible to deactivate any wished condition and analyse what kind of implications would arise for the cluster. For instance, if a given fuel option is not integrated in industrial processes because its price is slightly higher compared to other alternatives, it is possible to deactivate the contract condition monitoring price comparisons. In this way, less restrictions allow the solver to evaluate whether the integration of such fuel would be beneficial for the involved actors –as it is possible that a slight decrease in one actor's cash flow produces high gains for the cluster.

Contract conditions can also be fine-tuned to the specific interest of the researcher. In this way, our contract implementation finds a relevant application in redesigning contracts and testing their effects on the modelled system.

In this research, we made the choice to specifically focus on the effects of revenue contracts, and assess which contract form is best suited to provide a revenue stream to finance investment projects. The same kind of analysis can be performed by focusing on investment-based contracts, leaving revenue contracts as constant, and specifically evaluating which strategies for shared costs and ownership would stimulate investment projects in decarbonization options.

Thus, generally speaking, we observe that the proposed contract implementation in MILP allows to gain insights in various contract dynamics underlying the energy transition, and it is adjustable to different research purposes.

It is relevant to reflect on potential challenges arising if more realism was added to the contract representation. As previously mentioned, our implementation includes a general set of building blocks, which on the one hand make the implementation flexible and facilitate results' interpretation, but at the same time do not take into account more detailed contract clauses which may be relevant for a more realistic analysis. These could be implemented using same logic as for other, more generic, conditions, without hampering the ease of results' interpretation significantly –unless the number of explicit conditions is extremely high or if such conditions are dependent on other contracts' conditions. Elements such as contracts' duration may also be introduced to provide more realism, if dealing with long-term contracts. Implementation-wise, a simple data product modelled as a stock with an upper bound equal to the duration of the contract and an outgoing data link with a "$\oplus$" multiplier should do the work. Thus, this addition would not increase the complexity of our contract representation. However, the interpretation of results might become less obvious at first sight, as parties would be more constrained to stick to a specific exchange overtime based on the duration of the underlying contract. Finally, although we have made relevant distinctions in the proposed contract typology, it is possible that contracts that were not included in our classification (Table 4) may require a different kind of representation. This is an important limitation of this study, which should be addressed in further research to extend our implementation efforts to novel/more complex contracts, requiring specific additions to the proposed methodology.

6.2.4. Reflection on the Linny-R model

The modelling of the Rotterdam cluster under various contractual structures is accompanied by a series of simplifications of real-world dynamics.

Firstly, the model does not represent the entire Rotterdam cluster, focusing only on part of its petrochemical complex and power generation activities. Such choice was made due to scoping reasons and time constraints associated with the nominal duration of a thesis research. Nevertheless it should be noted that, given the objective of this research, using a stylised representation of the Rotterdam cluster did by no means constitute a barrier to answer our research questions.

Keeping the scope in mind, additional assumptions were made with respect to the representation of investment projects. Although the assumptions presented in Section 5.2 were based on solid arguments, we are aware that certain simplifications would present a major shortcoming if the analysis was conducted from the perspective of single actors. In fact, using the modelled system, single cluster participants would not gain detailed insight in the specific implications of their participation in a project. However, the aim of the model is not to conduct an investment evaluation from the perspective of each actor, but to provide a method to assess the transition from a system perspective.

It should be noticed, however, that the model can be adapted relatively easily to include a higher level of detail, if necessary. In fact, Linny -R offers the possibility to use nested modelling to further specify the process components and their interrelations. Nevertheless, our model already presents a relatively high number of binary variables, which exponentially increase the computation time. Thus, the trade-off between level of detail and computing time deserves particular attention when expanding the model. In this research, such balance was found based on the computing time obtained by using LP_solve, since most of the system was modelled before June 2021. Had this analysis been performed using the new solver, Gurobi, a higher level of detail could have possibly been incorporated without substantially slowing down the computation time.

The same consideration applies to other modelling choices, such as the choice of the size of the model time-step. With LP_Solve, increasing the number of time-steps in the model made running times unfeasibly long, hence we opted for a representation using *t=1 year.* The solver Gurobi would most certainly allow to run the model adopting a smaller time-step, such as *t=1 quarter* or *t=1 month*. This adaptation would also allow to capture more fluctuations in datasets, performing a more detailed analysis of the response of actors to price peaks under different contracts.

6.2.5. Reflection on societal and managerial implications

6.2.5.1. Societal and managerial relevance

This research contributes to the societal need for the decarbonization of the industrial sector and the reduction of carbon emissions. Specifically, this research contributes to the intended industrial transition to hydrogen as fuel and for power generation. However, the developed methodology is replicable and oriented towards the application, with the necessary adjustments, to virtually any set of investment projects for decarbonization options, eventually extending its potential beyond the study of hydrogen integration solely. Thus, society and industry can hugely benefit from the possibility to identify and test contractual structures that efficiently support various decarbonization projects, assessing the resulting CO_2 reduction potential and how it can vary based on the chosen contract form.

From the discussion above, we believe it is possible to take away some general conclusions relevant to next steps for investors and policymakers.

Although our findings suggest that there may not be a universal, one-size-fits-all approach in establishing a set of contracts that is best suited to support hydrogen projects, this research is effective in providing direction in interesting dynamics that might develop when considering multiple hydrogen projects from a system's perspective. Specifically, insights in the general attractiveness of blue and green hydrogen projects are provided, highlighting which kind of interactions may arise overtime and what factors could improve the incentives for their integration in industrial processes, as discussed in Section 6.2.1.4. Managerially, this signals possible opportunities to combine different investments in decarbonization technologies that could strengthen each other. From a policy perspective, specific areas of need for policy support can be identified, discussed below. Such insights are particularly valuable in a post-pandemic context in which governments want every bit of subsidy to generate the greatest possible value. In addition to that, results hint at the need to adopt different contractual structures based on market maturity. This observation has implications on the need to carefully rethink the relationship between producers and off-takers to gradually adapt it to market developments.

6.2.5.2. Policy recommendations

Our research results show that high hydrogen prices, combined with minimal CO_2 savings derived from hydrogen integration create unfavourable conditions for hydrogen use as fuel in refining processes. This signals specific areas of need for policy support.

Besides offering CAPEX support, high hydrogen prices could be addressed by means of regulated revenue support, such as contracts for difference including end-users' conversion costs or other variable costs passed on to off-takers. Additional measures could be taken to narrow the price advantage of carbon alternatives and provide higher savings for processes integrating hydrogen. This could be done, for instance, by increasing carbon prices on fossil fuels or by recognising the higher social value of green products. Policy makers should reward them accordingly via price premiums or carbon contracts for difference in price, which offer investors a higher benefit from CO_2 reductions than the prevailing price in current CO_2 trading systems. Finally, governments could preferentially buy products produced using clean technologies, such as green hydrogen.

Targeted policy action would create higher economic incentives for hydrogen integration in several industrial processes, eventually overcoming the barriers identified by this research. Combining policy developments with the analysis of the effects of contractual structures could result in additional insight in the general attractiveness of investment options.

6.2.6. Reflection on theoretical implications

In the beginning of this research, inter-firm collaboration was framed as a multi-motive game, based on the theoretical framework of game theory. More precisely, our research was put into perspective by defining non-cooperative and cooperative strategies via the key concepts of Nash equilibria and Pareto-optimal outcomes. With these premises, we considered contracts as an effective measure to deal with misaligned incentives and to distribute wealth fairly.

The proposed contract representation is the result of a deep analysis of scientific literature on game theory combined with a careful inspection of the possibilities offered by Linny-R. As a final outcome of this research, the devised contract representation allows the establishment of win-win situations for all the contractual parties. In this aspect, this research aligns with the methodology adopted by Albino et al. (2015), in which contractual mechanisms are modelled to assure win-win conditions in the context of Industrial Symbiosis (IS). Although their study is performed by simulating IS networks via Agent-Based Modelling, inherently not suitable for optimization, both this research and the study from Albino et al. (2015) contribute to the open discussion in literature regarding the role of contractual mechanisms in industrial clusters to solve the misalignment incentive problem. This objective is achieved in our research by giving relevance to the interests of individual actors via fair contract conditions, while maximizing the cluster welfare.

As a result, an optimal collective strategy is identified, which in our perspective constitutes a particular case of a Pareto-optimal strategy. In fact, no situations that are highly detrimental for specific actors, but particularly profitable for the rest of the cluster are eligible as optimal solutions –a situation that could have materialized as a traditional Pareto-optimal outcome. The traditional definition of Nash Equilibrium does not apply to our research outcomes either, as contractual agreements are inherently meant to generate a stable cooperation among actors, while Nash Equilibria arise as a result of non-cooperative strategies. Based on the perspective of Holt et al. (2004), however, the outcomes of our contract representation could be considered as an example of a "correlated equilibrium", namely an extension of the Nash equilibrium. In this case, jointly (rather than independently) randomized strategies allow the coordination of the strategies of groups of players, determining an equilibrium. Thus, the results of our contract representation could also be interpreted in the light of this perspective. To conclude, it is possible that, in Holt's (2004) vision, our whole research represents an attempt to bridge economic and evolutionary game theory. This results from the fact that the modelled contract conditions could be understood as an effort to incorporate fairness and non-selfish preferences in standard modelling, mirroring the outcomes of contracts' negotiation.

6.2.7. Reflection on research limitations

Some research limitations have already been discussed in the previous sections, with respect to the experimental setup and modelling choices. In this section, we specifically focus on limitations arising from the research methodology and research design.

Regarding the research methods, one of the premises of this research is the use of MILP to model the Rotterdam cluster and optimize its performance. This method inherently implies some degree of simplification of the actual (non-linear) relations in a cluster. In fact, the analysis of industrial processes is normally carried out using flowsheeters such as AspenPlus, resulting in non-convex MINLP models. With this research, we propose MILP as a means to get rid of information in excess, reducing the model complexity from the standpoint of single processes and enabling the analysis of the integrated cluster.

Various scoping decisions were made in order to avoid overcomplicating the model relatively to the research objective.

First of all, some simplifications were made in the contracts' classification (Table 4) and their representation. Specifically, we have made relevant distinctions in the proposed typology with respect to hydrogen contracts, but it is possible that contracts that were not included in our classification may require slight changes (or even a different kind of representation). This is an important limitation of this study, which is worth being explored in further research to extend our implementation efforts to novel contracts or to incorporate more specific contract clauses.

Moreover, having used a stylized representation of the cluster, a research limitation arises in the generalizability of results regarding projections on the transition of industry. For instance, the model does not include many of the existing processes operating in the Rotterdam industrial complex. As a result, the model does not allow an analysis of the consequences of blue and green hydrogen adoption and diffusion on the grey hydrogen sector and large-scale supply to industrial consumers. In this research, it was not possible to address this limitation given time constraints and a lack of access to information on current market dynamics and participants. This limitation, however, can be addressed in future research by extending the model boundaries.

In addition to that, our model specifically provides insight in the evaluation of options available for private-private arrangements. Due to time constraints, private-public arrangements and governmental support were left out of the scope of this research. This represents a major research limitation, as we realize that hydrogen's cost competitiveness can only be realised with sufficient policy support to accelerate its scale-up. Moreover, carrying out an unsubsidized analysis came at the cost of losing insights in the effects of interactions between policies and contracts. It is possible that, by introducing policies that provide economic incentives for hydrogen integration, contracts can play a more central role. This important knowledge gap signals additional opportunities for further research. However, the reader should be reminded that, by incorporating policies, insights in contracts' effects would have been influenced by additional policy factors that could have facilitated the adoption of certain contracts against others. Thus, this limitation can be considered as minor shortcomings when considering the research objective.

7. Conclusions

7.1. Main contributions

This thesis explored the implications of modelling contractual structures in MILP by developing a methodology for contracts' implementation in Linny-R and providing a proof of concept for its application to the industrial cluster in the Port of Rotterdam.

7.1.1. Addressing the research sub-questions

By combining insights from the scientific body of knowledge and from the analysis of the existing contractual network in the Port of Rotterdam, an overview of contractual structures that shape inter-organizational collaboration parties was provided in Table 4, summarizing the answer to the first SQ. Contractual structures were distinguished in (i) bilateral and (ii) multilateral agreements, based on the number of contractual parties involved in the investment and financing of a project. Additionally, based on the incentive coordinated by the contractual agreement, contracts were further categorized in (i) investment-based contracts and (ii) revenue contracts. Typical configurations assumed in practice for hydrogen projects were specified by defining distinctive characteristics of bilateral contracts under a tolling model, sale-and-purchase agreements, multilateral contracts with a standardised price per commodity and multilateral contracts with a single standardised price.

Possible impacts of different types of contractual structures on clusters' transition were identified based on the performed scientific and grey literature scan, answering SQ2. Based on risk of price exposure and demand risk, sale-and-purchase agreements were found to be preferable to tolling models, while multilateral contracts with a single hydrogen price was recognized as less attractive compared to multilateral contracts with different prices per commodity. An overview of the effects reported in literature is provided in Table 5.

Such foreseen effects were used as a basis to address SQ3. We concluded that the effects of contractual structures can be tested in a structured manner by formulating hypotheses focused on the effects of revenue contracts on a system including multiple investment-based contracts. More precisely, tolling agreements were hypothesized to generate lower cash-flows compared to sale-and-purchase agreements, due to the higher risk exposure from the side of end-users. Regarding multilateral contracts, a single standardized contract price for hydrogen was assumed to hamper the economic performance of the cluster, as it would potentially cause a lock-in of blue hydrogen, increasing (monetized) CO_2 emissions thus lowering the total cash flow. We designed an experimental setup for hypotheses testing, consisting of two models used to quantify the effects of bilateral and multilateral contract forms, respectively. An overview of the formulated hypotheses and the planned simulations is provided in Table 6.

In order to test the formulated hypotheses, a methodology for the representation of investments and contractual agreements on Linny-R was proposed and discussed. Investment-related constraints were successfully included in the Linny-R representation by considering investments as semi-continuous variables with a non-zero lower bound, associated to a binary variable to include start-up costs in the objective function of the MILP problem. Based on the same logic, a Linny-R representation of investment-based contracts was provided. Finally, a methodology to model revenue contracts was introduced, using constraint lines to link contract conditions to the activation of a contractually-regulated transaction. In this way, an answer to SQ4 and SQ5 was provided, adding an appreciable element of novelty to this research.

The last research step provided a proof of concept of the methodology for contracts' implementation. This implied specifying the model workflow and ultimately building and executing the models by applying the devised methodology. As a result, the effects of adopting different contractual structures to support investment decisions for the transition of the Rotterdam cluster were quantified, answering SQ6. By benchmarking cluster cash flows obtained under multiple contracts (Figure 52), we concluded that contracts do have an effect on the transition of the industrial sector: adopting different contractual structures shifts investment decisions overtime, affecting the timescale of investments and the associated CO_2 reduction. As a result, SQ6 was addressed.

More specifically, both hypotheses were rejected at the end of this research. In fact, (i) effects of different pricing mechanisms in bilateral contract forms were not detected by the model, resulting in the same net effect of tolling models and sale-and-purchase agreements on the cluster cash flow. This behaviour was justified by several factors, the first one being the modelling choice to set the same contract price under both types of agreements, while only varying the proportions of the underlying components. This, combined with absence of unpredicted price fluctuations in the datasets, made the Linny-R solver allocate the same material flows, hence the same cash-flows, to the cluster actors in both the experiments.

On the other hand, results showed that (ii) the degree of price standardization in multilateral contract prices constitutes a factor that differentiates the economic performance of the cluster – although with a minimal effect. This was traced back to the fact that the different degree of price standardization determines a shift in investment decisions to different moments overtime, producing a slight increase in individual cash flows of hydrogen producers (Air Liquide, Nouryon, Shell and Uniper), reflected in higher total cash flows. Had the system included more actors for which hydrogen integration is convenient, much more visible differences in the end results would have been identified.

7.1.2. Addressing the main research question

The identification and application of the proposed, novel methodology to implement contractual agreements in MILP allowed to gain significant insight in its implications from a system's optimization perspective. Several implications are discussed below, answering the main research question.

First, the provided methodology adds value to MILP-based approaches to model the transition of industrial cluster, as it allows the identification of optimal solutions that better reflect the behaviour of rational actors. Specifically, the implementation of contracts optimizes the sequence of investments for all actors by aligning their incentives and identifying possible win-win situations. In this way, skewed, distorted and highly price-sensitive cash flows' distributions are avoided, compared to the situation in which no contracts are incorporated in MILP. Results obtained in the latter case are clearly misleading in the identification of optimal transition path, and would not be directly applicable in a real world setting. Thus, a preliminary implication that can be drawn from this research lies in its added value to results obtained from MILP.

Secondly, our methodology generates insights in investment's analysis from a system perspective, adding value to traditional investment evaluation methods. In fact, our method allows to identify a transition path that optimally takes advantage of potential synergies between investment options. Thus, the method performs a dynamic analysis of investments that, via optimization, intrinsically takes into account potential externalities in the activation of new assets, while taking into account the alignment of partners' incentives in investing in decarbonization options. This creates important insights for decision-makers which would hardly emerge from other methods, enabling greater coordination of multi-actor decisions.

Moreover, this research shows how to conduct a systematic assessment of the factors determining contracts' effects on the economic and, indirectly, the environmental performance of a cluster. It was shown that, in addition to the implications of contracts' representation, the implementation of this methodology allows a reflection on other factors that play a role in contracts' effectiveness, such as price fluctuations or market density. Also insights on the general attractiveness of investments could be provided, based on the regularities observed across scenarios under different contractual structures.

