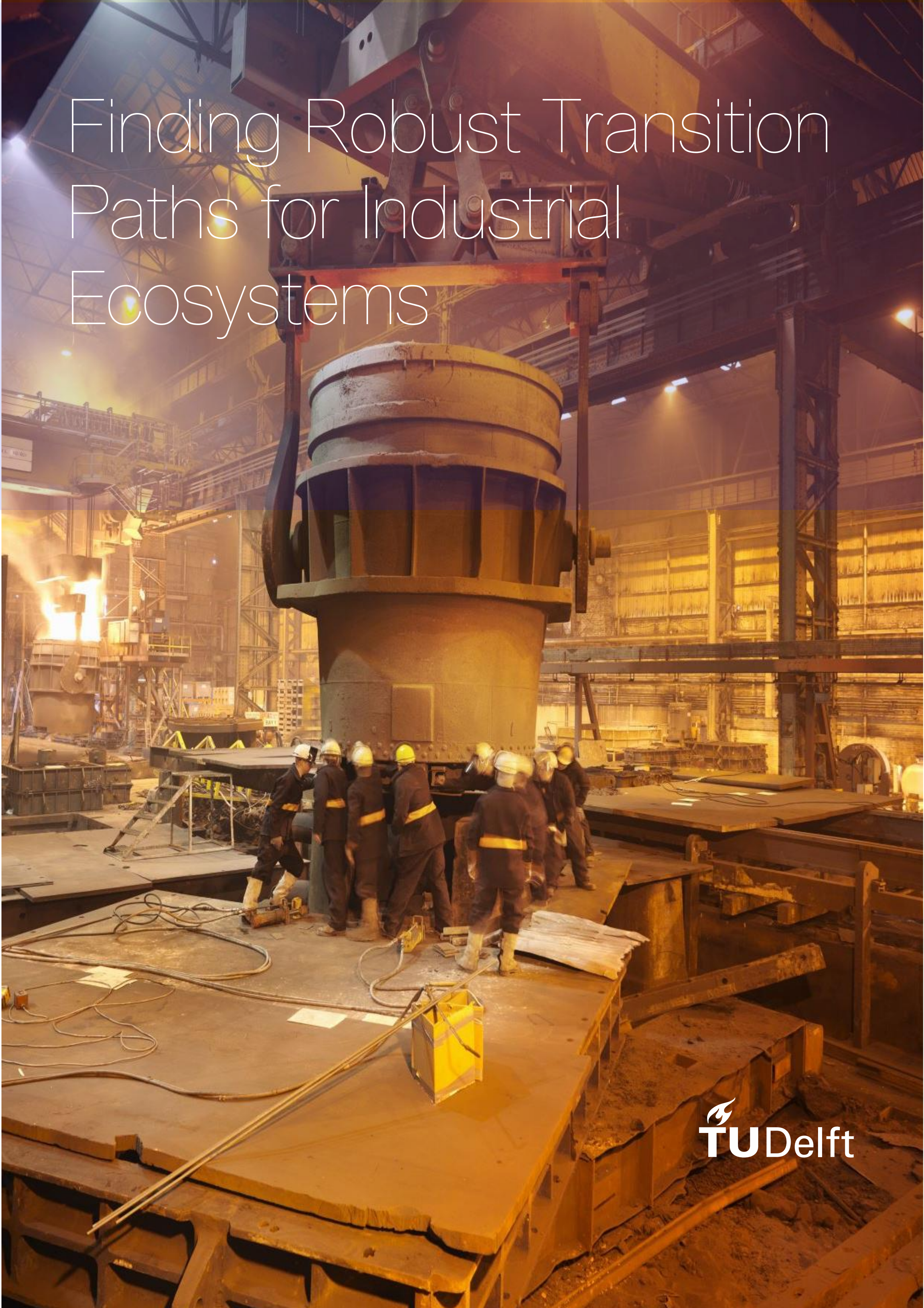
Finding Robust Transition Paths for Industrial Ecosystems



TU Delft

Finding Robust Transition Paths for Industrial Ecosystems

By

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“प्रत्येक प्रवास हा काहीतरी शिकवणारा असतो.” At the end of this long and arduous journey I feel exhilarated not only because I’m done but because I feel I’ve grown as an individual. There’s a long list of people I want to thank for being part of my journey. First and foremost, my parents Ranjeet and Sandhya for never quitting on me. My beautiful and talented sister Ashna, you are my pillar of strength. I know you’re always there. To my Chanda mama, I miss getting my hair combed by you. You are to me the most successful person because you have mastered the art of patience. To my beloved grandparents, Roza and Bani, I wish you were here to see me graduate and grow. Not a moment goes by when I don’t think of the talks we had on politics, physics and of course about Dee. Thank you for your wisdom. Thank you to Kumar and Raju mama for backing and encouraging me. To Simran for being there at every step. If I fall, I know you’ll throw me a rope. Thank you for never saying no. P.S. You 3000.

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“स्वतः चा विकास करा, लक्षात ठेवा, गती आणि वाढ हीच जिवंतपणाचे लक्षण आहेत.”

Varun Advani
The Hague, November 2020

Summary

In order to achieve the goal of sustainability, industries will have to make a transition to renewable energy and a more circular production. This requires substantial investments as well as constructive cooperation between the various companies in industrial clusters. The problem addressed in this thesis is to find ways of determining optimal investment paths for industrial clusters under specific constraints: the investments should contribute to sustainability (e.g., reduce emissions), provide a positive return for a cluster as a whole, and allow for a distribution of costs and benefits (e.g., through contracts) such that the companies that make the investment have strong incentives for cooperation.

The idea that underlies this thesis is to represent industrial clusters as networks of processes that are owned and operated by different companies, and interdependent via their input-output flows. Such representation should then facilitate analysis from an industrial ecosystem perspective, and identification of potential investment options that would improve the cluster's sustainability. From a game theory perspective, these investment options can then be seen as potential moves, and the companies as players. Assuming a time horizon (e.g., somewhere between 10 and 40 years), any combination of investments in that period constitutes a strategy, while for each company the difference in cumulative cash flow for that company with/without these investments constitutes the players' payoffs. Analysis of such a multi-company investment game will reveal rational strategies.

We have elaborated and tested this idea by using the Linny-R modelling language and its associated MILP optimisation tool that is being developed at TU Delft first to represent and analyse a variety of simple process configurations with only one or two investment options. Conducting this first series of small-scale simulation experiments, and verifying their outcomes has demonstrated the feasibility of our approach. Subsequently, we have applied the same approach to a realistic, albeit simplified and stylised, industrial cluster that comprises three companies. After identifying a set of potential investment options, we have used the resulting Linny-R model to conduct a second series of experiments to simulate and analyse solitary investment strategies per company, a cluster-wide cooperative strategy, as well as competitive strategies with various contractual arrangements.

The results of this study show that we can indeed use Linny-R as a modelling language and simulation tool to represent and analyse investment decisions as multi-actor games, which then allow us to infer and evaluate cooperative as well as competitive investment strategies.

This study has several limitations. We did not investigate the scalability of the method. We experimented with a relatively small and simplified cluster; upscaling to a cluster with 10 or 100 times more processes could become computationally infeasible. Another limitation is that we did not test in practice whether models in the Linny-R notation will indeed effectively support communication and negotiation between companies. Thirdly, the set of categories of investment options that we have identified is not exhaustive. Our recommendations for future research hence are to explore the computational limits using a state-of-the-art commercial solver, and to conduct real-world case studies, meanwhile extending and refining the categories of investment options that can be instrumental in furthering the transition towards more sustainable industrial clusters.

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1 Introduction

In this first chapter we discuss the energy transition, more specifically the Dutch case, and highlight the difficulties associated with an energy transition. We then conceptualise the energy transition by applying the Multi-Level Perspective (MLP) framework for analysing socio-technical transitions to sustainability, and argue that there is a natural 'inertia' in energy transitions. In doing so, we define what is required to overcome this inertia. This defines the focus of this thesis. Finally, we outline the structure of the thesis document.

1.1 The Dutch energy transition

Greenhouse gas emissions are caused by human activity all around the world, and climate change is in part a result of these emissions. (Hof et al., 2012). The effects of climate change are unquestionable, and the rate at which it is taking place is increasing worldwide. This has put society as a whole under pressure (UNEP, 2018). The Paris convention in 2015 marked the beginning of taggable action to reduce greenhouse gas emissions. A total of 196 countries pledged to attain the goal of limiting the global average increase in temperature to a value below 2 °C.

The Netherlands has vowed to reduce its emissions by 50% until 2030 according to the Paris agreement signed in 2015. This roughly translates to a national emission reduction of 48.7 megatons of CO_2-equivalents We know that the industrial sector ranks third in terms of amount of emissions, after the agricultural and transport sectors. The focus of this thesis is on the industrial sector, which should contribute to 30% emission reduction out of the 50% pledged by the Netherlands. These changes are not instantaneous, not a 'technical fix' that can be applied. Instead, a combination of economic, political, institutional and socio-cultural changes will be required (Berkhout et al. 2009). For the Netherlands, this implies that the energy system in the Netherlands requires rather drastic changes (Ros & Schure, 2016). Such drastic changes can be achieved through a process of gradual change guided by long-term policy perspectives that are grounded in present developments (Faber et al., 2016).

This gradual change in an energy system is termed as an 'energy transition' in climate policy literature (Verbong et al., 2012). The term refers to a pathway towards the transformation of the global energy sector from mainly fossil based to zero-carbon sources and/or CO_2 storage. Transitions to renewable sources are at the centre of policies in many countries. The spotlight on renewables has certainly grown in the past decades. Issues of acceptability and viability for options such as nuclear power and carbon capture and storage have only added to the focus on renewables (REN21, 2010). In spite of the promising potential of renewable energy sources and advanced technologies to utilise them, transitions towards renewables have been slow.

In the Netherlands, the industrial sector is divided into a few clusters. Each cluster contains multiple companies producing a variety of products. Some of these clusters are the Smart Delta Resources (SDR) in the province of Zeeland, the Rotterdam/Moerdijk cluster, Chemport Delfzijl, Chemelot and the Amsterdam cluster. In order to make a significant impact through this thesis, we focus on energy transitions in this type of industrial cluster.

1.2 Conceptualising the energy transition

Let us consider the example of the Rotterdam cluster. We recognise that there is a need for an energy transition in this cluster. The first question that arises from the information presented above is: Why, in spite of the Paris agreement, are the emissions not reduced to the desired amount? In order to answer this question, we refer to the Multi-Level Perspective framework for transitions proposed by Geels and Kemp (2000).