Although the findings suggest that there may not be a universal, one-size-fits-all approach in establishing a set of contracts that best supports hydrogen projects under all possible conditions, conclusions are effective in providing direction for the next steps to make hydrogen projects an investable prospect. Specifically, insights are provided in what factors should be improved to create a competitive advantage for a specific hydrogen technology and what incentives should be created to stimulate its integration in different industrial processes. This understanding has important implications from a policy and managerial perspective, providing guidance to policy makers and regulators on how to adjust levers for stakeholders to facilitate the development of a hydrogen market. More specifically, as an implication of this research, barriers identified via the implementation of contractually-regulated transactions specify areas of need for targeted policy action, addressing the creation of greater economic incentives for hydrogen integration. For instance, regulated revenue support, such as contracts for difference, in combination with policies recognising the higher social value of low-carbon or green hydrogen products may be relevant options to take into consideration. From a managerial perspective, the model allows to identify possible dependencies among investment options which may strengthen or jeopardize each other: thus, opportunities to improve the business case of specific decarbonization options are signalled. A relevant example is the need to complement green hydrogen with additional measures to capture refinery fuel gases to improve the attractiveness of such investment projects from the perspective of end-users. Additional implications arise in the need to carefully rethink the relationship between producers and off-takers to gradually adapt it to market developments. Price standardisation deserves special attention when adapting the current commercial framework based on bilateral agreements to a multilateral perspective that will possibly favour a future commodity wholesale trading.

As a general conclusion, implementing contractual structures in MILP enables a more accurate representation of the behaviour of rational actors, allowing for a dynamic analysis of the system's behaviour. Not only the incentives arising for each contracting party are taken into account in the identification of optimal transition paths, but also synergies and externalities arising from the combination of technical options are optimized. This generates insights that are more realistic from a multi-actor and system perspective. As a result, opportunities for concrete action are signalled, ultimately providing this research with high societal relevance.

7.2. Future research opportunities

Several opportunities for further research stem from the discussion in the previous chapter, following mainly two research avenues.

Firstly, future research can address the limitations of the study, to obtain more sophisticated results. Specifically, based on the highlighted limitations in capturing risk exposure of contract partners, the model could be improved to efficiently incorporate incentives to switch between contracts. To this end, datasets could be improved to include price fluctuations, or additional supply agreements could be modelled to allow for further price differentiation across contracts.

Additionally, the performed study could be replicated by expanding the model to a different system, in order to (i) improve the scalability of the model and (ii) conduct a cross-case analysis for clusters in different locations, to reveal whether location significantly influences the identification of contractual structures to support optimal transition paths.

Secondly, further research can build upon the research results. Following our general remarks on contractual structures, future research could adapt the proposed research framework to simulate a shift in contractual structures that follows the hydrogen market developments. Specifically, a model could be constructed that gradually includes market participants to simulate the evolution from a thin to a thick hydrogen market. Bilateral and multilateral contracts could be modelled as alternative options to be chosen by the solver based on which one would be best suited to support hydrogen integration overtime. In this way, the optimal switching moment from a bilateral to a multilateral framework could be identified.

In addition to that, other adjustments to the model could be performed with further research to examine the consequences of blue and green hydrogen integration on the incumbent grey hydrogen suppliers. The existing grey hydrogen market is often characterized by long-term (10-20 year) contracts: thus, interesting research opportunities arise in shedding light on what duration of new contractual agreements would allow green and blue hydrogen producers to break into the grey hydrogen sector. For instance, consumers may have an incentive to contract over a shorter term in order to have the opportunity to switch from blue to green hydrogen overtime.

Importantly, further research should be conducted to provide understanding of possible consequences of combining various policies with contractual structures. If policies that provide economic incentives for hydrogen integration are introduced, it is likely that contracts will play a greater role in determining the revenue generation of investment options in hydrogen. Thus, an analysis of their interrelations is recommended.

The models developed throughout this research could also be adapted to a different research objective, such as the identification of an optimal hydrogen price. This purpose could be achieved by making use of a recently introduced feature in Linny-R that allows to combine Linny-R models via an external Python script. The script could be used to iterate the model's execution while gradually changing the contract price, until the price that maximizes the cluster profit under a given contractual structure is identified.

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Appendix A: Notes on investments' representation

A.1. Explanation of the adopted investments' representation

This section further elaborates on the investment representation provided in Figure 14, and presented again below to facilitate the explanation.

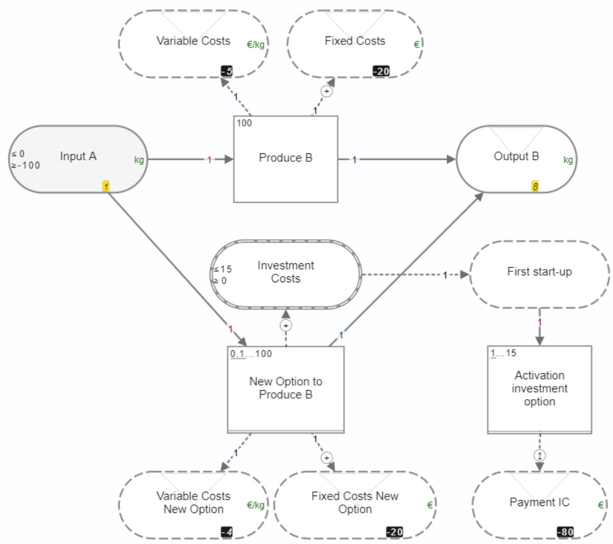


Figure A.1. Single-decision, single-actor model for investments' conceptualization

A chain of data products and processes was included to incorporate the investment option and associated investment costs immediately upon switching to the alternative process. Specifically, when the *New Option to Produce B* is active, a flow equal to 1 (due to the selected multiplier) fills the data product *Investment Costs*. The data product is modelled as a stock (denoted with a double dashed line) that keeps track of the number of time steps in which this option is active. In this simplified example, assuming a time step of 1 year, we limit the operation of the new option to 15 years: in fact, by specifying that the ingoing link adds 1 unit each year that the asset is in operation and limiting the upper bound of the stock by N, the process can only produce for N time steps. Thus, this configuration can be used as a specification of the economic life span of an investment option.

For every time-step in which *New Option to Produce B* is active, the unit added to the data stock flows into the process *Activation investment option*, modelled as a semi-continuous variable with a lower bound of 1. We associate a binary variable u_{it} with this process (1 = *on*, 0 = *off*), which is used to include start-up costs in the objective function of the MILP problem, as seen in Section 4.1.3. Start-up costs typically represent the additional resources required by industrial processes when resuming production after being inactive – even for a short period. Evidently, this aspect becomes relevant when simulating operations with a smaller time step (for instance, in an hourly model). In this research, the 'start-up' feature of Linny-R is used to represent the binary decision to invest. Using a time-step of 1 year, the MILP solver will start up an investment option only if the additional cumulative cash flow it generates (given the investment horizon) is able to at least recover the investment cost.

Investment costs are incorporated in the objective function by linking the semi-continuous process *Activation investment option* to a data product that specifies the capital investment costs as a negative price. The link between the process and the data product presents a "start-up multiplier", denoted by a circle with an upward arrow ↥: in this way, a data flow from *Activation investment option* to the data product *Payment Investment Costs (IC)* will occur only in the year that *New Option to Produce B* switches *on* –i.e. when the new process is active in time step *t*, but was inactive in time step *t*−*1*.

A.2. Model iterations to select the final investments' representation

The process used to derive a satisfactory model to incorporate investment decisions involved the implementation of various model iterations. Two basic issues arose when implementing a standard investment model in Linny-R:

i. The solver allowed the payment of investment costs every time the production unit would resume production after being inactive
ii. The solver would not allow the production unit to be switched on again after ceasing production at a time-step where producing would have been disadvantageous

We used the same simple model presented in Chapter 4 and simulated a situation in which each process would alternatively become more economically convenient than the other, based on the fluctuations of their respective variable costs (Figure A.2). Although unrealistic, the simulated situation allowed to test the model functioning with respect to the payment of investment costs after resuming production once the alternative process unit had been shut down –being its variable costs temporarily higher than the costs of the initial process.

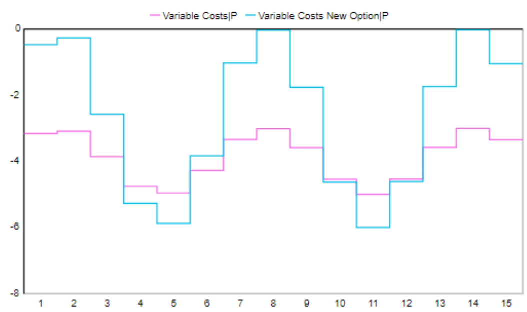


Figure A.2. Fluctuations in costs

<u>Configuration 1 and 2: data product (with or without stock option)</u>

In this configuration, only a data product with a negative price for investment costs was used. In this situation, the solver alternates production between the two processes based on the level of variable costs, however it never shuts down the investment option completely to avoid repaying the investment costs when resuming production. Thus, the solver allocates a flow equal to the (very low) lower bound to this process, even at moments when the production unit should be inactive. Although the resulting costs are negligible compared to the total cash flows of the actors, this representation inaccurately models production patterns.

Figure A.3. Configuration 1: data product

The same issue arises if the data product is turned into a stock.

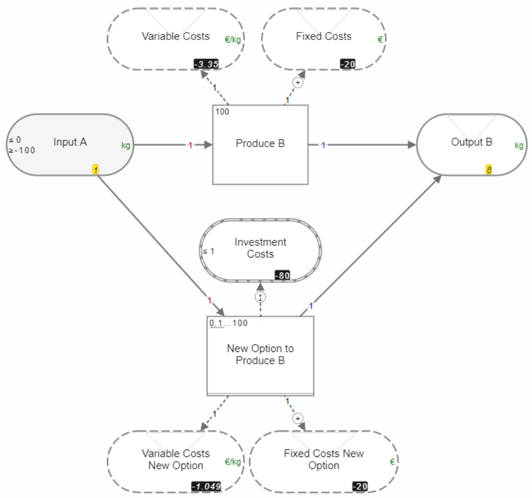


Figure A.4. Configuration 2: data stock

Note that these issues materialize when modelling actors with perfect foresight by setting the block length of the optimization equal to the time horizon. If the block length is decreased, configuration 1 shuts down the new process when its variable costs exceed the ones of the initial process. However, the investor bears the investment costs multiple times, when production is resumed. In configuration 2, the solver initially switches off the new process at the same moment as in configuration 1, but does not allow to start it up when needed, as the data stock keeps memory of previous decisions, thus limits the number of start-ups to 1. In any case, with any solver settings the same two issues arise, making the two configurations unsuitable for our purpose. Notwithstanding the simplicity of these two models, the tested configuration allowed us to gain insights on the functioning of several Linny-R tools, enabling us to arrive to the final configuration as displayed in Chapter 4.

Configuration 3: investment paid in instalments

This representation allows switch off the production unit and resume production without incurring capital investment costs again. Furthermore, the investment costs can be spread over a longer timespan (for instance, 12 months), representing an investment being paid in instalments. An interest rate component has also been added. An example of this conceptual representation is displayed in Figure A.5.

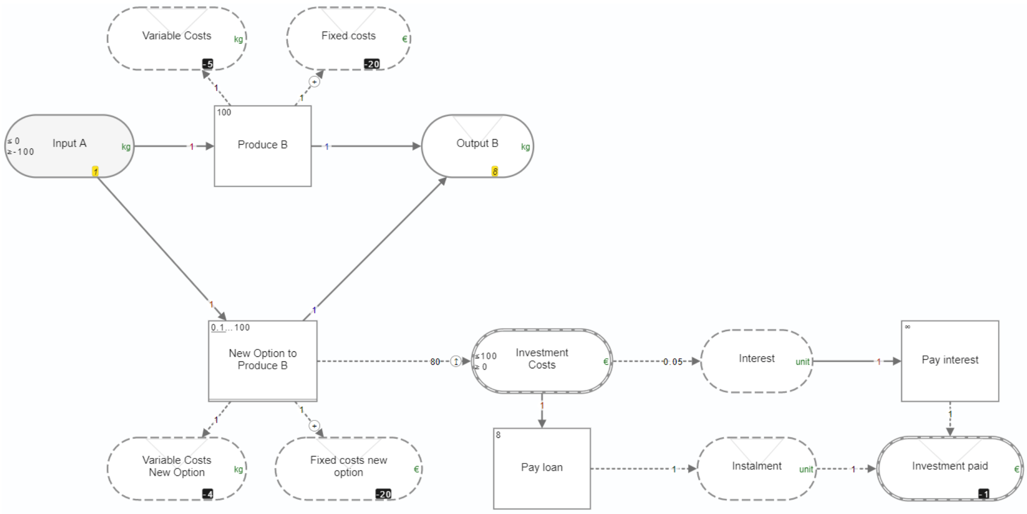


Figure A.5. Investment paid in instalments, including interest rate

This representation would be suitable for our purposes in case we decided to use a smaller time-step to model the transition over a 30-year time horizon (e.g. a time-step of one month). During the initial stage of the research, when the granularity of the model had not been selected yet, we decided to develop both the conceptual representations of investments, with the aim to select the most efficient one at a later stage, once the full structure of the model would have been developed. This is because the ambition to model a system including multiple investment options would have inevitably led to an increase in computation time. Hence, definitive decisions could not be made immediately, but only through an iterative process of testing various model configurations. In addition to binary variables, the number of time steps of the model is a determinant of computation time: thus, depending on the number of investment options to be modelled in the system, the granularity of the model would be selected. This decision would then impact the choice of our investments' representation.

In this example, assuming a time step of 1 month, an investment of (say) 80 is made at time step $x \in T$. The owner of the process is allowed to operate the investment from time step *x*, but does not pay the entire amount of the capital investment costs at once. Rather, the sequence of data products and processes allows to only pay 1/10 of the investment at each time step (since the upper bound of the process *Pay loan* is set at 1/10 * 80). As a result, the full investment costs will be entirely paid after 10 months. In addition, the process owner will pay an interest rate on the amount left to be paid at every time step. This investment representation works as intended, allowing the process owner to shut down and resume production without incurring any investment costs multiple times. This is made possible by the fact that, after switching on for the first time, the level of the process *Activation investment option* becomes positive and stays as such for the whole lifetime of the investment option. Thus, the difference between the binary start-up variables will always be 0 for every time step *x>t,* making the investment costs null in the objective function.

$$i_{ix} = 0.5 * i_i * \left[\left(u_{ix} - u_{i,x-1}\right) + \left(u_{ix} - u_{i,x-1}\right)^2\right] = 0 \ \ \forall x > \ t \in T$$

A.3. Explanation of JV representation

This section further elaborates on the provided example for the Linny-R representation of JV agreements provided in Figure 17, and presented below for reasons of clarity.

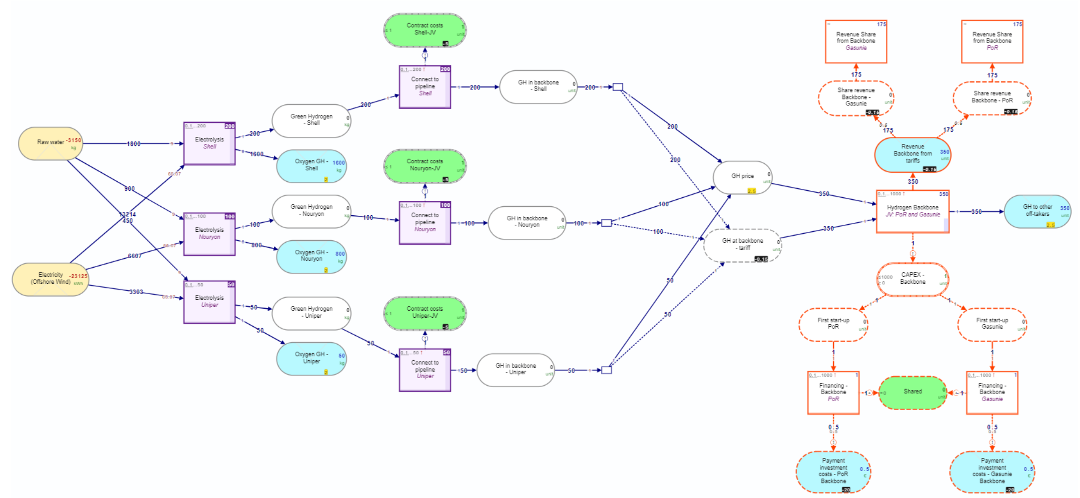


Figure A.6. Example of investment decision under a JV agreement (executed)

The investment realized under a JV is integrated in a system in which three PUs produce green hydrogen via electrolysis, to be sold on to other hydrogen off-takers via the pipeline. The exchange of materials is regulated by means of revenue contracts, which have been simplified in this representation using the processes *Connect to pipeline*, in combination with the data product *Contract costs* to allow the payment of start-up costs. This process allows the output of the electrolysers to be sold via the backbone at a price, which can be either set independently for every hydrogen producer, or in a standardized manner. The latter situation was modelled in the example. Each hydrogen producer, in this way, gets a revenue that is equal to the amount of hydrogen sold, multiplied by the standardized price. For the amount of hydrogen being transported via the backbone, each producer has to pay a tariff consisting of a price per unit of product. Note that this is not the definitive representation of revenue contracts that we will employ in our study: this simplification has been temporarily made for the purpose of our explanation of the investment-based contract (i.e. the JV), highlighted in red in Figure A.6. A more elaborate representation of revenue contracts will be formalised in the next section.