According to Geels and Kemp (2000) there are multiple layers that play a vital role in the transition of a system. This study was on technological transitions in the context of environmental policy plans, and it conceptualises transitions as evolutionary processes that improve with constant reconfiguration. According to this study, the energy transition is viewed as "a socio-technical development with processes on three layers; the landscape level (macro), the regime level (meso) and the niche level (micro)" (Geels, 2002).

The macro-level – also called 'landscape' – states that a transition needs fundamental changes in social thinking, and having common goals and concerns. For an energy transition, this implies an increase in awareness towards climate change and the detrimental effects to the environment (Ros, 2015). An example of this aspect is the positive change in perception of the public towards the Paris Agreement.

The meso-level – also referred to as the 'patchwork of regimes' – is viewed as a relatively stable social network. This is a stable technical system that interacts with different entities within the system. This level is mainly driven by two aspects: companies that make decisions, and consumers that drive change through their personal behaviour and preferences (Geels, 2002). In the context of the energy transition, different stakeholders interact with each other and with consumers to drive change. Taking the previous example of the Dutch industrial sector, these stakeholders are companies producing goods and services, electricity providers, agencies such as the Port Authority of Rotterdam that monitor companies, and consumers that (indirectly) use energy by consuming goods and services produced by these companies (Ros et al., 2016).

The micro-level – also referred to as 'niches' – is where new innovations and ideas are conceived and developed on a relatively small scale. In the context of the energy transition, these niches may be research organisations and incubators working at the grassroot level. According to Geels (2002), it is at this level that the cost of new technology is found to be extremely high. This increases the barriers to innovation, and also prevents the trickle effect from the micro- to the meso-level.

This trickle effect is critical for the transition process as envisioned by Geels (2002). One of the features of the multilevel perspective is that the success or failure of a new technology is not just driven by the process within the niche but also influenced by the regime and landscape levels. "It is the alignment of developments (successful processes within the niche reinforced by changes at regime level and at the level of the sociotechnical landscape) which determine if a regime shift will occur" (Geels et al., 2001).

1.3 Understanding 'inertia' in transitions

According to Geels (2002), a transition to a new and/or existing (not currently in use) technology occurs when there are interactions between the macro-, meso- and micro-levels. A transition in the socio-technical regime can be set into motion when there is a need for change at the macro-level (landscape signals). As a result, multiple path-breaking innovations occur in the niche level as shown in Figure 1 by the arrows. These arrow 'swarm' to indicate that multiple innovation options will be needed, because some will prove unsuccessful. The innovations that are successful in niches at the micro-level break out and interact with the meso- and macro-levels. This process is termed as a 'window of opportunity' by Geels (2002). These windows are created in the micro-level, and together with interactions with events in the macro-level they drive change in the meso-level (socio-technical).

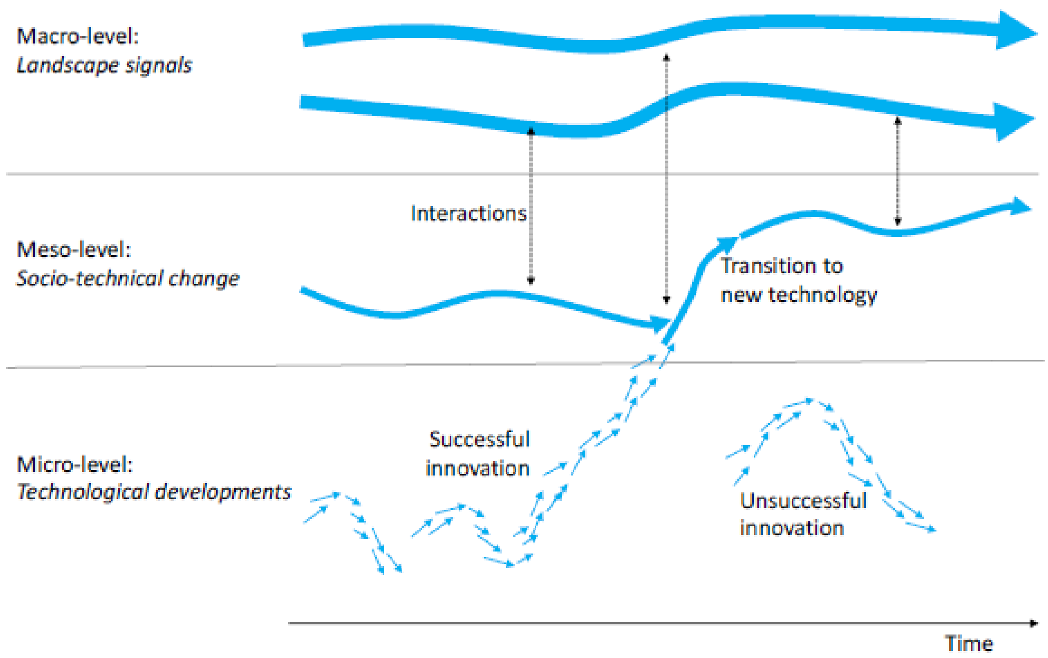

Figure 1. Dynamics in transition theory (adapted from Geels et al., 2002)

When we look at industrial clusters, we see that the emissions are not decreasing at an acceptable rate (UNEP,2018). This can be explained using the perspective of landscapes, regimes and niches established by Geels. According to Geels, a transition can occur when there is a successful alignment of radical changes at the nice and the landscape levels. At the landscape and niche levels there have been no major changes because of the inertia that is present at these levels. For example, at a landscape level, as long as the price of CO_2 remains constant due to weak government policy, companies will continue to produce high CO_2 emissions.

The reason for this inertia at the niche level is the long term investments made by companies. Typically, companies invest in assets that have a long economic life span. In industrial clusters there are hundreds of such assets with a high investment cost. When a company decides to invest in a new state-of-the-art technology, it does so with a view to use that technology for a long period of time, say 20-30 years. Since this investment is so expensive, it prohibits the company from investing in new assets during the 50 year period mentioned above.

Another important aspect is the interdependencies of companies within the industrial cluster. Continuing with the same example, if one company that is part of a cluster invests in a new asset, this could create a problem for another company that is dependent on the first company. This dependency can be on utilities such as steam, electricity, but also the availability of raw materials. The decision of one company to invest in a new asset might potentially affect multiple companies, causing a domino effect in the cluster. Companies hence seek to stabilise their environment by making long-term contractual agreements. Thus, it is not only the long term lifetime of assets that is responsible for the inertia, but also long-term agreements between companies in the cluster.

In sum, we have seen that transitions in industrial clusters can occur through a combination of government policy (landscape changes) and investment in technology (niche levels). In this thesis, will not consider what government policies could be effective, nor do we aim at identifying and suggesting promising novel technologies to companies in industrial clusters. Instead, we focus on the *decisions* of companies to invest in new and/or existing technologies, aiming to support companies within industrial clusters in making informed decisions about investment in new assets. To address the problem of inertia, we specifically consider investments that would be favourable for the companies to make, but do not take place in reality.

Assuming that every company aims to maximise its profit, the only way transitions can occur is by developing what we will call 'transition enabling win-win situations': arrangements of investments and contractual agreements on financial compensation between companies that make the investments favourable for all companies involved. Such situations require that the investments should (1) contribute to sustainability (e.g., reduce emissions), (2) provide a positive return for the cluster of companies as a whole, and (3) allow for a distribution of costs and benefits (e.g., through contracts) such that the companies that make the investment have strong incentives for cooperation.

The specific knowledge gap that we address in this thesis is how such transition enabling win-win situations can be identified for a particular industrial cluster.

1.4 Structure of this thesis

We will explore this gap in Chapter 2, where we review literature on industrial ecosystems and game theory to further conceptualise our research. We also select Linny-R as the modelling language and tool for representing industrial clusters and evaluating potential investments in such clusters. This leads to a set of research questions and a research approach that may produce plausible answers.

In Chapter 3 we focus on using Linny-R to represent and analyse industrial clusters as multi-player games. Building on the concepts we borrow from industrial ecology, we start with representations of what we will call elementary 'building blocks', typically a simple production chain and a single investment that will improve its performance. We demonstrate the feasibility of our approach by developing a generic building block that involves potential investments by two companies, and analysing it from both single-actor and multi-actor perspective. We then develop other types of building block.

In Chapter 4 we use Linny-R to model and analyse moderately complex cluster of three companies, inspired on a real life case. This model combines several of the building blocks discussed in Chapter 3, and allows to investigate the consequences of interdependencies and financial compensations between companies in more depth. In this way, Chapter 4 provides a genuine ‘proof of concept’ for our approach to developing ‘transition enabling win-win situations’.

In Chapter 5 we discuss the implications of the research in terms of its relevance and limitations. In Chapter 6 we conclude by revisiting the research questions, and providing some recommendations for future research.

2 Conceptualising the Research

In this chapter we first use literature on Industrial Ecology and Industrial Ecosystems to elaborate what types of change in an industrial cluster will effectively contribute to the energy transition, and to what extent this may cause disruption within a cluster. We then review game theory to see how this can support companies in making joint win-win investment decisions. Based on these ideas, we review methods that could be suitable for modelling investment decision making in industrial clusters, and argue why we opt for using Linny-R. This then enables us to formulate the research question and sub-questions for this thesis, and outline our research approach.

2.1 Industrial ecology and industrial ecosystems

Industrial ecology is a concept that functions under the field of sustainable development (Frosch, 1989) (Graedel, 1995) (Korhonen, 2004). The systems that are studied in industrial ecology are known as *industrial ecosystems*. These systems include system actors, such as companies and organisations. There are material and energy flows that link these actors with each other and with the economic, social, and ecological systems (Korhonen, 2005).

The importance of concepts such as industrial ecology and industrial ecosystems is growing in the fields of economics, policy, and management (Graedel, 1995). Historically, industrial systems operated with linear flows and unsustainable practices. Over time, there has been a shift to recycling and cascading material and energy flows. Understanding this evolution of systems from unsustainable to sustainable operations is crucial for environmental performance, future policy, and management (Korhonen, 2001, 2005). There are four basic principles of development of industrial ecosystems: *roundput*, *diversity*, *locality* and *gradual change*.

The concept of *roundput* in ecosystems can be understood from the example of the carbon-oxygen cycle. Plants consume carbon dioxide, and produce carbohydrates and oxygen as a waste product. Animals on the other hand, consume carbohydrates and oxygen, and produce carbon dioxide as a waste product. In this ecosystem, the waste product of plants is the ‘food’ or intake for animals, and vice versa. In terms of industrial ecosystems this can be understood as the recycling of matter, and making more efficient use of energy through sharing between the actors in a system. For industrial ecosystems, achieving roundput could mean that a side product that was previously not used (and hence emitted from the system) is now being recycled and used within the system as an input for another process.

For example, consider a company X that has a process that outputs a primary product and a waste gas that it currently torches (with associated emissions). Company X would then achieve roundput if it would invest in a CHP (producing heat and electricity from natural gas) that will accept waste gas from the primary process of X as feedstock. This investment would be economically interesting only if (1) using this waste gas as an input for the CHP process does not disrupt the flows of the primary process, while (2) the CHP produces heat and electricity so efficiently that company X can recover the investment costs by saving on energy imported from the grid and on CO_2 emission rights.

Ecosystems stand a better chance of survival if they have more *diversity*. In an ecosystem, diversity means the variety and number of species, organisms, and interdependencies between organisms. A variety of species in an ecosystem would offer flexibility and adaptability when exogenous conditions change so rapidly and radically that particular species cannot survive. The extent to which this extinction will cascade through the ecosystem is a function of the system's diversity. For example, when species X takes a unique position in the food chain, then all species who depend on X for food will perish as well, and this effect can cascade. But if the ecosystem offers alternative species to feed on that are not affected by the same exogenous change, then the extinction of X will not cascade. Thus, diversity can be viewed as conditions that favour the survival of ecosystems.

In the context of industrial clusters diversity can be understood in terms of technologies, companies, material, and energy flows. If there are changes in conditions, then the clusters possessing a higher variety of options have a higher chance of survival. Consider the same example as in the previous case, but now company X is situated in a cluster with a variety of other companies. In such a cluster it is probable that some company Y already has a CHP that can process waste gas. In that case, company X could transport its waste gas to the CHP of company Y rather than investing in its own CHP, and thus solve its problem at a relatively lower cost.

Locality refers to the idea that natural ecosystems need to adapt to their local natural limiting factors and environmental conditions. Taking a lake as example, the organisms populating this natural ecosystem are considered as local, but the water on which the ecosystem depends through rainfall or from a river is *not* local since it has to be 'imported' or received through an external source. If the rainfall stops or the river dries up, the ecosystem of the lake cannot survive. If resources on which the ecosystem depends have to be imported, or if these resources are lost through exports, then the ecosystem is less 'local' and so will be the chances of its survival. Being vast enough to affect the local climate, a sustainable rainforest ecosystem will generate its own rainfall. Thus, the water cycle of such a forest is closed in the same location. This illustrates that the idea of locality is tightly linked to roundput: complete roundput implies complete locality.

In industrial ecosystems, the term locality refers to the local nature of the industrial activity. Continuing with the same example that we used in the preceding paragraphs, consider that there would be many companies that produce waste gas on a large scale. As these companies produce more waste gas, their dependency on the imports of natural gas would reduce. This would increase the locality in the system. Eventually these companies would produce waste gas to the extent of becoming potentially independent of the natural gas that they required as input. Reducing the greenhouse gases emissions by switching to electricity as a source of energy could be another example of the application of locality in industrial clusters. The reduction of imports and exports would reduce the overall emissions in the cluster. More generally, industrial ecosystems can achieve locality by substituting imported resources with local side streams, waste material, and local energy sources.

Gradual change refers to the idea that the survival of an ecosystem depends on the flow of resources and the evolution of functions in accordance with the renewal rate of the ecosystem. In a natural ecosystem, the renewal rate of the ecosystem depends on the rate of reproduction of the organisms that populate it. If the rate of change is so high that the adaptation that is possible through reproduction cannot keep up with the changing conditions, then the ecosystem cannot thrive.

In the context of industrial ecosystems, the renewal rate can be interpreted in two ways. For a batch process, the production rate can be interpreted as renewal rate. For a batch process, a low production rate implies a long cycle time, which means that batches will be exposed longer to potential disruptions, while the loss of a batch that takes 2 months to produce will typically be felt stronger than the loss of a batch that can be produced overnight. The second interpretation of renewal rate in an industrial ecosystem relates to the economic life cycle of the assets. In this interpretation, the rate of change in an industrial ecosystem is inversely proportional to the economic lifetime of the assets. For example, if the assets of company X have an economic lifetime of 10 years while those of company Y last for 40 years, then company X is more flexible and can be more responsive, and will hence be less vulnerable to changes in the environment or the system.

If we relate our interpretation of the four ecosystem principles established by Korhonen (2001, 2005) to the Multi-Level Perspective framework proposed by Geels et al. (2002), we see that the *roundput* principle is most applicable at the micro (niche) level. It is at that level that technological innovations or novel ways of using existing technologies emerge that create new recycling opportunities for industrial ecosystems.

The *diversity* principle likewise applies to the micro-level, not only because when diversity is interpreted as ‘more investment options for an investor to choose from’, but also – and more importantly – because successful innovations often comprise a combination of technologies developed by a coalition of niche companies. The higher the number and variety of such companies, the more likely that synergetic combinations will be discovered.

The *locality* principle applies to both micro and meso (regime) level. At the micro-level, it corresponds to the idea that niche innovations occur in small groups that include technology developers, users as well as venture capitalists, and hence can operate as relatively independent niche players. At the meso-level, locality then relates more to the idea that industrial clusters typically form around a kernel (e.g., a refinery; a blast furnace) that transforms high volumes of raw materials (crude oil; ore, coke and limestone) into intermediate products (various oil fractions; iron) that are then processed by more specialised companies. The locality principle entails that these ‘downstream’ companies will attract new companies that process their products locally, provided that savings on transport and conditioning are superior to investment costs.

The principle of *gradual change* would then be most applicable to the macro (landscape) level and its interactions with the meso-level. According to this principle, policies should not change faster than that industries at the meso-level can adjust, as the consequence could be a disruptive collapse of the regime. But policies should change fast enough to facilitate ‘windows of opportunity’ that permit mature niche innovations to become part of the ‘patchwork of regimes’, thus smoothing the transitions in industrial ecosystems.

The combination of ecosystem principles and the Multi-Level Perspective as discussed above provides inspiration for identifying potential investments in an industrial cluster. At the micro-level, the principles of *roundput* and *locality* inspire a search for technologies (existing or novel) that can make (better) use of side products, while the *diversity* principle cautions us that investments that favour one particular subcluster C may make the cluster as a whole more vulnerable to changes in the demand for the products of C. Moreover, achieving *roundput* for some side product P within subcluster C may be disruptive for companies that use P as input (as until now it was superfluous and hence cheap).

This example illustrates that increasing locality in a subcluster (via a micro-level innovation) may put established companies elsewhere in the larger cluster (meso-level) out of business, thereby decreasing the overall diversity of the cluster. Note that such disruptive changes may also be caused by new companies entering the cluster, which could at the same time increase the diversity. This cautions us to consider to what extent *roundput* investments and investments by new entrants that in themselves appear to contribute to sustainability, may cause disruptions elsewhere that decrease sustainability. The *gradual change* principle cautions us to also consider the time dimension, and assess the (remaining) life time of assets.

Putting ecosystem principles such as roundput, diversity, locality and gradual change into practice within an industrial cluster will typically require coordination between companies to achieve win-win situations for all these companies. This coordination aspect remains largely implicit in the Multi-Level Perspective framework. Dubina & Carayannis (2015) argue that game theory helps to gain insight in the innovative entrepreneurial behaviour at the micro-level, and how this interacts with policies at the macro-level. In the next section, we therefore look how the basics of game theory can be applied to investment decisions in industrial clusters.

2.2 Game theory

Game theory is defined as a discipline that aims to model situations in which decision-makers have to make decisions from a pool of possibly conflicting outcomes (Fudenberg & Tirole, 1991, Gibbons, 1992). It conceptualises multi-actor decision situations in terms of *players*, *moves*, *strategies*, and *payoffs*. In the context of industrial ecosystems, the companies in an industrial cluster are the players, the investment decisions that these companies can make are the moves, any particular combination of such investments (possibly at different moments in time) is a strategy, and the additional profit (or loss) that a company would make after the investments comprised by a strategy is the payoff of that strategy for that company. Note that by choosing for return on investment as the payoff variable, we assume that companies decide on the basis of economic rationality. This means that if we also want to take into account other dimensions of sustainability, these must be monetarised.

Game theory differentiates between *cooperative* games and *competitive* games. Cooperative games imply that all individual players choose their moves such that the resulting strategy (i.e., combination of these moves) generates the highest total payoff (i.e., the sum of the payoffs for the individual players). Although – still assuming economic rationality – this would be the rational strategy for the cluster as a whole, it need not be a win-win situation for all players. It may very well be that the strategy works out so well for some players that their payoffs amply compensate for the negative payoffs of some of the other players.

Cooperative games presume collective decision-making. The optimal strategy for a cooperative game will be adopted in a real-world setting only if the companies are willing to share information and negotiate. If the companies involved can reach agreement not only on their individual moves, but also on how the overall profit of the cluster will be distributed, and then consolidate their agreements in contracts, then the cooperative strategy has indeed become a win-win situation.

Without cooperation, companies are assumed to act solely on the basis of their own profit, which means that they may not always do what is best for the cluster. Such settings can be represented as a competitive game: all players will maximise their individual payoff, anticipating that the other players will do likewise. Game theory then offers various algorithms, e.g., iterated elimination of (strictly) dominated strategies, that will predict which individual strategies are rational, and how these strategies will then play out. Depending on the specific setting, analysis can identify Nash equilibria: strategies that allow none of the players to gain additional payoff by any unilateral move. The typical example is the prisoner’s dilemma: a setting in which two rational players both miss out on the optimal collaborative outcome because they have no means to build trust.

Game theory would seem to fit our purpose of representing investment decision making of companies in an industrial cluster such that we can provide insight in their options, the existence of potential of win-win situations, and the need for collaboration to achieve them. However, the typical representations used in game theory (payoff matrices as normal form, and trees as extensive form) rapidly become so large as to be unsuited for human communication. As an example, consider the three-player game in Figure 2, where each player (X in red, Y in blue, Z in black) can choose from three moves. Each strategy then would be a combination of three moves that would result in a particular payoff for each player as indicated by the colours e.g., strategy X2Y3Z1 would result in payoffs 7 for X, 3 for Y, and 9 for Z.