In this example, we apply the conceptual representation of the JV agreement provided in Figure 16. The only costs incurred by the contractual partners are represented by the investment costs, while the only source of revenue is represented by the transport tariff. For reasons of ownership transfer, the JV does not retain any additional profit from transporting the commodity, as operator of the transport pipeline infrastructure. Thus, to ensure a correct allocation of cash flows, we attached a price to hydrogen before being transported via the backbone: this makes sure that each hydrogen producer obtains its revenue from selling the amount produced. Since the green hydrogen product is connected to the investment option *Hydrogen Backbone*, owned by the JV, the solver assumes that the venture partners are purchasing hydrogen from the electrolyser facilities. However, the JV should not incur any costs for transporting the product. For this reason, that same amount of hydrogen is modelled as an outflow from the hydrogen backbone, applying the same price specified by the producers. In this way (i) the JV will not incur any additional costs for providing its transport services and (ii) hydrogen producers will profit from selling their product. Finally, the JV makes profit from the received tariffs, which is then distributed to the JV partners according to their shares. Therefore, our representation of the JV in Figure A.6. correctly divides the investment costs and the revenues by means of the same set of (data) products and processes shown in Figure 16.

Appendix B: contract module verification results

B.1. Proposed contract representation under diverse multi-actor configurations

The first experiment was run using the most simple system configuration, consisting of one blue hydrogen producer and one refinery interested in using the product of the ATR facility (namely, the investment option) for desulphurization of its products. The integration of blue hydrogen takes place under a revenue contract, represented either under configurations (a), (b) or (c):

a. *Contract module consisting of activation costs only*: no conditions to monitor profitability or economic convenience of the transaction are implemented;
b. *Contract module consisting of activation costs and conditions to monitor cash flows' positivity:* this representation ensures that no actor operates at loss when engaging in a transaction. However, no price comparisons of fuel options are explicitly modelled as an additional condition to evaluate the economic convenience of the transaction;
c. *Contract module consisting of activation costs and conditions to monitor cash flows and to perform fuel price comparisons:* this corresponds to the contract module discussed so far.

Such configurations are visualized below, considering the described system.

Experiment I: Configuration (a) - no explicit conditions

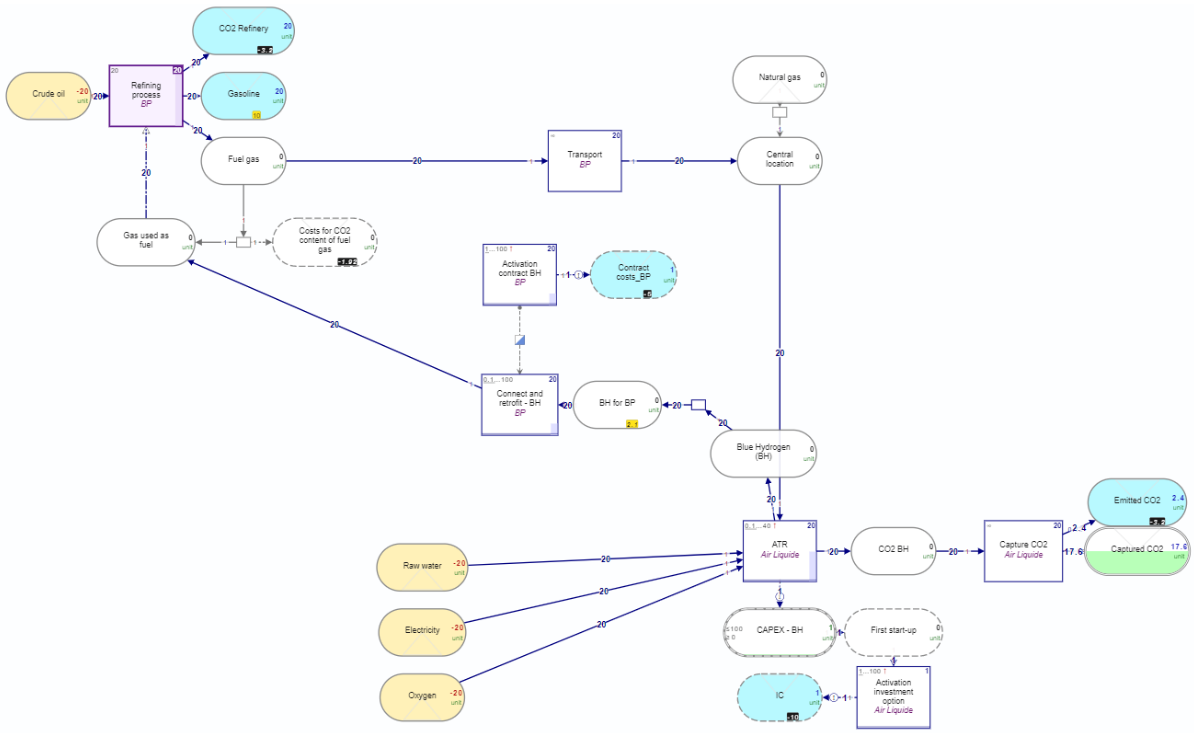


Figure B.1. Configuration (a), verification experiment I

Experiment I: Configuration (b) - explicit conditions on cash flows' positivity

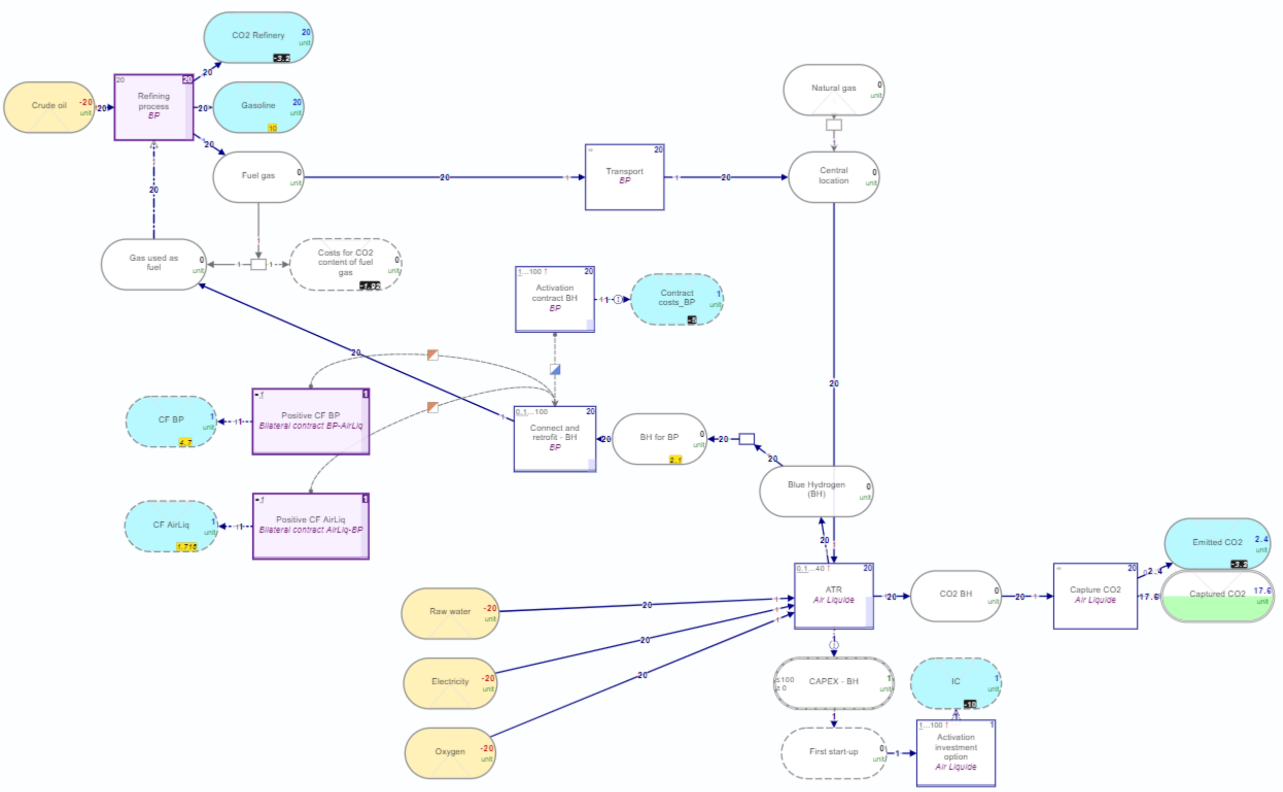


Figure B.2. Configuration (b), verification experiment I

*Experiment I: Configuration (c), **contract module** - explicit conditions on cash flows and fuel convenience*

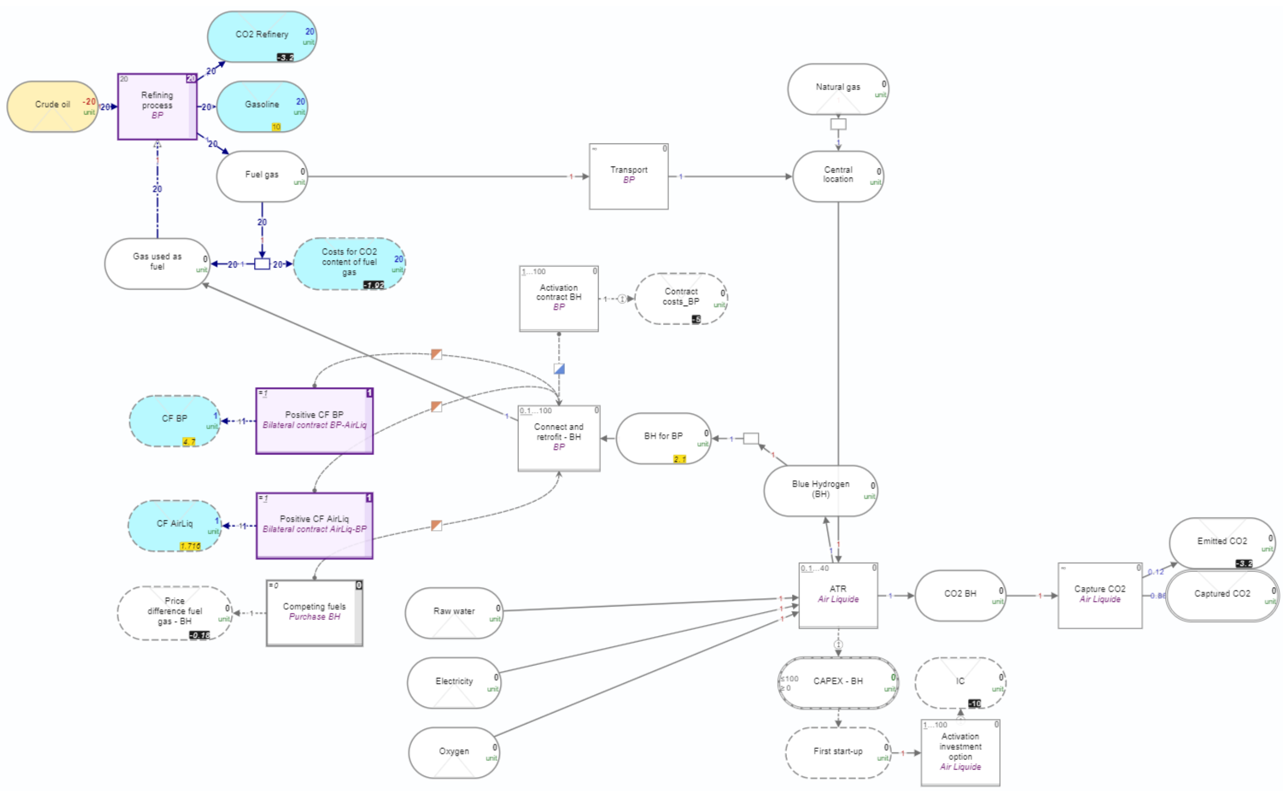


Figure B.3. Configuration (c), verification experiment I

B.2. Proposed contract representation under extreme scenarios

In this section, further details on the experimental results displayed in Table 7 are provided. We remind that the aim of these verification experiments is simply to test if the contract module functions as expected under extreme scenarios.

B.2.1. Manipulating blue hydrogen contract price for refineries

We started by testing the contract module's behaviour under various contract prices for the exchange of blue hydrogen with refineries.

Expected results

Our expectation for the behaviour of the contract module is as follows:

1) High blue hydrogen price (p=100 €/kg H_2): Integrating blue hydrogen in the refineries is never convenient for the off-takers, thus the contract module allows the refineries to keep producing relying solely on reusing refinery fuel gases;

2) Low blue hydrogen price (p=0.1 €/kg H_2): Integrating blue hydrogen in the refineries is never convenient for the producer, thus the contract module allows the producers to only sell hydrogen at a price that allows to at least cover the costs of production;

3) Periodic blue hydrogen price fluctuations (with positive and negative prices): Whenever the price is not convenient (too high) for the refineries or not convenient for the producer (too low to cover costs of production), blue hydrogen is not integrated in refineries.

Although the expected outcomes might seem an obvious result, we should keep in mind that without the contract module the solver optimizes the total cash flow of the cluster without considering the effect on individual actors. Thus, blue hydrogen may be integrated in the refining processes regardless of the effects it has on single actors' cash flows, as long as their sum is maximized.

Verification results

The results of our verification experiments complied with our expectations:

1. High blue hydrogen price (p=100 €/kg H_2): As blue hydrogen integration is never convenient for the refineries, it is never purchased by this category of off-takers. In the backbone, selling hydrogen at a standard price (p=2+0.1*t €/kg H_2, following an increasing trend as derived from reports) is profitable both for the hydrogen producer (Air Liquide) and for the pipeline operator, the Port of Rotterdam (PoR), hence blue hydrogen is produced from natural gas (no reuse of refinery fuel gases) in the initial time steps, and sold via the backbone to other end users. Refineries keep operating reusing refinery fuel gases until green hydrogen becomes cheaper (p= 6.5-0.25*t €/kg H_2, following a decreasing trend as derived from reports): at this point, refinery fuel gases are captured and reformed in the ATR facility (which keeps selling hydrogen via the backbone), while green hydrogen is integrated in the refineries. In this way:
    a. Refineries don't pay the negative price associated with CO_2 content of refinery fuel gases, because they still capture the gases via the ATR facility;
    b. The green hydrogen producer (Nouryon) and the refineries both make profit.

    Note that this situation does not materialize when the contract module is not implemented in Linny-R, as the solver allows blue hydrogen integration in the refineries since it creates huge revenues for the hydrogen producer, which increases the total cluster cash flow. This obviously comes at the expense of the refineries, whose losses however are amply compensated by the gains of Air Liquide. A comparison of the obtained cash flows with and without the contract module is displayed below. The graphs are not self-explicative but we include them in this section with the attempt to show what kind of situations would materialize hadn't the contract module been implemented.

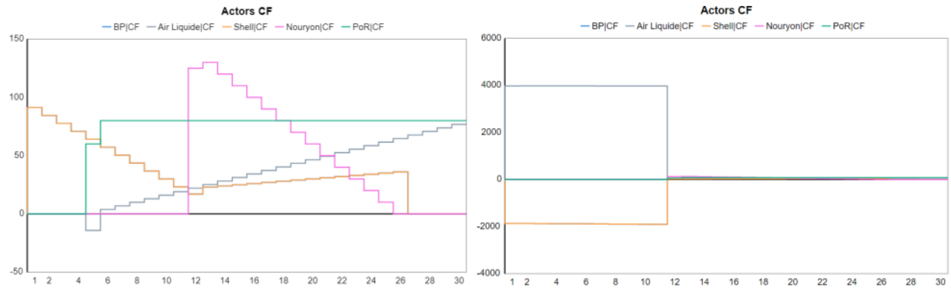


Figure B.7. Actors' cash flows– implementing contract module (left); without contract module (right)

Again, this proves that our proposed methodology to implement contracts in Linny-R prevents from obtaining optimal solutions characterized by an extremely distorted allocation of cash flows.

2. Low blue hydrogen price (p=0.1 €/kg H_2): In this case we observe a similar behaviour as in the previous case. While in the previous situation, refineries did not have an incentive to integrate blue hydrogen, as it would cause a substantial loss for their processes, in this case its integration does not take place because the losses would be for the hydrogen producer. In fact, the contract price is too low to cover production costs, thus it is not convenient for the producer to engage in a transaction at the given contractual price. Blue hydrogen is only sold to other end-users via the backbone. When green hydrogen becomes cheaper than reusing refinery fuel gases, green hydrogen is integrated at refineries.

   A comparison of the obtained cash flows with and without the contract module is displayed below.

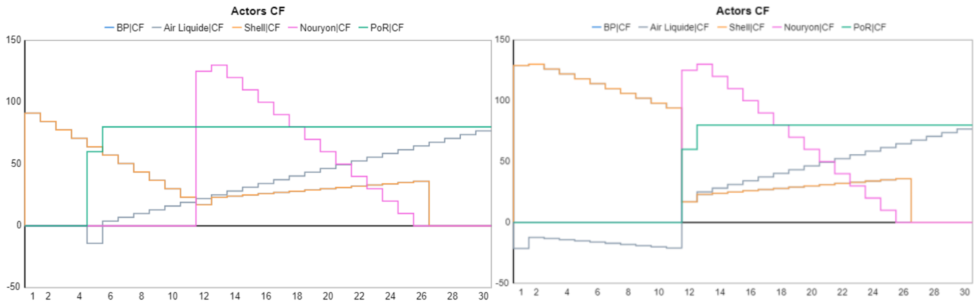


Figure B.8. Actors' cash flows– implementing contract module (left); without contract module (right)

   It is clear that the contract module prevents from obtaining optimal solutions that force some actors to keep producing at a loss (notice the negative cash flow of the hydrogen producer for the first 12 time-steps).

3. Periodic blue hydrogen price fluctuations (with positive and negative prices): Blue hydrogen is integrated in the refineries only when the refineries have an incentive to do it, substituting refinery fuel gases or green hydrogen. This only happens when the price blue hydrogen is lower than the cost associated with negative environmental performance of using refinery fuel gases (based on CO_2 content) and lower than the price of green hydrogen, exactly as expected.

   A comparison of the obtained cash flows with and without the contract module is displayed below.