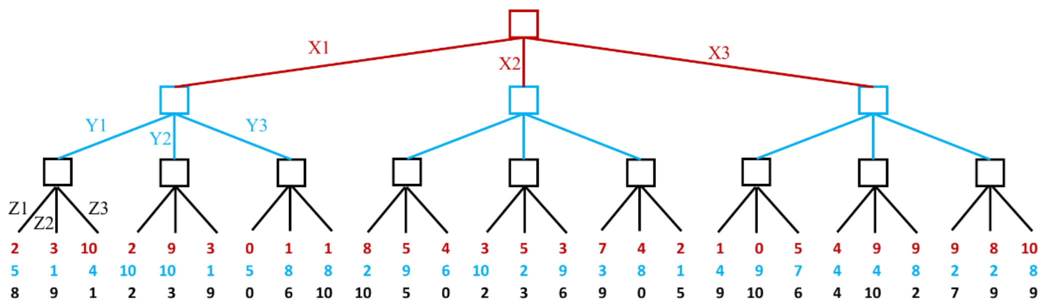

Figure 2. A 3-player game in extensive form with players X, Y and Z each having 3 moves

The example shows that for these small numbers of companies and options, the cooperative strategy can fairly easily be identified as X3Y3Z3, having the highest total payoff of 27. But inferring the outcome of this game if it is competitive is *not* easy. For example, the blue payoffs show that company Y would be better off with strategies like X1Y2Z1 (payoff 10 for Y), while company Z would gain more with strategies like X1Y3Z3. If companies Y and Z would form a coalition, they would prefer strategy X3Y1Z2, as their individual payoffs would both be superior compared to the collaborative strategy. So if the game were sequential and X would have to move first, investing in X3 would expose X to the risk that Y and Z then play sub-strategy Y1Z2, resulting in payoff 0 for X. If X does not trust Y and Z, it could opt to maximise its minimum payoff by playing X2, as then in the worst case it would still gain 2, and more likely 3 because Y and Z (if still cooperating) then would prefer Y2Z3.

So game theory puzzles become complicated even for small numbers of players and options. But that can be solved by means of computational tools (Bošanský et al., 2016). What is more important is that the representation of investment decisions as games must be comprehensible, and easy to understand by decision-makers. When applied to investment decisions in industrial ecosystems, game trees can indeed visualise the investment options, but then the same option typically occurs many times in the graphical tree representation (see Figure 2). And even when the less redundant normal form is used, the payoff matrices do not make transparent how the payoffs for the respective companies are generated. Neither representation provides any (visual) representation of the industrial ecosystem, in particular the interdependencies between companies.

To achieve our goal of supporting decision makers to find and appraise what at the end of §1.3 we have termed 'transition enabling win-win situations', we need methods and tools that can represent industrial ecosystems in a communicative manner, and afford analysis of investments by multiple companies as strategic games. We found this combination in the modelling method and supporting tool called Linny-R. In the next section, we will motivate why for our purpose Linny-R is superior to other tools.

2.3 Review of existing modelling techniques

To permit effective communication with companies in industrial clusters about their production processes and assets as industrial ecosystems, we will have to represent the interdependencies between companies, and also in more detail between specific production processes, as quantified input-output flows. Quantification of processes and is needed to infer, for example, energy use, emissions, and other performance indicators. Then from this representation, it must be possible to infer the payoffs for each company on investment strategies. This means that the representation must include financial information (e.g., annual cashflows) per company both before and after investments. Ideally, it should then also afford overall optimisation of the cluster (being the cooperative strategy) as well as optimisation for one specific company, or a particular coalition of companies.

In search for a such an executable specification language, we have compared three modelling techniques and associated software tools: Agent Based Modelling (ABM) using *Netlogo*, System Dynamics (SD) modelling using *VenSim*, and Mixed Integer Linear Programming (MILP) using *Linny-R*. We selected these particular modelling techniques based on a review of modelling approaches and tools that have been used by other researchers to study industrial ecosystems (Boix et al., 2014; Demartini et al., 2016), and also on our own first-hand experience in applying these methods. It should be noted that in our brief review of the advantages and disadvantages of each of these modelling methods, we refer only to the specific software tools that we have used ourselves. This does not indicate that this tool is the only one available.

Judging by the number of studies we found in the Industrial Ecosystems literature, ABM, appears to be the mainstream modelling tool. Studies related to, for example, sustainability (Zheng & Jia, 2017), systems evolution (Bichraoui, 2013; Nikolic, 2010), economic theory (Fraccascia, 2020) all make use of this type of model. As ABM are agent-based, capturing actor perspectives is intrinsic to this method. The inherent object orientation of ABM platforms would also enable modellers to represent an industrial cluster as aggregations of subclusters that would again be aggregations of specific processes and assets.

However, being in essence process *simulation* software, ABM modelling platforms like *NetLogo* lack the ability to perform model optimisation. Although parameter values that result in (near) optimal system performance (on some indicator) can still be inferred using heuristics (Raimbault et al., 2020) or a generate-and-test approach similar to Exploratory Modelling and Analysis (EMA, cf. Kwakkel et al., 2017b), this would be very demanding in terms of computational resources. Additionally, as ABM models are specified in programming code, rather than some graphical specification language, it does not meet our requirement that models should be easy to communicate and validate with decision makers.

Several studies into industrial symbiosis represent industrial ecosystems using System Dynamics models. A common trait appears to be that the industrial ecosystem is represented first using a process flow chart, while the dynamic evolution of the ecosystem is represented using SD models (causal loop diagrams and stock-flow diagrams). The study by Cui et al. (2018) is a typical example.

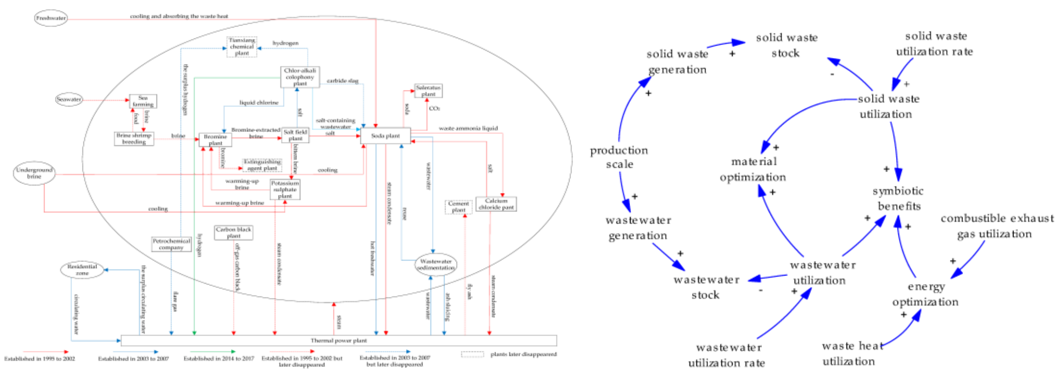

Figure 3. Process flow chart and causal loop diagram as used by Cui et al. (2018)

As can be seen in Figure 3, these types of models, based on *de facto* standards used in both industry and academia, would fulfil the requirements of being fit for communication. However, only the SD models are executable; there is no direct computational link between the process flow chart (where new investments as well as decommissioning of assets over time are indicated using colours) and the SD model. A tool like *VenSim* would allow computation of the symbiotic benefits due to, e.g., achieving roundput, but only if parameters such as reuse of side streams like brine, flare gas and fly ash are entered as input parameters.
Figure 4 shows that in this particular study, the stock flow diagram in VenSim is used to visualise how the model calculates the symbiotic benefits, rather than that it visualises the actual production processes in the cluster.

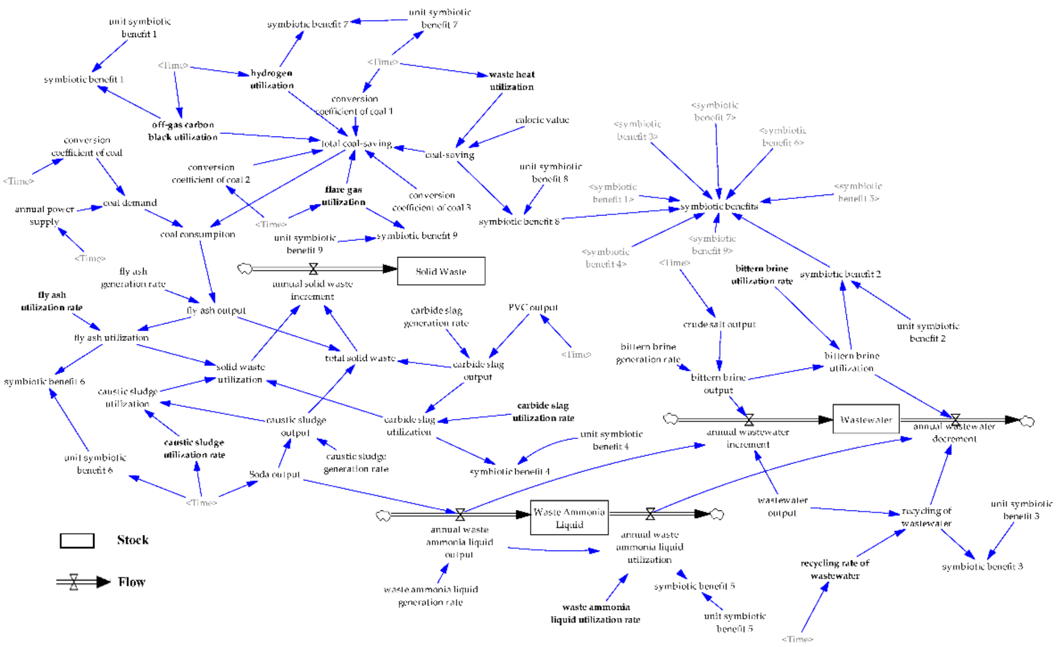

Figure 4. Stock-flow diagram as used by Cui et al. (2018)

As SD models typically represent continuous flows, it would certainly be possible to represent the actual production processes depicted in the left diagram in Figure 3 as stocks and flows. However, it would then be the flows (i.e., the double arrows) in the diagram that depict the plants that in a process flow chart are typically represented as boxes.

Moreover, SD software such as *VenSim* itself does not perform optimisation. Although, similar to ABM, optimisation using heuristic strategies or a generate-and-test approach would in theory be possible, it makes SD tools less suitable for our purpose.

We found several examples of the use of MILP models to simulate and/or optimise industrial ecosystems. Most appeared to be based on ‘hard coded’ models in the form of mathematical equations (Theo et al., 2016; Lee & Lin, 2019), but some used intermediary tools (Karlsson, 2011). Of these tools, Linny-R provides the most generic graphical specification language, and also allows layered modelling (i.e., clusters within clusters within clusters). It is visually appealing, making a clear distinction between processes and product flows and stocks. In addition, it also allows to optimise cash flows for selected companies, while allowing for commitment of only a selection of assets. Being based on MILP, Linny-R is inherently fit for optimisation, albeit that when the number of binary variables in a model increases, solver times will become unfeasibly long.

The advantages and disadvantages of each of these modelling methods and tools are summarised in Table 1. Since Linny-R fits all of the requirements described in the previous section, it is selected as the most appropriate tool for the study that we will elaborate in the next section.

Table 1. Assessment of Modelling methods and tools

Modelling method (Tool)	Advantage(s)	Disadvantage(s)
Agent Based Modelling (NetLogo)	- Allows layered/ hierarchical modelling. - Intrinsically capable of analysing multi-actor perspectives.	- Not adequate for visual representation/diagrams. - Essentially simulation software and not optimisation.
System Dynamics (Vensim)	- Highly suitable for modelling flows of a system. - Captures the dynamic nature of problems. - Allows layered/ hierarchical modelling.	- Does not perform optimisation
Mixed Integer Linear Programming (Linny-R)	- Allows layered/ hierarchical modelling. - Linny-R provides visually appealing process diagrams. - Highly suitable for optimizing processes. - Suitable for modelling flows of a system, including cash flows. - Intrinsically capable of analysing multi-actor perspectives.	- High number of investment options will clutter diagrams. - High number of investment options results in computational issues.

2.4 Research questions and approach

The specific knowledge gap that we address in this thesis is how transition-enabling win-win situations can be identified for a particular industrial cluster. In this chapter we have explored this gap by combining the Multi-Level Perspective framework with concepts from Industrial Ecology, and argued that the coordination that will be required of companies to identify, appraise, negotiate, and finally agree upon an investment strategy can be framed using game theory. We then argued that representing and analysing multi-company investments as collaborative as well as competitive games introduces specific modelling requirements. This led us to select the Linny-R method and tool currently developed at TU Delft to explore its potential as a tool for simulating investment decisions in industrial clusters.

We can now formulate the main research question for this thesis:

What are the strengths and weaknesses of using Linny-R to represent, analyse, and facilitate communication about transitions in industrial ecosystems driven by investment decisions?

To find an answer to this question, we address four more specific sub-questions:

1. *How can we represent investment options in industrial ecosystems using Linny-R?*
   One of the requirements of our research is to effectively represent investment options in industrial ecosystems. In our literature scan, we did not encounter any work on optimisation of decisions on investment in new assets. The optimisation problems addressed in the literature typically seek to optimise production in a cluster. The approach that we take to answer this sub-question is to conceptualise investments as *optional* production processes having associated start-up cost equal to the investment cost, so that the MILP solver can choose, given a time horizon, whether or not to commit this new process. We test this approach for a generic example in §3.2. Later, we develop our set of basic 'building blocks' further by looking how we can use the Linny-R notation to represent types of investments in industrial ecosystems that can be inferred from the ecosystems we principles discussed in §2.1. This leads us to discuss not only recycling options (§3.4), but also storage options (§3.5) and options that take into account the economic life time of assets (§3.6).

2. *How can we frame sets of multiple investment decisions as multi-actor games using Linny-R?*
   As we argued in §2.2, multiple investment decisions that will be made by multiple companies can be framed as games, provided that the payoffs can be calculated. If Linny-R can indeed maximise the total cash flow – including investment costs – over the full set of investment options, the 'committed' investments will constitute the cooperative strategy, and the resulting total cash flow will be the total payoff. We investigate this in §3.3 by adding two or more 'building blocks' to the same generic example of a simple production chain that we also used in §3.2. The key to framing this example as a multi-player game is to adequately represent the division of investment costs. We achieve this by explicitly adding financing processes for investments in shared assets.

3. *How can we analyse these games cooperatively as well as competitively, using Linny-R?*
   As Linny-R can also optimise cash flows for selected companies, and allows for selective commitment of assets, we expect that it can likewise infer competitive strategies. The question is whether the "Actors" settings of Linny-R suffice to also make the MILP solver infer the optimal investment strategies for individual companies using the same representation of the cluster. We test this first in §3.3, and find that Linny-R can indeed optimise our generic example for the companies collectively as well as individually. In Chapter 4, we test it more fully by applying our approach to a more realistic case study (inspired on the Chlorine cluster in the port of Rotterdam) with three companies having more interdependencies and a wider range of investment options. This demonstrates that we can also use Linny-R to represent and analyse multi-actor investment decisions as both competitive and cooperative games for somewhat larger clusters.

4. *How can we support effective communication between companies using Linny-R?*
   To answer our main research question, we should also establish whether Linny-R tool indeed enables parties to communicate about material flows and associated cash flows, interdependencies between accompanies, multiple investment options, and win-win strategies towards a more sustainable cluster.

A minimum prerequisite is that companies find it easy to comprehend these models thereby enabling informed decisions. Given the time constraints of this thesis project, we will address this sub-question only superficially, reflecting on our own experiences while representing and analysing the Rotterdam Chlorine cluster, and referring to reported experiences with Linny-R in other case studies.

The final outcome of this study is what we consider to be a valid ‘proof of concept’ that Linny-R is indeed an effective tool to identify, simulate and assess what in §1.3 we have termed ‘transition enabling win-win situations’.

3 Representing Investments as Games

In this chapter we demonstrate that the evolution of an industrial ecosystem can be viewed, represented and analysed as a multi-player game. We start by framing investments as decision situations in industrial ecosystems. These decision situations are in turn framed as multi-player games. The investment decisions become the moves, while the Net Present Value determines the payoffs. We then use Linny-R to represent and analyse a simple production chain improvement, first as a single-player game and then as a multi-player game. This provides the basic proof of concept for our approach to represent and analyse investments in industrial clusters as games. We then proceed by developing a variety of 'building blocks' in Linny-R that correspond to potential investments in industrial clusters that could be part of transition enabling win-win situations. As our first building block is generic, the same concept applies to all of these variants, and hence we need not analyse these variants separately as games.

3.1 Modelling Investments in Industrial Ecosystems

In this thesis, investments are viewed as drivers for transitions in industrial ecosystems as we have established in the previous chapter. In order to analyse these transitions, we must identify all potential investments over time. In this context we have to find a set of rational investments to be made by an investor. A rational investor is an investor who makes a decision so that the optimum level of benefit is reached. As described in the previous chapter, investments in new assets by an investor correspond to the moves of the game in game theory. To compute the payoff for strategies we use the Net Present Value (NPV), a measure that is commonly used when assuming rational behaviour of investors (Arnaboldi et al., 2014). NPV is defined as the present value of the future net cash flow from an investment in a project. The time value for money is represented using a discount rate **r**. This **r** is the decision-makers' time value for money, i.e., the return on investment they desire, also considering the risk of the investment not being profitable.

NPV is calculated as:

$$\mathbf{NPV} = \sum_{t=1}^{n} \mathbf{CF}_{t} / (\mathbf{1} + \mathbf{r})^{t-1}$$

where:

CF_t = net cash flow (cash in – cash out) at time t

n = number of time steps (typically years) over which the investment is evaluated

r = discount rate per time step

In this study, we assume that investments in assets are *instantaneous*, meaning that all investment costs are incurred at once, and that the asset is available and productive. This means that an investment generates a negative cash flow at the beginning of the first time step (t=1), but also a positive cash flow during that first time step. Hence, the cash flow at time t=1 equals the additional production revenue of 1 time step minus cost of the investment in the new asset.

All discounted cash flows are added over the entire time period and this results in a value of NPV. A rational investor will only decide in favour of an investment option if this investment option has NPV ≥ 0, as this indicates that the desired rate of return on investment is achieved.

In this thesis, we will assume that the rate of return **r** equals 0, and thus ignore discounting of cash flow. We do this for clarity, to keep our numerical examples simple. In §3.3 we will show by example that this simplification does not affect the validity of the method we describe, but still allows us to deliver our proof of concept.

With **r**=0, the cumulative cash flow will equal total revenue minus investment. As long as the cumulative discounted cash flow is greater than 0 the investment pays off, and the investor will decide to invest. However, since we use the concept of NPV, we need our model to have a time horizon. Throughout this thesis (unless specified otherwise) we will use an investment time horizon of **n**=40 years.

In this thesis, we represent processes in industrial clusters in two forms: the first is an existing ('brownfield') process, the second is a process representing an investment option. These 'option' processes have an associated investment cost, and they can be used for production only after this investment cost has been paid. Throughout this thesis, existing processes which have no investment cost are called **Process 1**, **Process 2**, etc., while process options having an investment cost associated with them are called **Option 1**, **Option 2**, etc.

In the following sections, we will present what we call 'basic building blocks' for industrial ecosystems. As we do this, we also explain the Linny-R graphical specification language (Bots, 2020). Each such 'building block' comprises a simple production chain (one or two 'brownfield' processes) plus one or more process options. For the first 'building block', we will first analyse it as a single-company investment, and then as a two-company investment. The latter allows us to demonstrate that Linny-R can simulate this as a cooperative game, and also as a competitive game.

3.2 Representing Investments: A Simple Production Chain

The idea of this research is that an industrial cluster comprises a network of production chains, that multiple companies each consider possible (combinations of) investment options, where each option involves a production unit of some kind, capable of converting some input (e.g., fossil fuel) into some output (e.g., electric power) in a way that adds value to one or more production chains in the cluster. This idea can be visualised using the Linny-R graphical notation. The diagram in Figure 5 depicts a simple production chain that consists of two production units: **Process 1** and **Process 2**. The chain converts product **A** into product **C** with product **B** as intermediary.

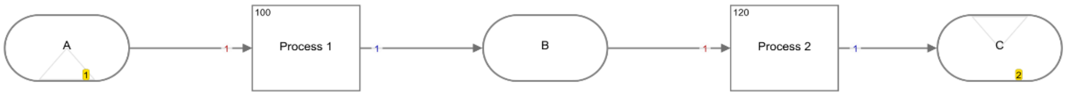

Figure 5. Representation of a simple production chain

The numbers in the upper left corner of the processes indicate the maximum capacities of the respective production units. Since the time period we use in cash flow calculations is 1 year, the number 100 denotes that at most 100 units of **B** can be produced *per yea*r. The numbers near the heads (red) and tails (blue) of the arrows denote input and output rates, which means that when a production unit is running at level X (with X between 0 and the unit's maximum capacity), it consumes X times the input rate while producing X times the output rate.

In Figure 5, all rates equal 1, so for each unit of **C** produced, one unit of **B** is consumed, and likewise for **B** and **A**. The numbers in the yellow boxes at the bottom of products indicate their market prices. Given that in this example the market price for **C** equals 2 while the market price for **A** equals 1, the production chain generates a net cash flow of 1 for each unit of **C** produced.

The triangle pointing up in the oval for **A** indicates that **A** is a 'source', which means that **A** can be obtained from third parties outside the cluster. The triangle pointing down in the oval for **C** indicates that **C** is a 'sink', which means that **C** can be exported to third parties outside the cluster. Since **B** has no triangle, it is neither a source nor a sink, which means that **Process 2** must consume all **B** produced by **Process 1**.