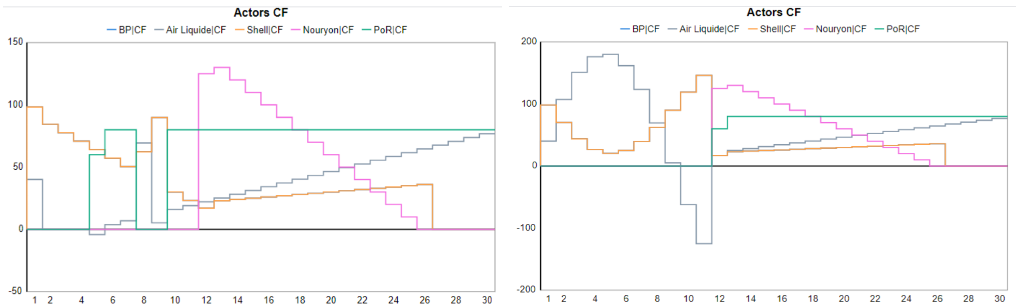


Figure B.9. Actors' cash flows– implementing contract module (left); without contract module (right)

It is clearly visible from the graph that, when the contract module is not implemented, the cash flows of actors are much more sensitive to price fluctuations: specifically, the hydrogen producer is clearly forced to produce and sell hydrogen even at a negative price, because of the resulting increase of refineries' cash flows. This is not a realistic situation, which is better approximated by the results on the left.

B.2.2. Manipulating green hydrogen contract price for refineries

Expected results

The same kind of behaviour presented in the previous section was expected for these verification experiments. Specifically, we expected that the contract module would prevent the hydrogen producer from selling hydrogen at a loss and/or prevents refineries from purchasing hydrogen at a disadvantageous (extremely high) price.

Verification results

The results of our verification experiments complied with our expectations:

1. <u>High green hydrogen price (p=100 €/kg H_2):</u> Green hydrogen is never convenient for the refineries so, as expected, it is never integrated in their processes. Refineries keep operating reusing refinery fuel gases until blue hydrogen becomes cheaper, then stop operating when using blue hydrogen becomes unprofitable. We do not show plots in this section because the kind of trends and behaviour of the model are very similar to what we have described with the other verification experiments.

2. <u>Low green hydrogen price (p=0.1 €/kg H_2):</u> Again, we observe a similar behaviour as in the previous case. While in the previous situation, refineries did not have an incentive to integrate green hydrogen, as it would cause a substantial loss for their processes, in this case its integration does not take place because the losses would be for the hydrogen producer. In fact, the contract price is too low to cover production costs, thus it is not convenient for the producer to engage in a transaction at the given contractual price.

3. <u>Periodic green hydrogen price fluctuations (with positive and negative prices):</u> as expected, when the price of green hydrogen is negative, the solver picks the cheapest option to be integrated in refineries between reusing refinery fuel gases and incorporating blue hydrogen. When the price of green hydrogen becomes positive, interesting insights are obtained. An interesting outcome that is worth being mentioned pertains the general attractiveness of green hydrogen integration in refining processes. More specifically, from our verification experiment it emerged that green hydrogen is only integrated in the refineries if their fuel gases are captured by the ATR facility, thus used for production of blue hydrogen to be sold to other end-users. This highlights an important aspect pertaining the debate on green hydrogen

competitiveness, with specific respect to its integration in refining processes: in fact, green hydrogen cannot decarbonize refinery fuel gases, thus it cannot significantly affect the environmental performance of refining processes. This is because the process of electrolysis used for green hydrogen does not reform gases, so the CO_2 from the refinery fuel gases would still be emitted (or would have to be captured in some other way). Producing blue hydrogen, on the other hand, does make it possible to also decarbonize refinery fuel gases.

Appendix C: simplified models for insights on experimental setup

This appendix further elaborates on how the integration of green hydrogen and blue hydrogen is modelled, using different revenue contract representations, which can be stipulated either bilaterally or multilaterally. The former is tested in Model I, the latter in Model II. In both models, the same system is represented, consisting of two existing refining processes owned by Shell and BP, which produce end products by reusing refinery flue gases as fuel. Shell and BP seek to decarbonize their operations by integrating blue hydrogen or green hydrogen as alternative fuel options. The former is produced by one, large-scale, ATR facility owned by Air Liquide. Green hydrogen, on the other hand, is supplied by two, smaller scale electrolysers owned by Shell and Nouryon. The processes that produce blue and green hydrogen are currently not present in the existing cluster configuration, and are being evaluated as investment options. Therefore, the purpose of these models is to test which kind of contractual structure would better support optimal investment decisions in hydrogen integration.

C.1. Model I

This model relies on the bilateral contract representation to enable the integration of blue and/or green hydrogen in the system described above. Specifically, Air Liquide stipulates a bilateral contract with each refinery interested in hydrogen use, as displayed in the figure below.

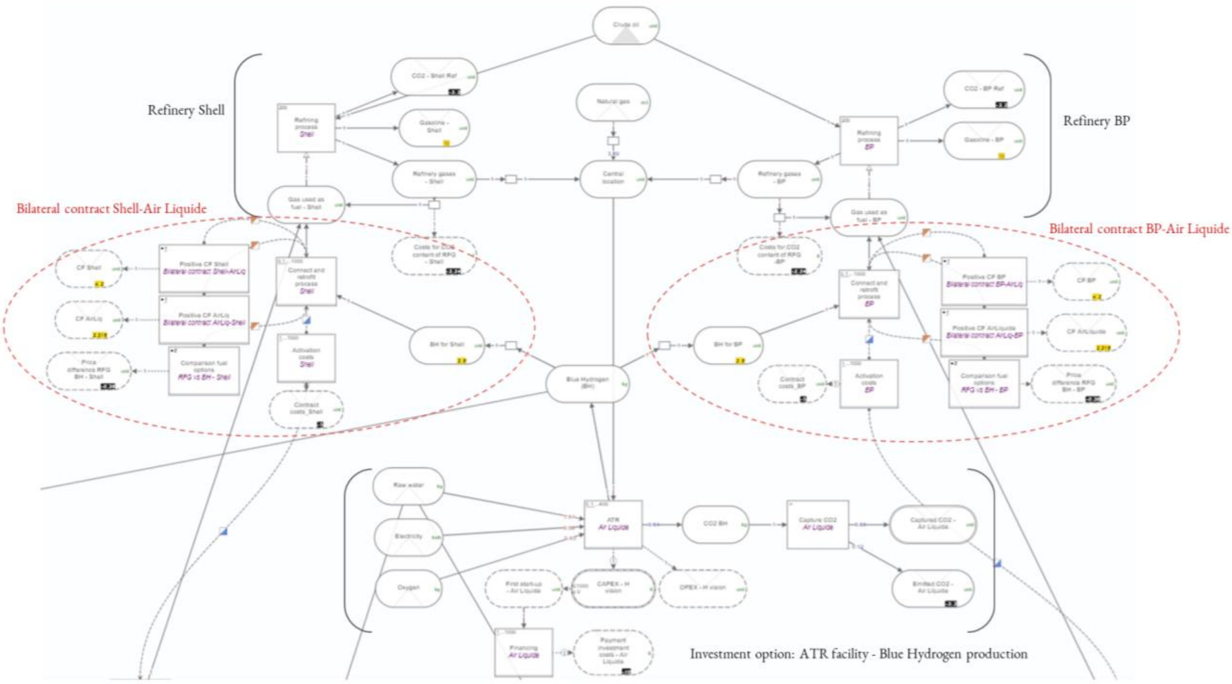


Figure C.1. Model I – bilateral revenue contracts for blue hydrogen integration

In the long run, H-vision plans to integrate into the Port's hydrogen backbone: thus, in our simplified model, Air Liquide establishes a bilateral contract with the Joint Venture that owns the backbone (Gasunie – Port of Rotterdam) to be allowed to sell blue hydrogen to other end-users via this regional pipeline, in exchange for a transport tariff.

The same logic is applied to the exchange of green hydrogen. Each electrolyser establishes a bilateral contract with the refineries for green hydrogen integration (Figure C.2.). At the same time, they make bilateral agreements to sell their hydrogen to other end-users via the backbone, in exchange for a tariff.

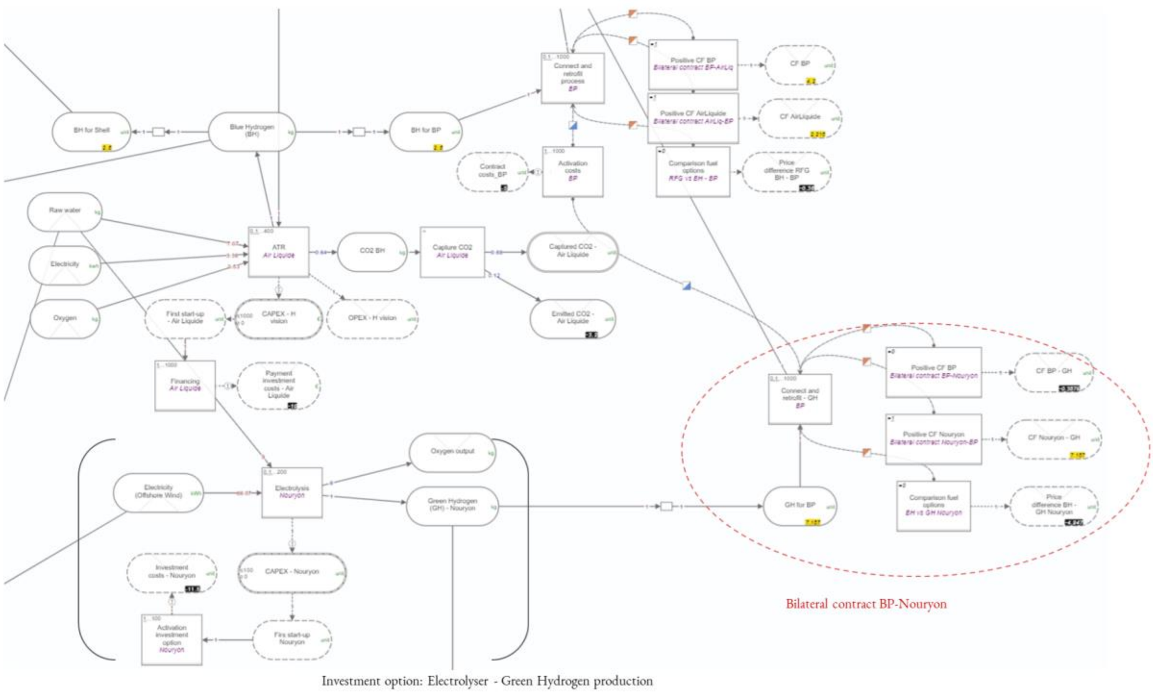


Figure C.2. Model I – bilateral revenue contracts for green hydrogen integration

This representation is replicated for every bilateral contract established between two partners in the cluster.

C.2. Model II

This model relies on the multilateral contract representation to enable the integration of blue and/or green hydrogen in the described system. Differently from Model I, in which Air Liquide stipulates a bilateral contract with each refinery, in this model Air Liquide established a multilateral contract with both the refineries interested in hydrogen use, as displayed in the figure below. Here, the same standardized price is applied to both off-takers, and they are subject to the same contract conditions (i.e. shared conditions with constraint lines, in Figure C.3). The only conditions that apply individually to each refinery are the ones monitoring their own revenue, and the retrofitting costs resulting from the contract's activation.

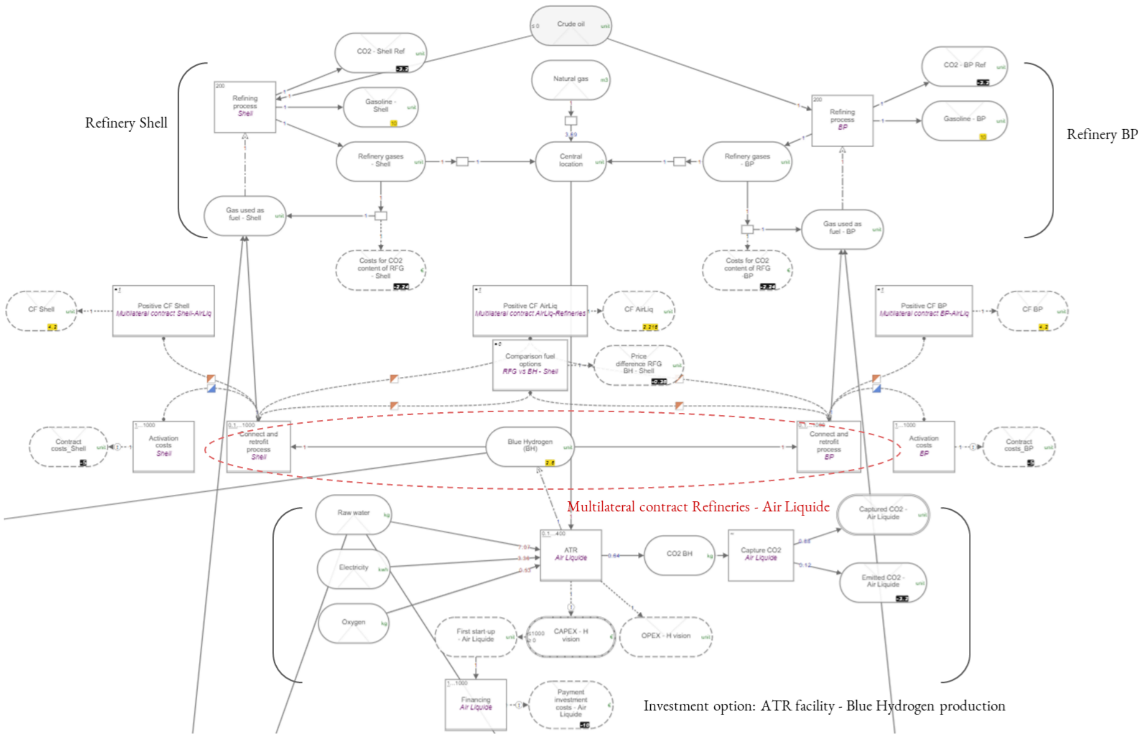


Figure C.3. Model II – multilateral revenue contract for blue hydrogen integration

Similarly, for the exchange of green hydrogen the two electrolysers establish a multilateral contract with the refineries for green hydrogen integration (Figure C.4). More specifically, green hydrogen producers pool their hydrogen production and sell it at the same standardized price to the end-users, as shown below.

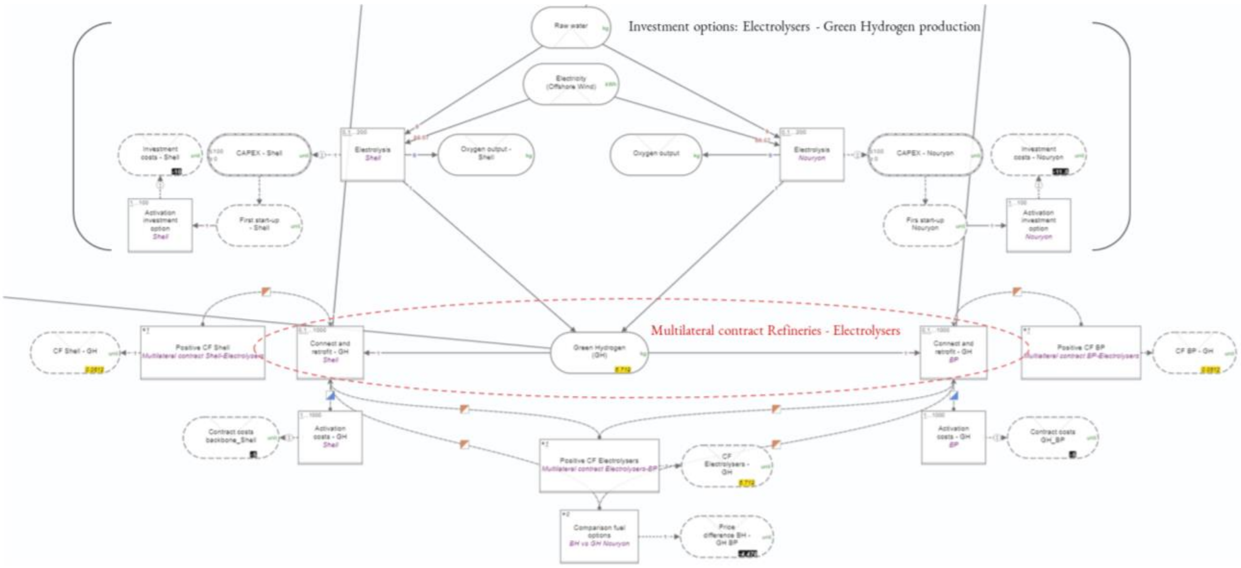


Figure C.4. Model II – multilateral revenue contract for green hydrogen integration

This representation is replicated for every multilateral contract established between *n>3* partners in the cluster.

Appendix D: Linny-R representation of industrial processes

D.1. Representation of refining process

The schematic representation of refining processes used in the Linny-R model is displayed below.