Evidently, **Process 1** constitutes the bottleneck in this production chain, since it can only produce up to 100 units of **B**, so **Process 2** cannot be used to its full capacity. This limits the production of **C** to 100 units per year, and this limits the net cash flow for the production chain to 100 per year.

The Linny-R notation can represent that a process can be ON or OFF. This tells the MILP solver to consider this process as a semi-continuous variable having a (typically but not necessarily non-zero) lower bound. This means that this process must either be inactive (production level = 0) or produce at least at the specified lower bound. The solver then also associates a binary variable with this process (1 = ON, 0 = OFF). This so-called 'start-up variable' can then be used to include start-up costs in the objective function of the MILP problem.

Start-up costs are typically used to represent that some industrial processes, when resuming production after being inactive – even for a short period – need significant additional resources. Evidently, this aspect becomes relevant when simulating operations with a time step of, for example, 1 hour.

In our study, with a time step of 1 year, we use the 'start-up' feature of Linny-R to represent the binary decision to invest. We use a near-zero lower bound so that the solver can deploy the asset with the same flexibility as it would a regular process. As we use a time step of 1 year, the MILP solver will 'start up' a process option only if the additional cumulative cash flow it generates (given the investment horizon) is superior to the investment cost.

We use the Linny-R notation to represent investment options as depicted in Figure 6. To distinguish them from existing production units, we label the rectangles that represent investment options as **Option N**. Moreover, Linny-R represents processes having the ON/OFF property as rectangles with a double rim at the bottom. In all other respects, investment options are similar to existing production units in that they have a maximum capacity (in this case 50 units per year), and that they consume and produce products at specified rates (in this case both 1).

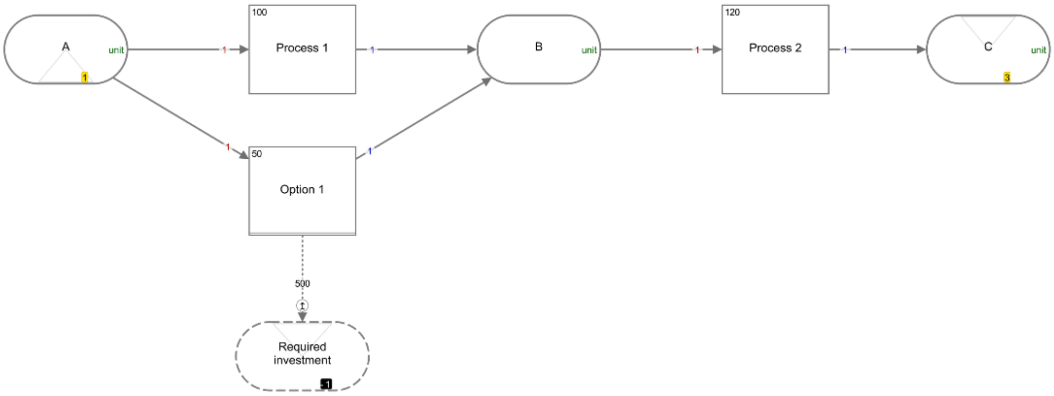

Figure 6. Representation of a production chain with one investment option

So in our research, when an investment option switches ON this means that the investor decides to invest in this option. To represent the financial consequences of this investment, we use what in Linny-R are called ‘data products’ and ‘data links’. To distinguish them from physical products, data products are denoted with a dashed rim. Likewise, ‘data links’ are dotted arrows, while links representing flows of physical products are solid arrows. The circle with the upward arrow ↥ near the arrowhead denotes that a data flow from **Option 1** to the data product **Required investment** will occur only in the year that **Option 1** switches ON. The rate of 500 on the arrow denotes that when this occurs, Option 1 ‘outputs’ a required investment of 500. To represent that this conversion constitutes a negative cash flow, we give **Actual investment** this a market price of -1. Note that in Linny-R, negative market prices are denoted in a black box, whereas positive market prices are denoted in a yellow box.

Given these semantics, the Linny-R diagram in Figure 6 specifies that **Option 1** represents the possibility for the investor to expand the present capacity for producing **B** from **A** by 50%, and that this expansion requires a single investment of 500.

The diagram also implies that this expansion will make **Process 2** become the ‘bottleneck’ in the production chain, because its maximum capacity is 120. This means that the additional revenue generated by **Option 1** will be limited to 20 times the net revenue from selling one unit of product **C**, which we already calculated as 1. This means that for the NPV to become positive, the total net revenue of 20 per year should exceed the investment of 500. Without considering the discount rate (so **r**=0), this would occur after 500/20 = 25 years. So, if **Option 1**, and also **Process 1** and **Process 2**, are expected to be productive for more than 25 years, it is rational for the investor to invest in **Option 1**.

Since Linny-R is an *executable* graphical notation, the model in Figure 6 can be executed. The diagram in Figure 7 shows the same model after execution with a simulation period of 40 years.

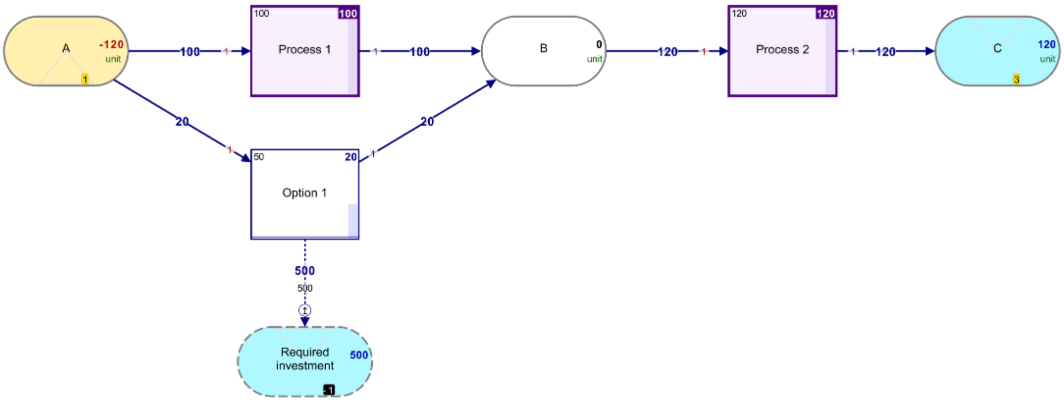

Figure 7. Executed Linny-R model (at t = 1, with N = 40 years)

The colours in Figure 7 should be interpreted as follows:

- Product **A** is orange to denote that, being a source, it is generating 120 units of A. Its 'stock level' (the number on the right) is negative (-120 in red) to denote that product **A** is imported from outside to be consumed by the production chain.
- Product **C** is light blue, and its stock level is positive (120 in blue) to denote that it is exported from the cluster.
- When the stock level of a product equals 0, the oval remains white.
- The same colouring conventions hold for 'data products'.
- The dark blue numbers in the upper right corner of processes denote their actual production level. The purple-shaded vertical bar on the right side represents its relative production level (40% for **Option 1**). A thick purple rim and complete shading indicates that a unit is producing is at its maximum capacity.

As expected, Figure 7 reflects that the investor chooses to implement **Option 1**, resulting in an actual investment of 500 at t=1 of, and a production at full capacity (limited to 120 by **Process 2**) for 40 years.

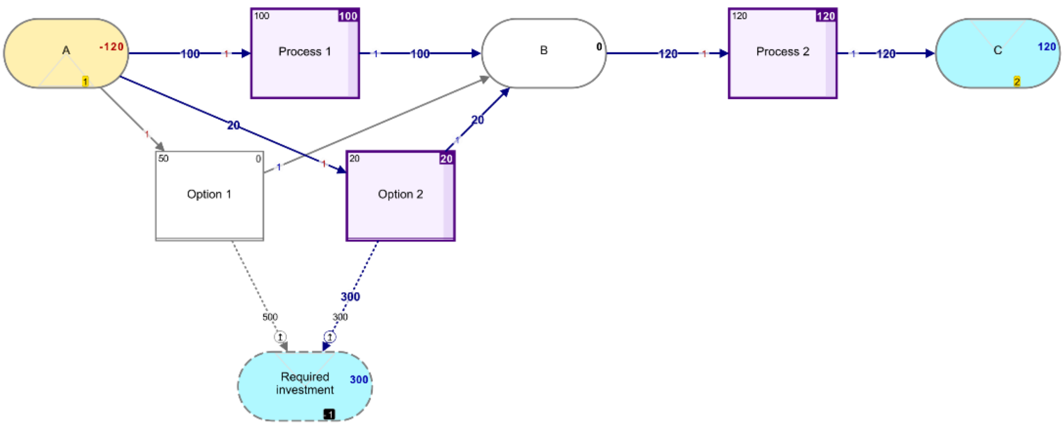

Figure 8. Executed Linny-R model with two investment options (at t = 1, with N = 40 years)

The diagram in Figure 8 extends the case by giving the investor an alternative way to expand the production capacity. This **Option 2** comprises a production unit with a capacity of only 20 units of **B** per year, and a required investment of 300.

Although the relative investment cost is higher (15 per capacity unit versus only 10 for **Option 1**), this option is more attractive because the limited capacity of Process 2 prohibits valuation of the excess capacity of **Option 1**. Hence, when this model is executed it shows that **Option 2** is chosen.

Sensitivity analysis with this particular two-option model reveals that the investor still prefers **Option 2** over **Option 1** as long as **Option 2** has a maximum capacity of more than 15 units per year. At less than 15 units per year, **Option 1** again becomes the preferred investment. This makes sense when we compare the marginal contribution to the NPV for both options:

- **Option 1** allows +20 units of **C**, which in 40 years generates a total additional net revenue of 20×40 = 800 minus a required investment of 500, so a marginal NPV of +300.
- **Option 2** with a max. capacity of only 15 allows +15 units of **C**, which in 40 years generates a total additional net revenue of 15×40 = 600 minus a required investment of 300, hence also a marginal NPV of +300.

3.3 Representing Multi-Actor Investment Decisions as Games

Having demonstrated that we can use Linny-R to represent investment options and simulate rational investment strategies of a single investor, we now turn to a setting that involves two different companies. The diagram in Figure 9 represents an industrial cluster with two existing production chains (highlighted in red) that are operated by two different actors: *X* and *Y*. The chain operated by *Actor X* is identical to the one we have used so far, and *Actor X* is now considering only **Option 1** as a potential investment.