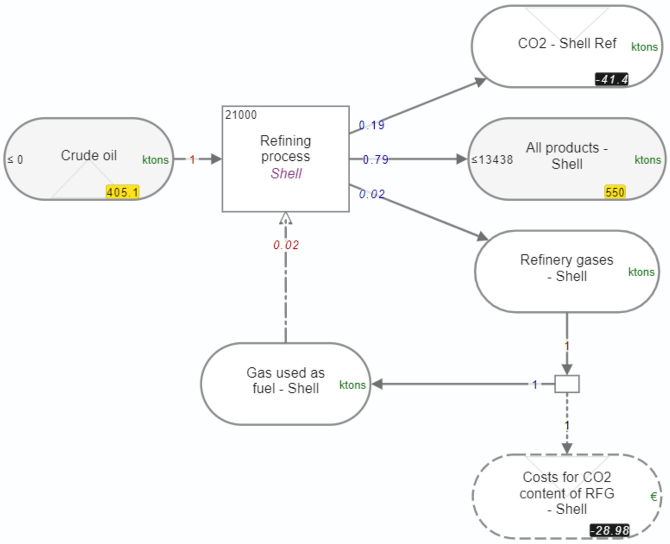


Figure D.1. Simplified Linny-R representation of refining process

The ratios in Figure D.1. are derived based on the following tables, used as input data:

Table D.1. Dutch refineries nameplate capacities and CO_2 emissions (Oliveira & Schure, 2020)

Refinery site	Crude oil nameplate capacity [kt/yr][1)]	Crude oil nameplate capacity [PJ/yr][2)]	Direct CO_2 emissions 2016 [kt/yr][3)]	Direct CO_2 emissions 2017 [kt/yr][3)]	Direct CO_2 emissions 2018 [kt/yr][3)]	Direct CO_2 emissions 2019 [kt/yr][3)]
BP Refinery Rotterdam B.V.	20,000	854	2,292	2,074	2,254	2,151
ESSO Refinery Rotterdam	9,100	389	2,106	2,068	1,583	2,376
Gunvor Petroleum Rotterdam B.V.	4,500	192	420	448	397	421
Shell Nederland Raffinaderij B.V.	21,000	897	4,254	3,831	4,211	4,357
Vitol B.V.	3,500[4)]	149	74	115	102	109
Zeeland Refinery N.V.	8,907[4)]	380	1,552	1,601	1,633	1,588
Total	**67,007**	**2,861**	**10,699**	**10,137**	**10,180**	**11,002**
Direct CO_2 emissions/ crude oil intake			0.197	0.189	0.185	0.194

Table D.2. Annual production volumes for the Dutch refinery sector (Oliveira & Schure, 2020)

Product	2016 [kt/yr]	2017 [kt/yr]	2018 [kt/yr]	2019 [kt/yr]
LPG	1,650	1,560	1,480	1,570
Naphtha	7,728	8,131	9,583	8,454
Gasoline	3,981	3,026	3,988	4,061
Kerosene (Aviation fuel)	8,220	7,988	9,099	9,064
Diesel/gasoil	19,162	19,272	18,599	20,753
Fuel oil	11,963	11,684	11,077	8,909

Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)

Blue hydrogen demand for power plants and industry: Reference scope		
Description	Max [MW]	Details
Engie Maasvlakte power plant	805	2 x 147 MWe gas turbines (36.5% open cycle efficiency) added to each power plant, running on hydrogen fuel and fully integrated with the existing boilers (topping cycle + heat integration), in addition to steam integration with the H-vision plant.
Uniper Maasvlakte power plant	805	
Pergen steam and power	286	Pergen has 2 x GE 9E.03 turbines with a total capacity of 200 MWe at 35% thermal efficiency. Assumed 50% replacement of NG with hydrogen.
BP refinery RFG	520	Maximum modifications for replacement of RFG and with hydrogen-rich fuel. Replacement of NG imported to balance the fuel gas grid (excluding NG duty of gas turbines).
BP refinery NG	40	
Pernis refinery RFG	650	Maximum modifications for replacement of RFG and with hydrogen -rich fuel. Higher replacement of NG imported to balance the fuel gas grid (excluding NG duty of gas turbines).
Pernis refinery NG	100	
Total demand (rounded up)	**3207**	

Based on Tables D.1, D.2. and D.3., the following calculations were performed:

Table D.4. Mass balance calculations: Shell refinery

Shell refinery	*Formula*	*2016*	*2017*	*2018*	*2019*	*Average*
Emissions based on nameplate capacity *(%)*	$\frac{Direct\ CO2\ emissions\ in\ year\ Y^{(1)}}{Crude\ oil\ nameplate\ capacity^{(1)}}$	0.160	0.151	0.152	0.164	*0.157*
Actual CO_2 emissions *(%)*	$\left(\frac{Direct\ CO2\ emissions\ in\ year\ Y}{Crude\ oil\ intake}\right)^{(1)}$	0.197	0.189	0.185	0.194	*0.191*
Capacity utilization *(%)*	$\frac{Emissions\ based\ on\ capacity}{Actual\ CO2\ emissions}$	0.811	0.800	0.821	0.846	*0.820*
Actual CH_2 emissions *(%)*	$Actual\ CO2\ emissions * \frac{14}{44}$	0.063	0.060	0.059	0.062	*0.061*
Total production volumes for the Dutch refinery sector *(ktons/y)*	$\sum_{i=1}^{\#\,products} \begin{matrix} Annual\ production \\ volumes\ of\ product\ i \end{matrix}^{(2)}$	52704.0	51661.0	53826.0	52811.0	*52750.5*
Total CH_2 emissions for the Dutch refinery sector *(ktons/y)*	$Crude\ oil\ nameplate\ capacity^{(1)} * Actual\ CH2\ emissions$	4200.121	4029.557	3944.276	4136.159	*4077.528*
Total crude oil intake for the Dutch refinery sector *(ktons/y)*	$Crude\ oil\ nameplate\ capacity^{(1)} * Capacity\ utilization$	54309.645	53634.921	55027.027	56711.340	*54920.733*
Total crude oil intake Shell *(ktons/y)*	$Crude\ oil\ nameplate\ capacity\ Shell^{(1)} * Capacity\ utilization$	17020.648	16809.189	17245.475	17773.339	*17212.163*
Total intake RFG Shell *(ktons/y)*	$\frac{Demand\ RFG\ (MW)^{(3)} * \frac{8760\ h}{year}}{0.00977\frac{m3}{MWh} * 0{,}554\frac{kg}{m3} * \frac{10^{-6}ktons}{kg}}$	-	-	-	-	*322.892*
Ratio RFG	$\frac{Total\ intake\ RFG\ Shell}{Total\ crude\ oil\ intake\ Shell}$	-	-	-	-	*0.019*
Ratio CO_2	$Actual\ CO2\ emissions$	-	-	-	-	*0.191*
Ratio end products	$1 - (Ratio\ RFG + Ratio\ CO2)$	-	-	-	-	*0.790*

1) Data source: Table D.1. Dutch refineries nameplate capacities and CO_2 emissions (Oliveira & Schure, 2020)
2) Data source: Table D.2. Annual production volumes for the Dutch refinery sector (Oliveira & Schure, 2020)
3) Data source: Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)

It should be noted that CH_2 emissions were calculated in this table to allow to perform a balance check of the performed calculations up to that point. This is because we had decided to use Table D.1. for

calculations regarding crude oil intake and CO_2 emissions, and Table D.2. for the ones pertaining to the refinery's outputs. However, it is clearly visible from the Table above that an imbalance is present when comparing the total crude oil intake with the total CH_2 emissions plus the total production volumes. As a result, we decided to only rely on calculations performed based on Table D.1. as input data, deriving the ratio of end products indirectly (last row), as a function of the ratio of by-products – i.e. Refinery Fuel Gas (RFG) and CO_2.
The total intake of RFG is calculated by converting the input data from MW to ktons/year, using conversion factors displayed in Table E.3.(Appendix E).

The same calculations are performed for the BP refinery. Same observations as for Shell apply to this case.

Table D.5. Mass balance calculations: BP refinery

BP refinery	*Formula*	*2016*	*2017*	*2018*	*2019*	*Average*
Emissions based on nameplate capacity *(%)*	$\frac{Direct\ CO2\ emissions\ in\ year\ Y^{(1)}}{Crude\ oil\ nameplate\ capacity^{(1)}}$	0.160	0.151	0.152	0.164	*0.157*
Actual CO_2 emissions *(%)*	$\left(\frac{Direct\ CO2\ emissions\ in\ year\ Y}{Crude\ oil\ intake}\right)^{(1)}$	0.197	0.189	0.185	0.194	*0.191*
Capacity utilization *(%)*	$\frac{Emissions\ based\ on\ capacity}{Actual\ CO2\ emissions}$	0.811	0.800	0.821	0.846	*0.820*
Actual CH_2 emissions *(%)*	$Actual\ CO2\ emissions * \frac{14}{44}$	0.063	0.060	0.059	0.062	*0.061*
Total production volumes for the Dutch refinery sector *(ktons/y)*	$\sum_{i=1}^{\#\,products} Annual\ production\ volumes\ of\ product\ i^{\ (2)}$	52704.0	51661.0	53826.0	52811.0	*52750.5*
Total CH_2 emissions for the Dutch refinery sector *(ktons/y)*	$Crude\ oil\ nameplate\ capacity^{(1)} * Actual\ CH2\ emissions$	4200.121	4029.557	3944.276	4136.159	*4077.528*
Total crude oil intake for the Dutch refinery sector *(ktons/y)*	$Crude\ oil\ nameplate\ capacity^{(1)} * Capacity\ utilization$	54309.645	53634.921	55027.027	56711.340	*54920.733*
Total crude oil intake BP *(ktons/y)*	$Crude\ oil\ nameplate\ capacity\ BP^{(1)} * Capacity\ utilization$	16210,141	16008.752	16424.262	16926.990	*16329.536*
Total intake RFG BP *(ktons/y)*	$\frac{Demand\ RFG\ (MW)^{(3)} * \frac{8760\ h}{year}}{0.00977 \frac{m3}{MWh}^{(4)} * 0{,}554 \frac{kg}{m3}^{(4)} * \frac{10^{-6} kton}{kg}}$	-	-	-	-	*258.214*
Ratio RFG	$\frac{Total\ intake\ RFG\ BP}{Total\ crude\ oil\ intake\ BP}$	-	-	-	-	*0.016*
Ratio CO_2	$Actual\ CO2\ emissions$	-	-	-	-	*0.191*
Ratio end products	$1 - (Ratio\ RFG + Ratio\ CO2)$	-	-	-	-	*0.793*

1) Data source: Table D.1. Dutch refineries nameplate capacities and CO_2 emissions (Oliveira & Schure, 2020)
2) Data source: Table D.2. Annual production volumes for the Dutch refinery sector (Oliveira & Schure, 2020)
3) Data source: Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)
4) Data source: Table E.3. Conversion table

D.2. Representation of repowering option of MPP3 Uniper power plant

The schematic representation of the MPP3 power plant used in the Linny-R model is displayed below. The existing steam cycle is represented in the upper-right corner. Below, we modelled an alternative set of processes derived from repowering the MPP3 plant with topping cycle.

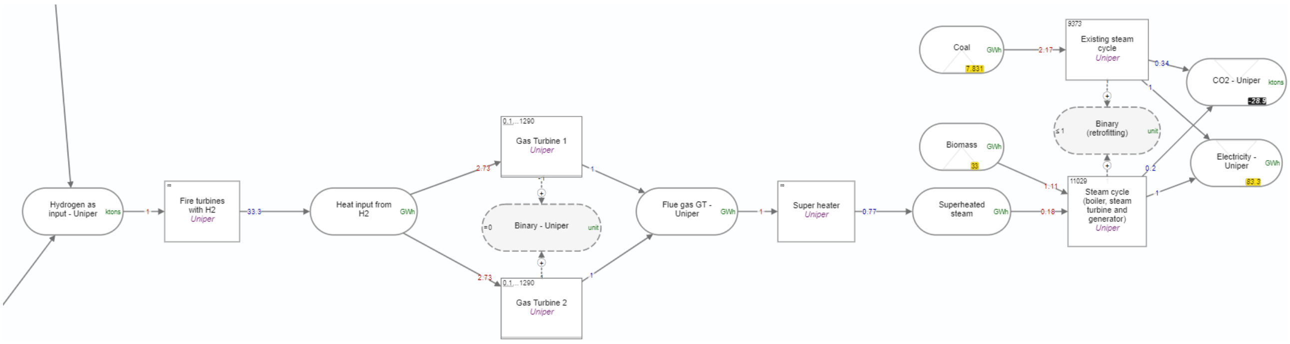


Figure D.2. Simplified Linny-R representation of MPP3 power plant and repowering option

The ratios in Figure D.2. are derived based on Table D.6., used as input data:

Table D.6. Model results for a repowered 1000 MW coal-fired power plant (H-Vision Consortium, 2019)

		1000 MW coal fired power plant							
				H-Vision low case		H-Vision reference case		H-Vision high case	
		Generic coal case	Minimum biomass case	Baseload operation	Max H2 use	Baseload operation	Max H2 use	Baseload operation	Max H2 use
Parameter	Units			Biomass + min steam integration	+ direct H2 firing + additional steam	Biomass + min steam integration	Full load + H2 GT topping cycle + additional steam	Biomass + min steam integration	Full Load + H2 GT topping cycle + direct H2 firing + additional steam
Heat input coal	[MWth]	2174		0	0	0	0	0	0
Heat input Biomass	[MWth]		830	830	613	830	1395	830	1069
Heat input hydrogen (direct firing)	[MWth]			0	217	0	0	0	326
Heat input hydrogen (GTs)	[MWth]			N/A	N/A	0	805	0	805
Steam from ATR HP steam (100 bar)	[tph]			52	84	112	225	210	302
Steam from ATR MP steam (30 bar)	[tph]			17	28	37	75	70	101
Heat input to steam turbine (HP steam, superheated at 600°C)	MWh]			52	84	113	227	211	303
Superheating heat extracted from the boiler	[MWth]			-11	-18	-24	-49	-45	-65
Heat input from ATR MP steam	[MWth]			13	22	29	59	55	79
Total heat input	[MWth]	**2174**	**830**	**884**	**918**	**948**	**2437**	**1050**	**2517**
Power output steam turbine	[MWe]	1000	340	360	395	382	965	418	1000
Power output gas turbines	[MWe]						294		294
Total power output	[MWe]	**1000**	**340**	**360**	**395**	**382**	**1259**	**418**	**1294**
Power production efficiency	[%]	46%	41%	41%	43%	40%	52%	40%	51%
Hydrogen GT incremental efficiency	[%]	N/A	N/A	N/A	N/A	N/A	59%	N/A	60%
Biomass energy input (relative to generic coal case)	[%]	0%	38%	38%	28%	38%	64%	38%	49%
Gas turbine size	[MW]					147		147	
Number	[-]	N/A	N/A	N/A		2		2	
Total capacity	[MW]					294		294	
Investment estimates									
Modification for direct H2 firing	[M€]			25				25	
Tie-ins + BOP for steam integration	[M€]			30		40 + 5		40 + 15	
Gas turbine	[M€]					120		120	

Based on the table above, the calculations in Table D.7. were performed. It should be specified that gas turbines and combined heat and power (CHP) systems are normally quoted by their electrical output in megawatt electric (MWe). Thus, the ratios used in Linny-R were adapted accordingly, by setting the flow rate of the power output at 1, and making the input flow rates proportional. The model was then executed and its output levels checked to ensure that the rates had correctly been used.

Table D.7. Mass balance calculations: MPP3 power plant

MPP3 power plant	*Input data*	*Unit*	*Calculated ratio*	*Ratio*	*Description*
<u>Repowered plant parameters</u>					
Heat input hydrogen	805	MW(th)	$\frac{Heat\ input\ hydrogen}{Power\ output\ GT} = \frac{1}{GT\ efficiency}$	2.73	Based on GT output
Power output GT	294	MW(e)	-	1	Based on GT output
Efficiency GT	0.365	-	-	-	-
Heat input biomass	1395	MW(th)	$\frac{Heat\ input\ biomass}{Total\ power\ output}$	1.11	Based on total power output
Heat input steam turbine	227	MW(th)	$\frac{Heat\ input\ steam\ turbine}{Total\ power\ output}$	0.18	Based on total power output
Power output steam turbine	965	MW(e)	-	-	-
Total power output	1259	MW(e)	-	1	Based on total power output
<u>Coal power plant parameters</u>					
Heat input coal	2174	MW(th)	$\frac{Heat\ input\ coal}{Power\ output\ steam\ turbine}$	2.17	Based on power output
Power output steam turbine	1000	MW(e)		1	Based on power output

Data source: Table D.6. Model results for a repowered 1000 MW coal-fired power plant (H-Vision Consortium, 2019)

Note that, as the pricing of coal, biomass and electricity is expressed in €/MWh, we converted the capacities of the processes used to model the MPP3 power plant from MW to MWh/year. Since the values for prices and material flows would be very high, a second conversion step was made to express capacities in GWh/year, and prices in k€/GWh. In this way, the calculated ratios stay the same and conventional units for prices (with minimal manipulations) can be used.

D.3. Representing ATR process

A schematic representation of the ATR facility employed in the Linny-R model is displayed below.

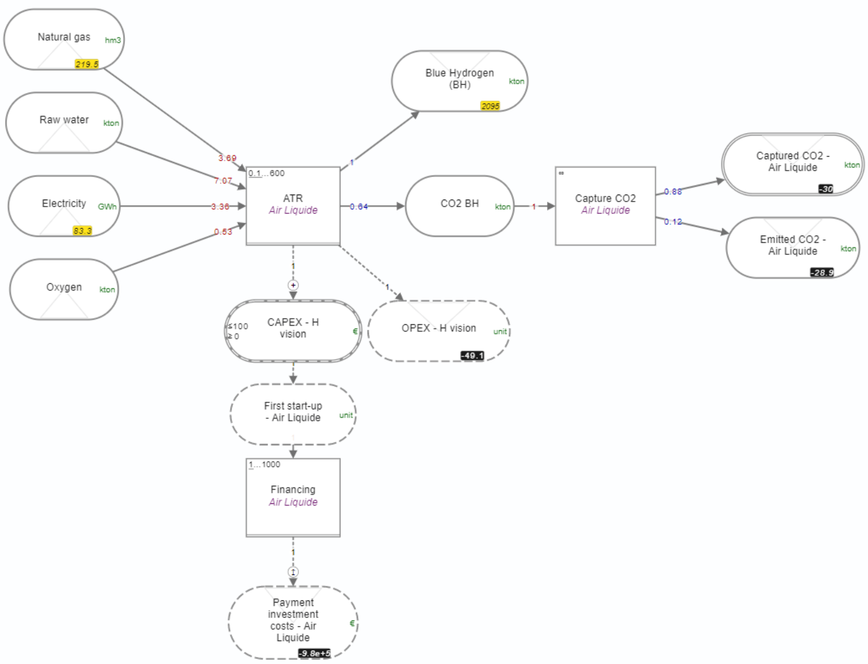


Figure D.3. Linny-R representation of ATR production facility

The flow rates used in the representation are derived from Table D.8, and converted according to Table D.10. The capture rate of CO_2 via Porthos (including residual carbon) is derived from Table D.9.

Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen, Croezen, & Rooijers, 2018)

Input	SMR	ATR	Electrolyzer 2017	Electrolyzer 2030
Inflow NG ($m^3/kg\ H_2$)	3.73	3.69	0,0	0,0
Inflow raw water ($kg/kg\ H_2$)	4.68	7.07	9.0	9.0
Inflow sea water ($m^3/kg\ H_2$)	1.18	0.0	0,0	0,0
Electricity demand (kwh/kg)	1.17	3.36	66.07	53.6
Oxygen ($kg/kg\ H_2$)	0.0	0.53	0.0	0.0
Output	**SMR**	**ATR**	**Electrolyzer 2017**	**Electrolyzer 2030**
Hydrogen (kg)	1.0	1.0	1.0	1.0
CO_2 process emission ($kg/kg\ H_2$)	0.99	0.64	0.0	0.0
CO_2 capture rate (%)	0.9	0.95	0.0	0.0
Waste water ($kg/kg\ H_2$)	1.83	0.0	0.0	0.0
Return sea water ($m^3/kg\ H_2$)	1.18	0.0	0.0	0.0
Oxygen ($kg/kg\ H_2$)	0.0	0.0	8.0	8.0

Table D.9. Key parameters of hydrogen production via ATR

Key parameters of hydrogen production via HP ATR		
HP ATR plant capacity (as hydrogen output)	700,000	$Nm^3/h\ H_2$
Hydrogen purity in the outlet stream	95.5	%
HP ATR plant capacity (as total fuel output)	2,400	MW_{th} (LHV)
Overall thermal efficiency	78	% on LHV basis
	~82	% on HHV basis
Total feedstock (input of NG + RFG) required	3,130	MWth (LHV)
Excess steam production (available for export, with 20°C superheating)	305	t/h HP steam (100 bar)
	100	t/h MP steam (30 bar)
Electricity import	128	MW_e
Direct CO_2 emissions at the H-vision plant	6	$t\ CO_2/h$
CO_2 captured at the H-vision plant	498	$t\ CO_2/h$
CO_2 capture & export factor	0.208	$t\ CO_2/MWh$
CO_2 purity in the export stream	99	%
Overall capture rate (including residual carbon)	88	%
Overall CO_2 emissions factor	0.028	$t\ CO_2/MWh$
Total plant cost	910	M€
Fixed OPEX (2.5% of CAPEX annually)	22.8	M€

Considering that hydrogen volumes produced and exchanged in Rotterdam will be in the scale of tons rather than kilograms, the units in used in Table D.8. need to be adequately converted. Moreover, having dimensioned the refining processes in ktons, it is convenient to use the same unit to dimension the capacity of the ATR facility. Units of natural gas and electricity inflows are converted accordingly, in order to maintain the same ratios as in Table D.8. An overview of the final units is displayed in Table D.10.

Table D.10. Input-output flow rates with converted units

Input ATR	*Unit*	*Conversion*	*Final ratio*
Inflow natural gas	$m^3/kg\ H_2$	$hm^3/kton\ H_2$	3.69
Inflow raw water	$kg/kg\ H_2$	$kton/kton\ H_2$	7.07
Electricity demand	$kWh/kg\ H_2$	$GWh/kton\ H_2$	3.36
Oxygen	$kg/kg\ H_2$	$kton/kton\ H_2$	0.53
Output ATR			
Hydrogen	kg	kton	1.0
CO_2 process emissions	$kg/kg\ H_2$	$kton/kton\ H_2$	0.64
CO_2 capture rate	(%)	(%)	0.88

The following tables were used as inputs for the calculations of financial parameters.

Table D.11. References for an ATR + CCS plant, all with high pressure CO2 capture (H-Vision Consortium, 2019)

Parameter	ATR+HP CCS [H21] (1.3 GW H_2) 1 ATR train	ATR+CCS [NTU] (0.7 GW H_2) 1 ATR train	ATR+PSA CCS [TNO] (0.4 GW H_2) 1 ATR train	HP ATR + HP Rectisol CCS [Air Liquide] (2.1 GW H_2) 1 ATR train
CO_2 capture [%]	94.5%	92.3%	94.0%	88%
CO_2 footprint [kg CO_2 / MWh H_2]	15.4	19.1	-	28
Efficiency (HHV) Efficiency (LHV)	76.0% 71.1%	87.7% (excl. CCS) 82.0% (excl. CCS)	81.9% 76.4%	82.3% 77.7%
Electric power import [MW_e]	53.8	27.1 (excl. CCS)	32.3	128
CAPEX per capacity [M€ / MW H_2]	-	1.40	-	0.43
OPEX per capacity [M€ / MW H_2 / year]	-	0.24 (incl. CCS)	-	-

Table D.12. Overview retrofitting costs (H-Vision Consortium, 2019)

	Capital Retrofitting costs Power plant A	M€	-	162.5	192.5
	Capital Retrofitting costs Power plant B	M€	55	162.5	192.5
	Generic O&M Costs Power Plant A	€/MWh	-	2.40	2.40
	Generic O&M Costs Power Plant B	€/MWh	-	2.40	2.40
	Capital Retrofitting costs Refineries	M€	101.6	214.3	389.3

Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)

Technology	Parameter	Units	Today	2030	Long term
Water electrolysis	CAPEX	USD/kW_e	900	700	450
	Efficiency (LHV)	%	64	69	74
	Annual OPEX	% of CAPEX	1.5	1.5	1.5
	Stack lifetime (operating hours)	hours	95 000	95 000	100 000
Natural gas reforming	CAPEX	USD/kW_{H2}	910	910	910
	Efficiency (LHV)	%	76	76	76
	Annual OPEX	% of CAPEX	4.7	4.7	4.7
	Emission factor	$kgCO_2/kgH_2$	8.9	8.9	8.9
Natural gas reforming with carbon capture	CAPEX	USD/kW_{H2}	1 680	1 360	1 280
	Efficiency (LHV)	%	69	69	69
	Annual OPEX	% of CAPEX	3	3	3
	CO_2 capture rate	%	90	90	90
	Emission factor	$kgCO_2/kgH_2$	1.0	1.0	1.0

From these tables, the financial parameters were calculated using the H-vision feasibility study for most of the inputs. Missing data was retrieved from the IEA G20 Hydrogen report. Financial parameters were calculated as follows:

- Capital investment costs were calculated from Table D.11. using the HP ATR + HP Rectisol CCS from Air Liquide as a reference;
- As no estimates for OPEX per capacity were present in the same Table, we used Table D.13, calculating the annual fixed costs of the reformed as 3% of the used CAPEX per capacity (from the previous step);
- Capital retrofitting costs were retrieved from Table D.12. Retrofitting costs for refineries were divided for Shell and BP based on the hydrogen demand of each off-taker

Table D.14. Overview of financial parameters associated with investment in ATR

Parameter	*Formula*	*Value*	*Unit*
Capital investment costs reformer	$\frac{CAPEX\ per\ capacity\ \left[\frac{M€}{MW}\right]^{(1)} * (Reformer\ capacity\ [tons]^{(2)} * 33.33\ \left[\frac{MWh}{tons}\right])}{8760\ MWh/y}$	981.6	M€
Annual fixed costs reformer (% capital costs)	$3\%^{(3)} * \frac{CAPEX\ per\ capacity\ \left[\frac{M€}{MW}\right]^{(1)} * 33.33\ \left[\frac{MWh}{tons}\right]}{8760\ MWh/y}$	49.1	€/ton
Capital retrofitting costs Shell refinery	$\frac{Capital\ retrofitting\ costs\ [M€]^{(4)} * Hydrogen\ demand\ Shell\ refinery}{Total\ estimated\ hydrogen\ demand^{(2)}}$	119	M€
Capital retrofitting costs BP refinery	$\frac{Capital\ retrofitting\ costs\ [M€]^{(4)} * Hydrogen\ demand\ BP\ refinery}{Total\ estimated\ hydrogen\ demand^{(2)}}$	95.2	M€
Capital retrofitting costs Uniper power plant	Capital retrofitting costs $[M€]^{(4)}$	162.5	M€
Default WACC	$Assumption^{(3)}$	8.00	%
Economic lifetime	$Assumption^{(3)}$	25	years

1) Data source: Table D.11. References for an ATR + CCS plant, all with high pressure CO2 capture (H-Vision Consortium, 2019)
2) Calculated from the sum of estimated hydrogen demand for the modelled processes using as Data source: Table D.3. Breakdown of estimated demand for blue hydrogen for the H-vision Reference Scope (H-Vision, 2019)
3) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
4) Data source: Table D.12. Overview retrofitting costs (H-Vision Consortium, 2019)

D.4. Representing electrolysis processes

A schematic representation of the green hydrogen conversion park is displayed below.

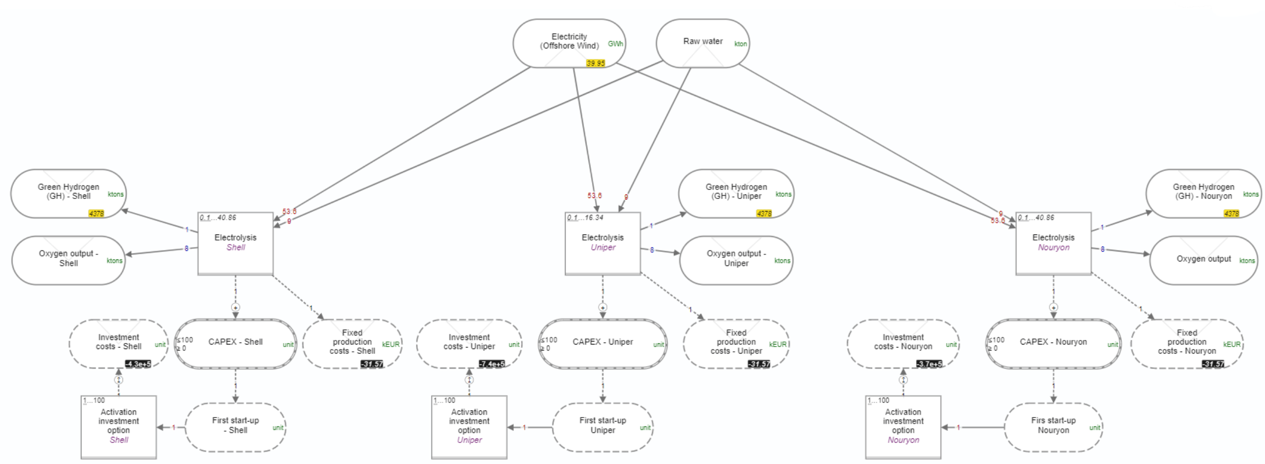


Figure D.4. Linny-R representation of electrolysers

Similarly to the ATR case, data reporting the input-output ratios was available, thus no additional mass balance calculations were performed –only unit conversions were needed. The flow rates used in the representation above are derived from Table D.8, and converted according to Table D.15, for the same reasons discussed in Section D.3.

Table D.15. Input-output flow rates with converted units for green hydrogen

Input	*Unit*	*Conversion*	*Final ratio*
Inflow raw water	kg/kg H_2	kton/kton H_2	9
Inflow electricity	kWh/kg H_2	GWh/kton H_2	53.6
Output ATR			
Hydrogen	kg	kton	1.0
Oxygen output	kg/kg H_2	kton/kton H_2	8

As explained in Section 5.2.2.2, green hydrogen production is modelled as an investment option in an electrolyser *strategy* for each of the investors. To this end, the capacity of each of the three processes in Figure D.4 is progressively increased to reach the required maximum output. The progression of capacity expansions for Shell's electrolyser strategy is shown in Table D.16. Investments in additional capacity were assumed to be made every 10 years, with the ambition to meet hydrogen demand for Shell Pernis. Specifically, we assumed the electrolyser strategy to be able to produce the amount of hydrogen required by the refinery by 2040. This choice was made to allow the refinery to possibly run solely on green hydrogen and eventually replace blue hydrogen produced by H-vision.

Table D.16. Overview key decisions and assumptions for green hydrogen strategy: Shell

Required capacity Shell	*Ktons H_2 output (=H_2 demand)*	*GW electricity input*	*Conversion*
Required capacity to meet hydrogen demand	170.8	1.04	$\frac{Hydrogen\ demand\ Shell\ refinery\ [ton] * Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]}{8760\ \left[\frac{h}{y}\right] * 10^3}$
Decision Shell	***MW electricity input***	***Ktons H_2 output***	***Conversion***
Initial capacity (Today)	250	40.86	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2030	500	81.72	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2040	1040	170.8	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$

Data source inflow of electricity: Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)

The same rationale applies to the assumptions made for the electrolyser strategy of BP.

Table D.17. Overview key decisions and assumptions for green hydrogen strategy: Nouryon

Required capacity BP	*Ktons H_2 output (=H_2 demand)*	*GW electricity input*	*Conversion*
Required capacity to meet hydrogen demand	136.7	0.837	$\frac{Hydrogen\ demand\ BP\ refinery\ [ton] * Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]}{8760\ \left[\frac{h}{y}\right] * 10^3}$
Decision Nouryon	***MW electricity input***	***Ktons H_2 output***	***Conversion***
Initial capacity (Today)	250	40.86	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2030	500	81.72	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2040	8370	137	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$

Data source inflow of electricity: Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)

A slight difference is present in the expansion plans for Uniper. In fact, in our model the use of coal stops from 2030 onwards due to the coal ban. As a result, Uniper's coal-fired plant needs to be repowered and converted to a biomass plant. Based on the modelled development concept, the new power plant needs hydrogen as secondary fuel. In order to avoid to suggest blue hydrogen as an implied solution for power plants' repowering (due to unavailability of sufficient green hydrogen), we assume that Uniper succeeds in scaling up its electrolyser strategy in order to produce enough green hydrogen by 2030 and successfully substitute coal. In this way, the solver can pick the hydrogen option that is more economically convenient based on its investment costs, fixed and variable production costs, and end-price –as related to the chosen contractual structure.

Table D.18. Overview key decisions and assumptions for green hydrogen strategy: Uniper

Required capacity Uniper	*Ktons H_2 output (=H_2 demand)*	*GW electricity input*	*Conversion*
Required capacity to meet hydrogen demand	211.6	1.29	$\frac{Hydrogen\ demand\ Uniper\ power\ plant\ [ton] * Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]}{8760\ \left[\frac{h}{y}\right] * 10^3}$
Decision Uniper	***MW electricity input***	***Ktons H_2 output***	***Conversion***
Initial capacity (Today)	100	16.34	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2025	500	81.72	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$
Expansion 2030	1300	211.6	$\frac{Electrolyser\ capacity\ [MW\ input] * 8760\ \left[\frac{h}{y}\right]}{Inflow\ electricity\ per\ ton\ H2\ [MWh/ton]} * 10^{-3}$

Data source inflow of electricity: Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)

A final assumption that was made regarding green hydrogen production is that enough wind capacity will be installed in time to guarantee that electrolysers are able to produce the required amount by the modelled off-takers. We are aware that such plans may seem too optimistic. However, for the purpose of this research it is more important that we do not constrain the choice of investing in green hydrogen production by external factors –such as insufficient technological progress for scale-up or unavailability of renewable capacity. We rather opted for the adoption of these assumptions, so as to let the economics be the decisive factor in investment decisions, combined with the contractual structures that make the economics more or less favourable.

Capital investment costs are calculated according to the assumed capacity expansions, by adding together all the capital investment costs. Expansions take into account future cost reductions, influenced by innovations in the technologies themselves (for instance, the development of less costly materials for electrodes and membranes), and by economies of scale. Therefore, each capacity expansion is associated to a specific CAPEX (€/unit capacity) estimate. An overview of the investment costs and the underlying calculations is presented in Table D.19, based on data input from Table D.13.

Table D.19. Overview of financial parameters for electrolyser strategies

Electrolysis **Parameter**	***Formula***		***Today***	***2030***	***2040***	***Unit***
CAPEX	$\frac{CAPEX\ per\ capacity\ \left[\frac{\$}{kW}\right]^{(1)} * 10^3 \left[\frac{kW}{MW}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(2)} * Discount\ factor^{(3)}\ )}{8760\ \left[\frac{h}{y}\right] * Efficiency^{(1)} * \frac{1}{33.33\ \left[\frac{MWh}{tons}\right]}}$		2104.7	1518.34	1203.60	€/ton
Fixed production costs	$1{,}5\%^{(1)} * CAPEX\ [\frac{€}{ton}]$		31.57	22.77	18.05	€/ton
Total CAPEX	***Formula***	***Initial investment***	***Expansion 2025***	***Expansion 2030***	***Expansion 2040***	***Total CAPEX***
Shell	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2140.7*40.9	-	1518.3*81.7	1203.6*171	415.8 M€
Nouryon	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2140.7*40.9	-	1518.3*81.7	1203.6*137	374.9 M€
Uniper	$\sum_{t=1}^{T} CAPEX\ [\frac{€}{ton}]$* *tons capacity expansion (t)*	2140.7*16.3	1829.5*(81.7-16.3)	1518.3*215	1203.6*215	738 M€

4) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
5) Assumed 0.85 €/$
6) Assumed 10 years lifetime and discount rate of 8%

Finally, it should be noted that green hydrogen produced via the electrolyser strategies is integrated in existing cluster processes, which require technical adaptations to their installations. Refineries and power plants may want to integrate either blue hydrogen or green hydrogen in their processes: in both cases, they will bear retrofitting costs, which have to be paid for only once, at the moment of first integration of one type of hydrogen –say, blue hydrogen. In the future, when green hydrogen is integrated, only small adaptations will be required due to similarities in the types of fuels and in the retrofitting process: thus, for the second integration, we do not consider these costs. This implies that, once the process has been repurposed for the integration of a fuel, no additional retrofitting costs are needed for integration of fuels with similar characteristics. This means that, on the other hand, if green hydrogen is the first fuel to be integrated, the same retrofitting costs derived from the H-vision feasibility study (Table D.14) will be paid by the off-taker. Then, if blue hydrogen is integrated in a second moment, no additional retrofitting costs will need to be paid, as the process has already been retrofitted for green hydrogen use.