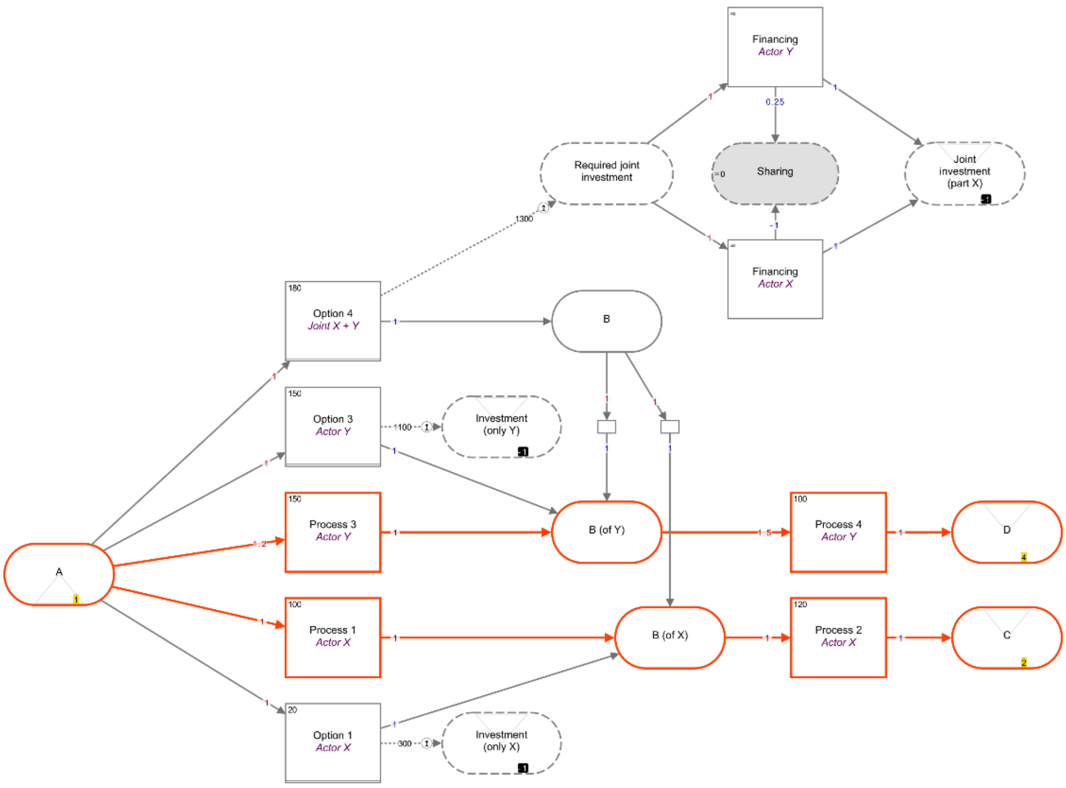

Figure 9. A two-actor cluster with three investment options

The chain operated by *Actor Y* is similar in that it also comprises a production unit that converts **A** into **B**. This unit (**Process 3**) has a higher capacity than **Process 1** (150 instead of 100) but is less efficient (consuming **A** at a rate of 1.2 instead of 1). *Actor Y* converts its **B** into end product **D** via **Process 4**, which has a maximum capacity of 100 units of **D**, and consumes 1.5 units of **B** to produce 1 unit of **D**. This means that when the chain is producing at full capacity, **Process 3** and **Process 4** both operate at full capacity.

Actor Y is considering replacing **Process 3** by a more efficient unit (**Option 3**) with the same maximum capacity of 150 units. The required investment would be 1100. Alternatively, since the two actors are producing for different markets (products **C** and **D**), they might consider a joint investment in the even larger production unit **Option 4** that can produce 180 units of **B** as efficiently as options 2 and 3. This **Option 4** requires an investment of 1300.

Note that in Linny-R, processes can be 'collapsed' to small rectangles. This feature is used in particular to denote 'transport', i.e., 1-to-1 processes (typically unconstrained) between two products. This notation is now used to represent that both actors *X* and *Y* can use the **B** produced by **Option 4** to supplement (for *Actor X*) or replace (for *Actor Y*) the **B** produced by processes 1 and 3.

Also note that in Linny-R, cash flows are ascribed to the processes that consume and/or produce products having a market price. This likewise holds for 'data products'. Therefore, to represent that this investment is shared, we must ensure that each company 'produces' its part of the investment. We achieve this by adding two processes that now *explicitly* represent the financing actions of the companies. As the 'data products' that represent the required investments are not sinks, the required investments *must* be 'consumed' by these financing processes.

In this example, we assume that the actors cost of realising **Option 4** is split 20%-80% between the two actors, so a 1:4 ratio. To achieve that the financing process of *Y* will 'produce' 4 times as much as the financing process of *X*, we introduce an extra 'data product' **Sharing**, and add two links: one from the financing process of *X* with rate -1, and one from the financing process of *Y* with rate 0.4. In this way, **Sharing** = 0 only if *Y* finances 4 times the amount that *X* finances. So by specifying this condition, we ensure the 20%-80% split.

Like in the previous examples, we compare the marginal contribution to the NPV for all three options:

- **Option 1** allows +20 units of **C**, which in 40 years generates a total additional net revenue of 20×40 = 800 minus a required investment of 300, hence also a marginal NPV of +500 for *Actor X*.
- **Option 3** consumes 30 units of **A** less than **Process 3**, which increases the annual net revenue by +30, which in 40 years amounts up to 1200. Minus the required investment of 1100, this means a marginal NPV of +100 for *Actor Y*.
- **Option 4** is as efficient as options 1 and 3, and its capacity suffices for both actors to produce at their maximum capacity, so it increases the total annual net revenue by +50. Over 40 years, the total marginal net revenue would be 50×40 = 2000. Minus the required investment of 1300, this means a marginal NPV of +700 if actors *X* and *Y* would invest jointly.

As 700 > 500+100, a joint investment in **Option 4** would outperform separate investments in the cluster. But alone, neither actor will invest in **Option 4**, as for *Actor X* it would mean a marginal NPV of -500, and for *Actor Y* a marginal NPV of -100. Thus, from a game theory perspective, the investment decision represented by the diagram in Figure 9 constitutes a game with the payoff matrices as specified in Table 2:

Table 2. Payoff matrix for Actors X and Y

	Actor Y		
Actor X	**Don't invest**	**Option 3**	**Option 4**
Don't invest	0, 0	0, 100	0, -100
Option 2	500, 0	500, 100	500, -100
Option 4	-500, 0	-500, 100	540, 160

For *Actor X*, **Option 2** dominates over **Don't invest**, as it has a higher payoff for *X* regardless of what *Y* does. Likewise, for *Actor Y*, **Option 3** dominates over **Don't invest**, as it has a higher payoff for *Y* regardless of what *X* does. Thus, the payoff matrix can be simplified to the one in Table 3:

Table 3. Simplified Payoff matrix for Actors X and Y

	Actor Y	
Actor X	**Option 3**	**Option 4**
Option 2	500, 100	500, -100
Option 4	-500, 100	540, 160

This reflects the well-known prisoner's dilemma: when *Actor X* and *Actor Y* do not trust each other, they will opt for options 2 and 3, respectively, as with the cooperative strategy (**Option 4**) each player will incur a significant loss when the other player defects.

One could imagine companies using different discounting factors, but we assume that **r**=0 in all our examples. This means that the financing processes all are equally 'efficient'. As a result, when Linny-R executes a model by maximizing overall benefit (this is the default setting of Linny-R), the solution is insensitive to the distribution of cash flows over actors. As it is more efficient for the cluster as a whole, **Option 4** will be committed even when the investment of 1300 is financed entirely by *Actor X*. Thus, by default, Linny-R infers the *cooperative* strategy.

From a game theory perspective, however, the payoff matrix would change as a function of the investment split: *Actor X* would no longer profit from **Option 4** when its investment share would exceed 3/13 ≈ 23%, as then its payoff for this move would drop below 500, and then **Option 2**. Would become the dominant strategy for *Actor X*.

To analyse this cluster with investment options as a competitive game, we must configure Linny-R in different ways. Figure 10 shows that the *Actors* dialog of Linny-R permits to specify not only how the cash flows of actors should be weighed in the MILP objective function (by default, all weights equal 1), but also whether the processes of specific actors should be ignored (i.e., not be committed by the solver). The third option ('Ignore interests') is for convenience only, as the same result can be achieved by giving actors weight 0.

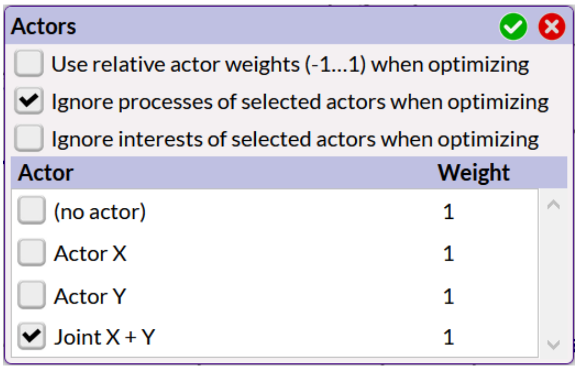

Figure 10. Configuring Linny-R to optimise the cluster without collaborative options

To make the game competitive, it suffices to ignore the collaborative options, which we have modelled as processes having actor *Joint X + Y*.

Figures 11, 12 and 13 allow comparison between the optimal solution for the cluster (= collaborative strategy), the optimal solution when all processes of *Actor Y* are ignored (= competitive strategy of *X*), and the optimal solution when all processes of *Actor X* are ignored (= competitive strategy of *Y*).