D.5. Representing the hydrogen backbone

A schematic representation of the hydrogen backbone as a joint venture agreement was already displayed in Figure 17 (Chapter 4).

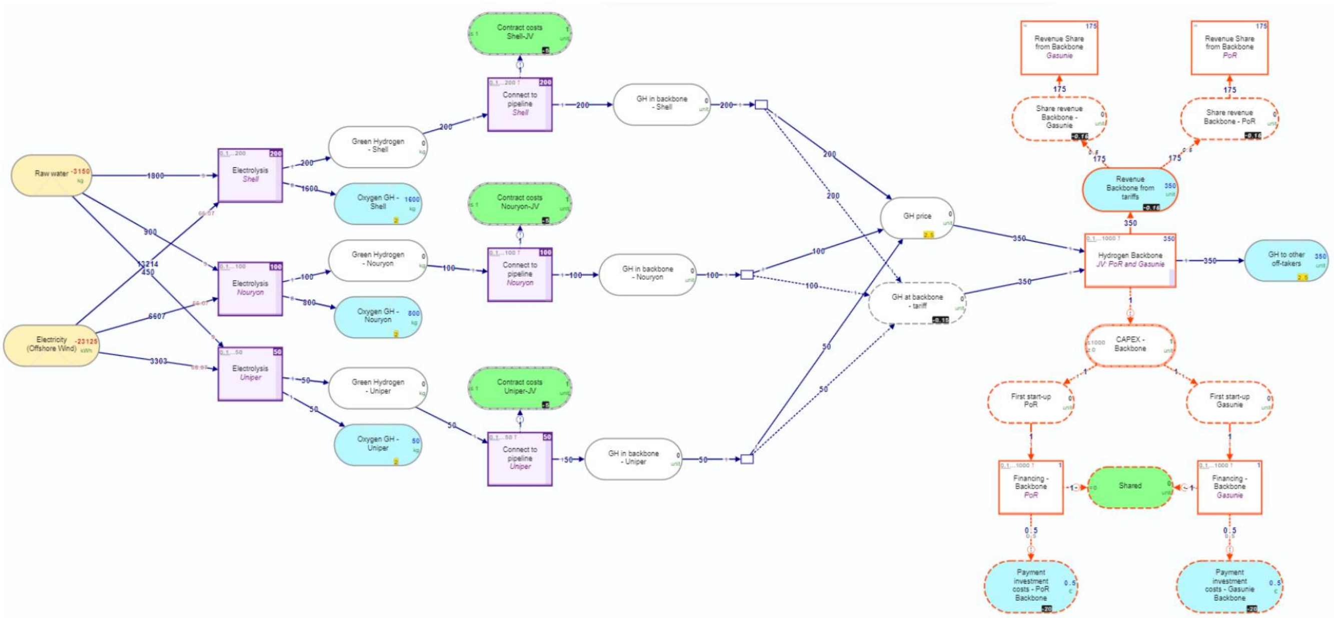


Figure D.5. Linny-R representation of hydrogen backbone

In our model, we use the same representation as above, with some minor adjustments:

i. Also blue hydrogen is sold via the backbone, in exchange for a tariff of 0.003 €/GJ
ii. The representation of revenue contracts is made according to the procedure explained in Chapter 4. More specifically, revenue contracts are implemented with the usual set of conditions that ensure that the transaction is always profitable or economically convenient for both the producer and the off-taker. In addition to that, since the end users of hydrogen have not been specified in the model, we add a threshold for the hydrogen price that mirrors the maximum willingness to pay of end-users. If the hydrogen price is higher than this threshold, hydrogen will not be sold via the backbone.

To be able to sell hydrogen via the backbone, hydrogen producers need to bear some contract costs, namely the connection costs of building smaller pipelines to connect their processes to the backbone. An overview of the financial parameters used is displayed below, using Table D.21 as input data.

Table D.20. Overview financial parameters to model the hydrogen backbone

Financial parameter	*Value*	*Unit*	*Assumption*
Capital investment cost regional backbone	100	M€	Only costs for the regional pipeline are taken into account. Costs of repurposing the existing gas network to constitute a national backbone are out of scope.
Equity share Port of Rotterdam	50	%	-
Equity share Gasunie	50	%	-
Capital costs of connection to backbone	1.21(1)	M€/km	Converted to M€ assuming that the smaller connections of 4km are needed. Distance estimation based on (Institute for Sustainable Process Technology, n.d.)
Transport tariff	0.003	€/GJ	-

1) Data source: CAPEX/km from Table D.21. Hydrogen transmission parameters (IEA, 2020)

Table D.21. Hydrogen transmission parameters (IEA, 2020)

Technology	Parameter	Units	Hydrogen	LOHC	Ammonia
Pipelines[1]	Lifetime	**years**	40	-	40
	Distance	**km**	Function of supply route		
	Design throughput	**ktH$_2$/y**	GH$_2$: 340	800	240
	Gas density	**kg/m^3**	7.9	-	-
	Gas velocity	**m/s**	15	-	-
	CAPEX/km	**USD million/km**	1.21	2.32	0.55
	Utilisation	**%**	75%	75%	75%

Appendix E: scenario definition

Three scenarios have been drawn up due to the uncertainty regarding future macro-economic developments influencing commodity prices –and, in turn, hydrogen prices. These uncertainties may swing the choice of the contract form that is best suited to support specific investments. An overview of the critical variables for scenario analysis is summarized in the uncertainty table below. Prices are expressed in the units that were used in sources from which data was retrieved. An overview of the conversions is displayed in Table E.2, based on the values reported in Table E.3.

Table E.1. Uncertainty table

Key uncertainties: commodity prices	Unit	Range of outcomes		
		Low	***Med***	***High***
Gas market price(1)	$/MBtu	7.3-7.8 *IEA Sustainable Development*	7.3-9.8 *IEA New Policies*	7.3-10.4 *IEA Current Policies*
CO_2 certificates(1)	$/ton	34-41 *IEA Current Policies*	34-49 *IEA New Policies*	34-191 *IEA Sustainable Development*
CO_2 transport and storage tariff(2)	€/ton	22.5	30	80
Electricity price(3)	$/MWh	98-58	98-123	-
			Assumed as constant	
Crude oil price(1)	$/bbl		65 *IEA Current Policies*	
Coal price(1)	$/ton		75 $/ton *IEA Current Policies*	
Biomass price(4)	€/MWh		32.6	

1) Data source: International Energy Agency. (2018). *World Energy Outlook 2018.*
2) Data source: H-Vision Consortium. (2019). *Annexes to the H-vision Main Report.*
3) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
4) Data source: Perner, J., & Van Der Poel, S. (2019). *PROFITABILITY AND DISPATCH OF MPP3 POWER PLANT WITH ALTERNATIVE FUELS - A report for Uniper Benelux.*

The considered scenarios are built out of combinations of the presented range of outcomes, resulting in Table 15. As the focus of our research is on sensitivities versus determinants of hydrogen contract prices, scenarios focused on variations of CO_2, natural gas and electricity prices. For coal and crude oil, prices of the IEA Current Policies scenario are applied. Biomass prices are assumed to remain constant in real terms at the level of today's forward prices (32.6 €/MWh). This assumption was made consistently with the Frontier Economics feasibility study on coal-fired power plants' conversion into biomass power plants (Perner & Van Der Poel, 2019). Moreover, this assumption allowed to avoid making debatable assumptions on the biomass price behaviour after the 2030 coal ban: when this tipping point is reached in real life, it is likely that a steady demand increase will in turn increase biomass prices. However, a relatively low biomass price compared to gas and CO_2 prices may still make biomass an economically attractive option. Such real-world effects are not included in our model, which assumes biomass as a viable option. Thus, conclusions about the future feasibility of biomass in coal-fired power plants lie outside the scope of this study. Results are only ´possible futures developments´, given the set of assumptions made.

The prices in Table E.1. were converted to match the units used in Linny-R for the system representation.

Table E.2. Overview of performed conversions

Commodity prices	Unit	Final Unit	Conversion	Range of outcomes		
				Low	***Med***	***High***
Gas market price(1)	\$/MBtu	k€/hm^3	$\frac{Gas\ market\ price\ \left[\frac{\$}{MBtu}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(5)} * 10^{-3}[k€]}{28.264^{(6)}\ \left[\frac{m^3}{MBtu}\right] *\ 10^{-6}[\frac{hm^3}{m^3}]}$	219-236	219-294	219-312
CO_2 certificates(1)	\$/ton	k€/kton	$\text{CO2 certificates}\ \left[\frac{\$}{\text{ton}}\right] * \text{Exchange rate}\ [\frac{€}{\$}]$	30-35	30-41	30-163
CO_2 transport and storage tariff(2)	€/ton	k€/kton	$CO2\ tariff\ \left[\frac{\$}{ton}\right] * Exchange\ rate\ [\frac{€}{\$}]$	22.5	30	80
Electricity price(3)	\$/MWh	k€/GWh	$Electricity\ price\ \left[\frac{\$}{MWh}\right] * Exchange\ rate\ [\frac{€}{\$}]$	83-66	83-105	-
				Assumed as constant		
Crude oil price(1)	\$/bbl	k€/kton	$\frac{Crude\ oil\ price\ \left[\frac{\$}{bbl}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(5)} * 10^{-3}[k€]}{0.1364^{(6)}\ \left[\frac{bbl}{tons}\right] *\ 10^{-3}[\frac{tons}{kton}]}$	405.06		
Coal price(1)	\$/ton	k€/GWh	$\frac{Coal\ price\ \left[\frac{\$}{ton}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(5)} * 10^{-3}[k€]}{8.141^{(6)}\ \left[\frac{MWh}{tons}\right] *\ 10^{-3}[\frac{MWh}{GWh}]}$	7.83		
Biomass price(4)	€/MWh	k€/GWh	-	33		

1) Data source: International Energy Agency. (2018). *World Energy Outlook 2018.*
2) Data source: H-Vision Consortium. (2019). *Annexes to the H-vision Main Report.*
3) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
4) Data source: Perner, J., & Van Der Poel, S. (2019). *PROFITABILITY AND DISPATCH OF MPP3 POWER PLANT WITH ALTERNATIVE FUELS - A report for Uniper Benelux*.
5) Assumed 0.85 \$/€
6) Data source: Conversion table (Table E.3)

Table E.3. Conversion table

Commodity	**Conversion factor**	**Unit**
Natural gas	28.264	m^3/MBtu
	0.00976	m^3/MWh
	0.554	kg/m^3
Coal	8.121	Tonne/MWh
Crude oil	0.1364	Bbl/ton
Hydrogen	33.33	kWh/kg

Appendix F: calculations for contract price determination

F.1. Tolling model

Hydrogen contract prices under a tolling model are determined by (i) capital investment costs and fixed production costs, (ii) variable production costs, represented by the feedstock price and (iii) a profit element, constituted by the conversion fee. The hydrogen contract prices (in €/ton) under a tolling agreement displayed in Figure 41 are derived based on the calculations presented in Table F.1. and Table F.2.

Table F.1. Calculations for blue hydrogen contract prices under tolling agreement

Price determinants	Formula	Today	2030	2040	2050	Unit
Blue Hydrogen						
CAPEX	$\frac{CAPEX\ [\frac{€}{MW}]^{(1)} * 33.33\ [\frac{MWh}{ton}]^{(2)}}{8760\ h}$	1636.1	1636.1	1636.1	1636.1	€/ton
OPEX	$3\%^{(3)} * CAPEX\ [\frac{€}{ton}]$	49.1	49.1	49.1	49.1	€/ton
Electricity price (grid)	$Electricity\ price \left[\frac{€}{MWh}\right]^{(4)} * 3.36\ [\frac{MWh}{ton\ H2}]^{(5)}$	*279.9*	*325.6*	*338.4*	*351.3*	€/ton
Natural gas price	$Natural\ gas\ price \left[\frac{€}{hm3}\right]^{(6)} * 3.69\ [\frac{hm3}{ton\ H2}]^{(5)}$	*810.1*	*909.9*	*998.8*	*1087.4*	€/ton
Total fuel costs		1089.9	1235.6	1337.2	1438.7	€/ton
CO_2 price	$CO2\ price \left[\frac{€}{ton}\right]^{(6)} * 0.12\ [\frac{ton}{ton\ H2}]^{(5)}$	*3.47*	*3.60*	*3.88*	*4.15*	€/ton
CO_2 storage tariff	$CO2\ tariff \left[\frac{€}{ton}\right]^{(7)} * 0.88\ [\frac{ton}{ton\ H2}]^{(5)}$	*26.4*	*26.4*	*26.4*	*26.4*	€/ton
Total CO_2 price		29.8	30.0	30.3	30.6	€/ton

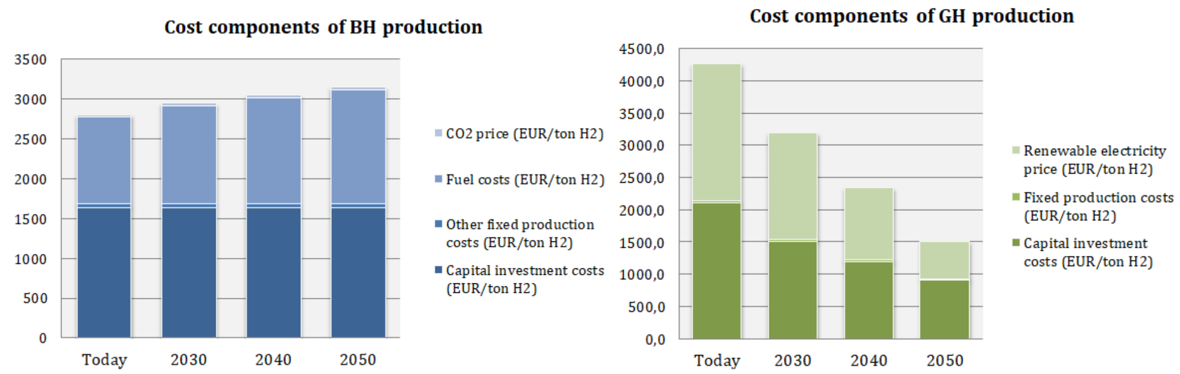
1) Data source: Table D.11. References for an ATR + CCS plant, all with high pressure CO2 capture (H-Vision Consortium, 2019)
2) Data source: Table E.3. Conversion table
3) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
4) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
5) Feedstock prices are multiplied by their respective flow rates, as reported in Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)
6) Data source: International Energy Agency. (2018). World Energy Outlook 2018.
7) Data source: H-Vision Consortium. (2019). *Annexes to the H-vision Main Report.*

Table F.2. Calculations for green hydrogen contract prices under tolling agreement

Price determinants	Formula	Today	2030	2040	2050	Unit
Green Hydrogen						
CAPEX	$\frac{CAPEX\ per\ capacity\ \left[\frac{\$}{kW}\right]^{(1)} * 10^3 \left[\frac{kW}{MW}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(2)} * Discount\ factor^{(3)}}{8760\ \left[\frac{h}{y}\right] * Efficiency^{(1)} * \frac{1}{33.33\ \left[\frac{MWh}{tons}\right]}}$	2104.7	1518.3	1203.6	910.1	€/ton
OPEX	$1.5\%^{(1)} * CAPEX\ [\frac{€}{ton}]$	31.6	22.8	18.1	13.7	€/ton
Electricity price (RES)	$Electricity\ price \left[\frac{€}{MWh}\right]^{(4)} * 53.6\ [\frac{MWh}{ton\ H2}]^{(5)}$	2141.3	1659.7	1124.6	589.6	€/ton

1) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
2) Assumed 0.85 €/$
3) Assumed 10 years lifetime and discount rate of 8%
4) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
5) Feedstock prices are multiplied by their respective flow rates, as reported in Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)

Summing all the elements presented in the table above, the plots in Figure F.1. are obtained.



Notes: Assumed WACC = 8%. Natural gas price of 7.3-9.8 $/MMBtu. CO_2 price of 35-40 €/tCO_2. Electricity price (grid) of 88-105 €/MWh. Renewable electricity price = 40-20 €/MWh; CAPEX and OPEX discounted over a 25y lifetime for ATR and 10y for electrolysers;

Figure F.1. Hydrogen production costs for Natural Gas + CCUS and Electrolysis Renewable

The contract price approximations displayed in Figure 41 are calculated by adding a profit element (i.e. the conversion fee) on top of the obtained hydrogen cost estimates. To the best of our knowledge, estimates for the value of such profit element are not yet available in literature. Therefore, we derived its value by performing multiple model iterations to identify a tipping point above which hydrogen integration is not a viable option in the cluster anymore. In this way, we identified an upper bound to the value of the profit element, equal to 200 €/ton. Thus, based on the model's assumptions and on our system's representation, the range of values that the conversion fee can assume is [0;200 €/ton]. To perform our experiments, we chose an intermediate value of 100 €/ton. We are well aware that the range of value is very limited: this is probably due to the low flow rates for hydrogen inflows in the existing cluster processes (see Appendix D). As a result, hydrogen integration only minimally contributes to cash flows of off-takers. If the hydrogen price, however, becomes too high, contracts for hydrogen integration will hardly be an attractive option.

Values in Figure F.1. are benchmarked against hydrogen costs projections from several reports (International Energy Agency, 2019; Renewable Energy Agency, 2020; Rijk & van Dinther, 2019). This benchmark analysis reveals that our total cost estimations correctly mirror future hydrogen cost trends. However, the proportions of costs components are not exactly aligned with estimates of future hydrogen costs. This deviation may be traced back to differences in the assumptions underlying the calculations. Nevertheless, it should be noted that the total estimate correctly represents hydrogen cost projections, as proved by the figure below, derived from the IEA report from which we derived part of our assumptions. Moreover, we should remind that this research does not aim to identify an optimal pricing procedure to support hydrogen integration, rather its objective is to provide a methodology on how to quantify the impacts of a contractual structure (where the contract price is given) on investment decisions. Thus, this approximation of contract prices adequately suits the research objective.

Note that Figure F.2. refers to hydrogen production costs in 2030. Several technology options are compared, but in our research we focus solely on electrolysis renewable (since electricity is provided by offshore wind parks in the north sea, connected to the electrolyser conversion park) and on natural gas with CCUS. As our assumptions are not completely aligned with the ones specified in the figure below, we compare the obtained values in Figure F.1. with the cost estimations derived in F.2. including the additional range resulting from combined sensitivity. By converting the upper bounds of ranges in Figure F.2. to €/ton, we obtain:

i. $4000 \frac{\$}{ton} * 0.85 \frac{EUR}{\$} = 3400 \frac{EUR}{Ton}$, only slightly higher than the estimate for green hydrogen costs in 2030 (Figure F.1.)

ii. $3300 \frac{\$}{ton} * 0.85 \frac{EUR}{\$} = 2800 \frac{EUR}{Ton}$, which corresponds to our estimate for blue hydrogen costs in 2030

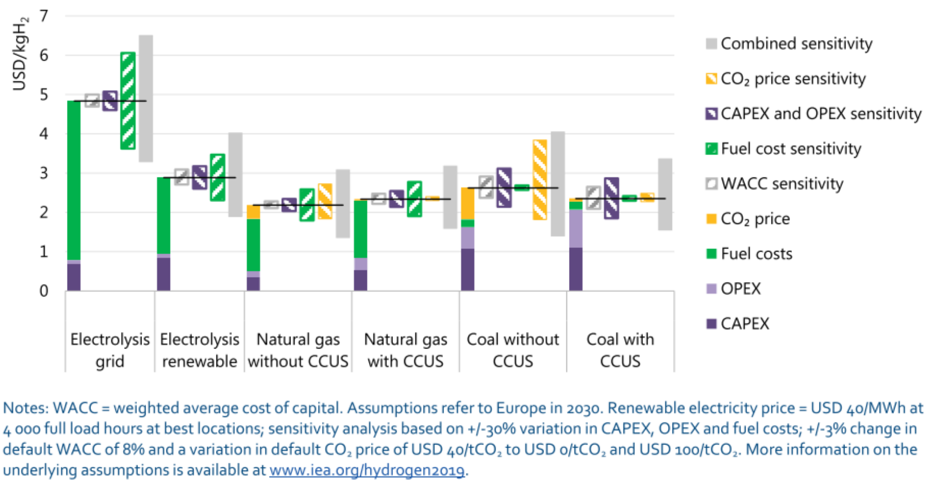


Figure F.2. Hydrogen production costs in 2030 for different technology options (International Energy Agency, 2019)

F.2. Sale-and-purchase model

Having validated the calculations for the derivation of contract price in the section above, we apply the same procedure to the sale-and-purchase agreement. The only difference lies in the lower impact of costs of raw materials on the contract price, to simulate lower price exposure (assumed 50%) from the side of the consumer. The following calculations are performed to derive the contract prices in Figure 42:

Table F.3. Calculations for blue hydrogen contract prices under S&P agreement

Price determinants	Formula	Today	2030	2040	2050	Unit
Blue Hydrogen						
CAPEX	$\frac{CAPEX\ [\frac{€}{MW}]^{(1)} * 33.33\ [\frac{MWh}{ton}]^{(2)}}{8760\ h}$	1636.1	1636.1	1636.1	1636.1	€/ton
OPEX	$3\%^{(3)} * CAPEX\ [\frac{€}{ton}]$	49.1	49.1	49.1	49.1	€/ton
Electricity price (grid)	$Electricity\ price\ [\frac{€}{MWh}]^{(4)} * 3.36\ [\frac{MWh}{ton\ H2}]^{(5)}$	*139.9*	*162.8*	*169.2*	*175.6*	€/ton
Natural gas price	$Natural\ gas\ price\ [\frac{€}{hm3}]^{(6)} * 3.69\ [\frac{hm3}{ton\ H2}]^{(5)}$	*405.0*	*454.9*	*499.4*	*543.7*	€/ton
Total fuel costs		544.9	617.8	668.6	719.4	€/ton
CO_2 price	$CO2\ price\ [\frac{€}{ton}]^{(6)} * 0.12\ [\frac{ton}{ton\ H2}]^{(5)}$	*1.73*	*1.80*	*1.94*	*2.07*	€/ton
CO_2 storage tariff	$CO2\ tariff\ [\frac{€}{ton}]^{(7)} * 0.88\ [\frac{ton}{ton\ H2}]^{(5)}$	*13.2*	*13.2*	*13.2*	*13.2*	€/ton
Total CO_2 price		14.9	15.0	15.1	15.3	€/ton

1) Data source: Table D.11. References for an ATR + CCS plant, all with high pressure CO2 capture (H-Vision Consortium, 2019)
2) Data source: Table E.3. Conversion table
3) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
4) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
5) Feedstock prices are multiplied by their respective flow rates, as reported in Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)
6) Data source: International Energy Agency. (2018). World Energy Outlook 2018.
7) Data source: H-Vision Consortium. (2019). *Annexes to the H-vision Main Report.*

Table F.2. Calculations for green hydrogen contract prices under S&P agreement

Price determinants	Formula	Today	2030	2040	2050	Unit
Green Hydrogen						
CAPEX	$\frac{CAPEX\ per\ capacity\ \left[\frac{\$}{kW}\right]^{(1)} * 10^3 \left[\frac{kW}{MW}\right] * Exchange\ rate\ \left[\frac{€}{\$}\right]^{(2)} * Discount\ factor^{(3)}}{8760\ \left[\frac{h}{y}\right] * Efficiency^{(1)} * \frac{1}{33.33\ \left[\frac{MWh}{tons}\right]}}$	2104.7	1518.3	1203.6	910.1	€/ton
OPEX	$1.5\%^{(1)} * CAPEX\ [\frac{€}{ton}]$	31.6	22.8	18.1	13.7	€/ton
Electricity price (RES)	$Electricity\ price \left[\frac{€}{MWh}\right]^{(4)} * 53.6\ [\frac{MWh}{ton\ H2}]^{(5)}$	1070.7	829.9	562.3	294.8	€/ton

1) Data source: Table D.13. Cost parameters for hydrogen production technologies (IEA, 2020)
2) Assumed 0.85 €/$
3) Assumed 10 years lifetime and discount rate of 8%
4) Data source: IEA. (2020). *IEA G20 Hydrogen report: Revised Assumptions. The Future of Hydrogen.*
5) Feedstock prices are multiplied by their respective flow rates, as reported in Table D.8. Input-output table for CO_2 footprint calculations (van Cappellen et al., 2018)

The profit element is derived by subtracting the contract price derived for the tolling model and the total cost components obtained in the tables above.

F.3. General considerations for bilateral contracts

Having calculated the contract prices under a tolling agreement based on Table F.1. and F.2., and under a sale-and-purchase agreement based on Table F.3. and F.4., contract prices are inserted in Linny-R as expressions in the hydrogen products' details. This ensures a realistic price representation, which varies with annual fluctuations in feedstock prices and with future cost reduction based on technological progress.

For the case of bilateral contracts, tailored prices for each bilateral exchange between producer and off-taker can be established. In this specific case, such price differentiations are due to the fact that cost components for hydrogen generation differ based on the actors involved.

For instance, blue hydrogen contract prices are differentiated based on the off-taker interested in hydrogen integration. In fact, blue hydrogen from the H-vision project is produced from refinery fuel gas, which supplements or completely substitutes natural gas as feedstock. This implies that blue hydrogen integrated at refineries will not make use of natural gas for production, thus this cost component is omitted from price calculations in bilateral contracts between Air Liquide and each of the refinery owners, Shell and BP. On the other hand, Uniper's power plant does not contribute to hydrogen generation through flue gases: thus, the amount of hydrogen that can be produced at a lower price, without using natural gas, is limited. As a result, Uniper's process will be supplied with hydrogen produced from refinery fuel gases only if Shell and BP do not need to integrate it in their process. Otherwise, Uniper can still make use of blue hydrogen, which however will be produced from natural gas, thus at a higher price. This is ensured by setting an appropriate if-condition in the price of blue hydrogen for Uniper.

Also green hydrogen contract prices differ based on the specific bilateral transaction. More specifically, each green hydrogen producer sets the output price to cover its costs and generate additional revenue. In Section 5.2.2.2, we have pointed out the main differences in electrolyser strategies by the three green hydrogen producers: specifically we noted that, due to the coal ban in 2030, Uniper plans to expand its electrolysis capacity earlier compared to other producers. The additional investment costs for the anticipated expansions are therefore reflected in contract prices and passed on to end-users, which will cover the additional CAPEX for Uniper. Such price with thus be differentiated from the one of green hydrogen by Shell or Nouryon.

F.4. Multilateral contracting: choice of pricing mechanism

In this research we derive multilateral contract prices by aggregating hydrogen prices calculated in the previous section, resulting in the standardized multilateral prices displayed in Figure 43 and 44. For these calculations, we rely on the pricing mechanism used for the tolling model, as this procedure is consistent with S&P Platts benchmark price assessments. In any case, as the contract prices under a tolling model or sale-and-purchase agreement are equal, the choice for a specific pricing procedure matters little to the determination of the multilateral contract price.

Several approaches to perform aggregations of bilateral contract prices and derive a standardized price of hydrogen are possible. We assume that a standardized price for every time-step can be derived by:

i. taking the lowest price among the prices calculated in F.1
ii. taking an average price among the prices calculated in F.1
iii. taking the highest price among the prices calculated in F.1

To derive a standardised price per commodity, this procedure is performed comparing prices of blue and green hydrogen separately (for every time-step):

i. $Min \{p_{GH1}; p_{GH2}; p_{GH3}...\}$; $Min \{ p_{BH1}; p_{BH2}; p_{BH3}...\}$
ii. $Avg \{p_{GH1}; p_{GH2}; p_{GH3}...\}$; $Avg \{ p_{BH1}; p_{BH2}; p_{BH3}...\}$
iii. $Max\{p_{GH1}; p_{GH2}; p_{GH3}...\}$; $Max \{ p_{BH1}; p_{BH2}; p_{BH3}...\}$

This allows to obtain different price estimates for each hydrogen commodity.

In the case of a single standardized price for hydrogen, this procedure is applied comparing all hydrogen prices together.

i. $Min \{p_{GH1}; p_{GH2}; p_{GH3;} p_{BH1}; p_{BH2}; p_{BH3}...\}$
ii. $Avg \{p_{GH1}; p_{GH2}; p_{GH3;} p_{BH1}; p_{BH2}; p_{BH3}...\}$
iii. $Max\ p_{GH1}; p_{GH2}; p_{GH3;} p_{BH1}; p_{BH2}; p_{BH3}...\}$

This allows to use a single price to market hydrogen as a single product.

In order to identify a suitable pricing mechanism, several model iterations are performed to assess the effects of pricing procedures (i), (ii) and (iii) on the cluster system across different scenarios (defined in Section 5.3.1). In this way, we aim to understand which pricing mechanism is more robust to price fluctuations and macro-economic changes. Such iterations were performed for both types of multilateral contracts. The results displayed in Figure F.3. and F.4. allow to assess the effects of each pricing mechanism on the total and individual cash flows, across different scenario situations.

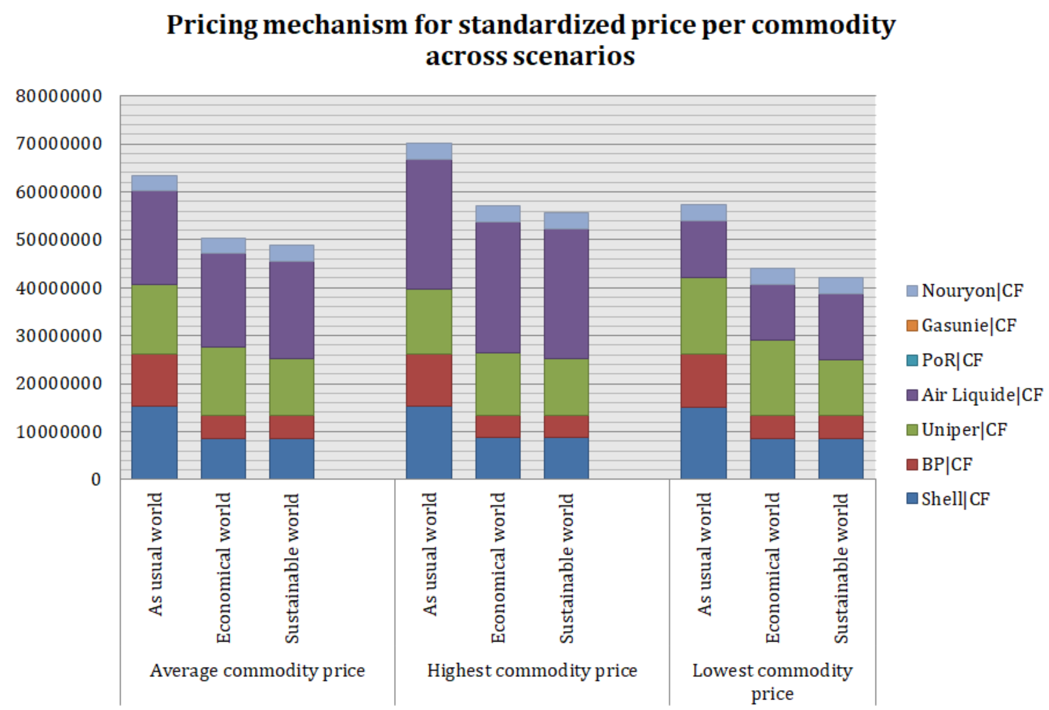


Figure F.3. Comparison of pricing mechanism for multilateral contract price per commodity across scenarios

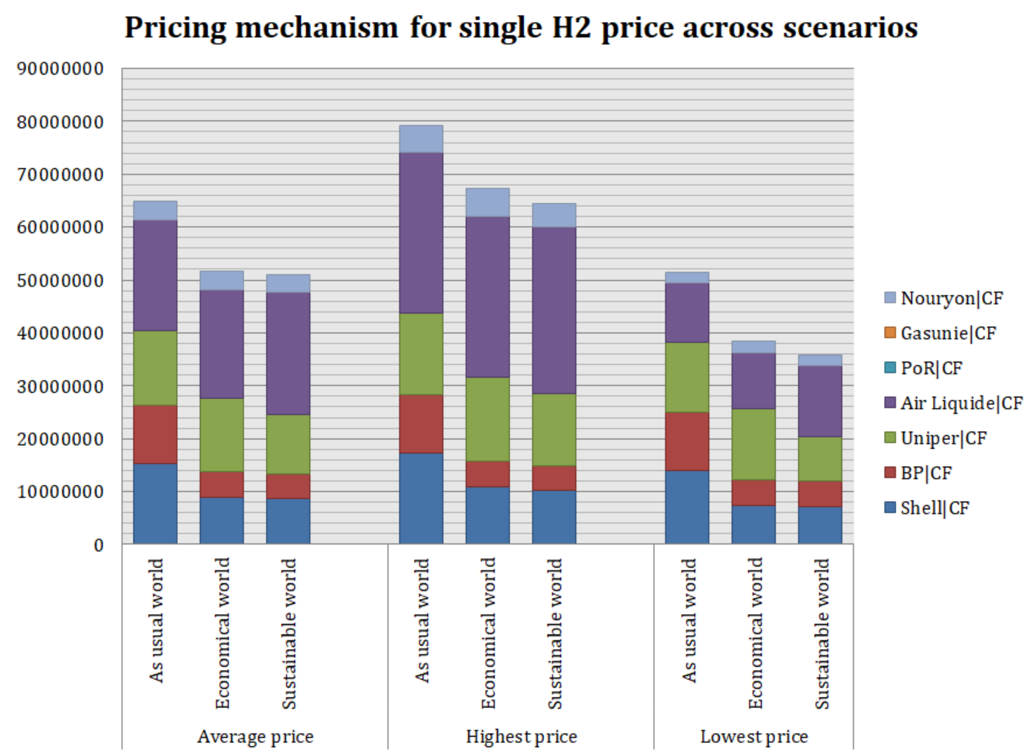


Figure F.4. Comparison of pricing mechanism for standardized multilateral contract price across scenarios

Comparing the variation in total and individual cash flows per type of pricing mechanism across scenarios, we conclude that using average prices in both cases results in the lowest variability, therefore in the most robust solution to establish a standardized multilateral price. This pricing mechanism is therefore adopted to derive contract prices displayed in Figure 43 and 44.