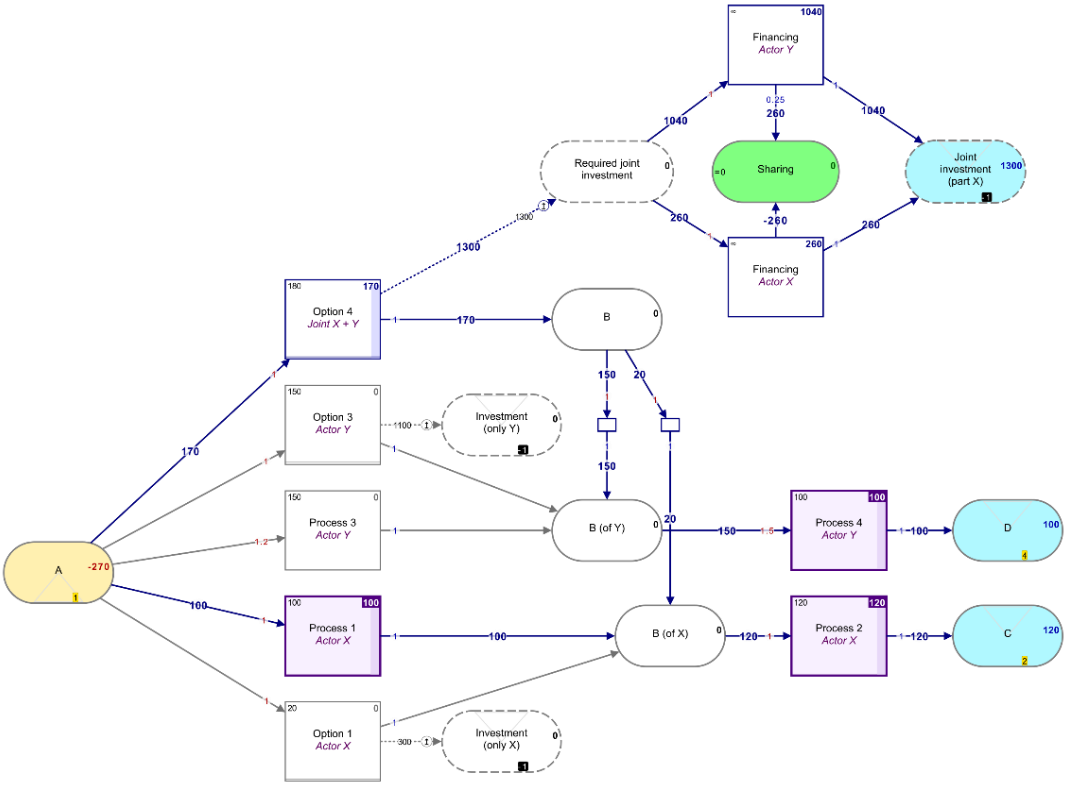

Figure 11. The Linny-R model from Figure 9 after execution (at t = 1, with N = 40 years)

Note that **Option 4** could conceivably so efficient that it would constitute a rational investment for either *X* or *Y* when acting alone. However, the constraint that ensures the 1:4 financing ratio would prohibit either actor to be the sole investor. Hence, when analysing joint investment options, such 'ratio constraints' should be lifted. We achieve this by making Sharing a source as well as a sink, so that it can become negative if *X* finances **Option 4**, or positive when *Y* finances it.

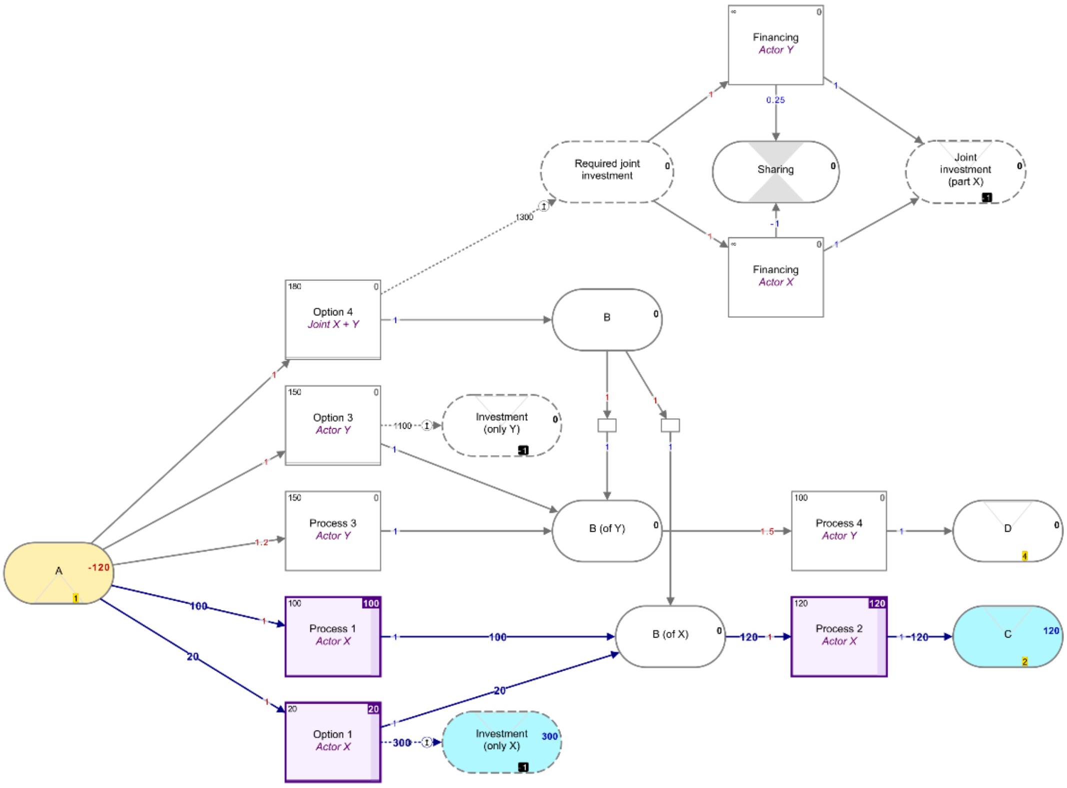

Figure 12. Same model executed while ignoring processes of Y (competitive strategy of X)

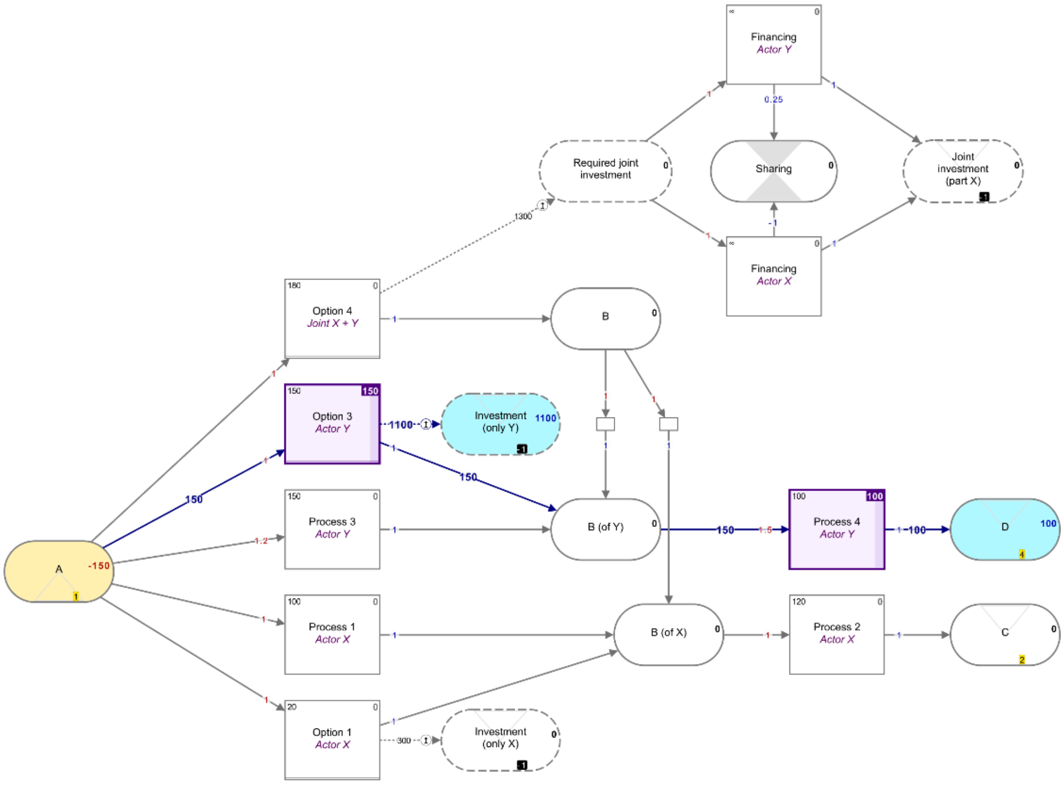

Figure 13. Same model executed while ignoring processes of X (competitive strategy of Y)

The two ‘competitive strategy’ model runs show solutions that are consistent with our earlier analysis of the game based on the payoff matrices. As a final check, we see what happens when we lower the investment cost of **Option 4** from 1300 to 1100, so that it is just as costly as investing in **Option 3**. As can be seen in Figure 14, *Actor Y* now appears to prefer **Option 4** over **Option 3**. Note that this preference is deceptive, as the two investments have equal returns. It so happens that the MILP solver comes up with this one particular solution.

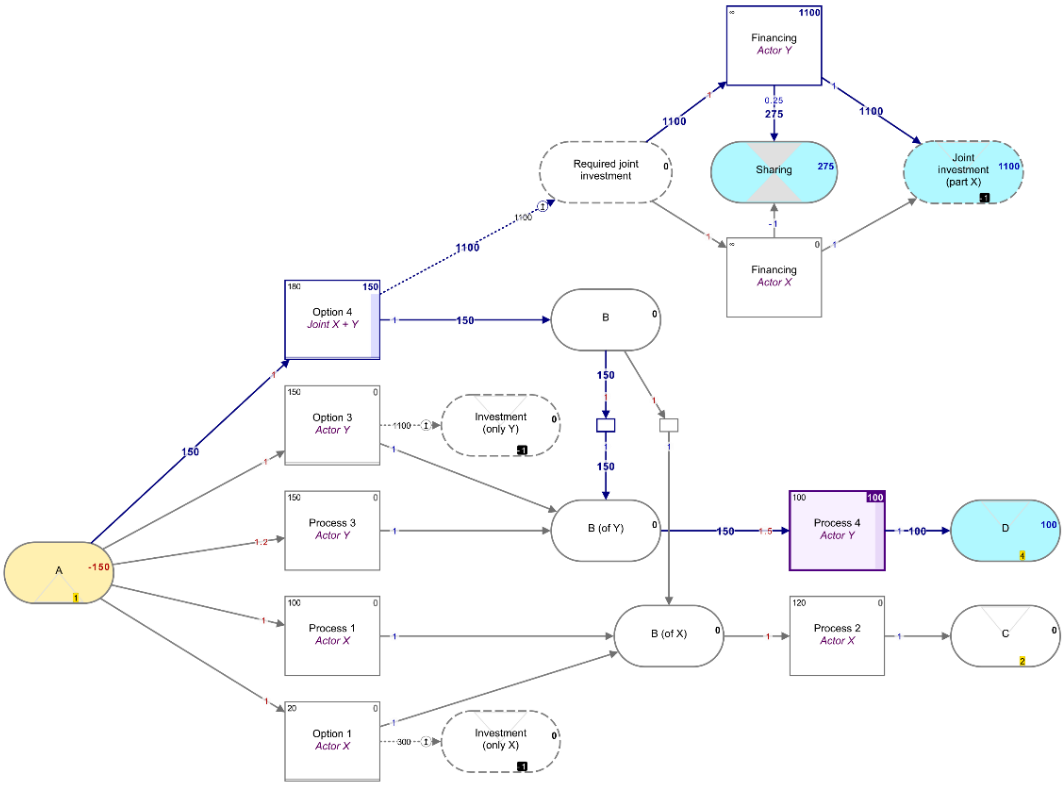

Figure 14. Competitive strategy of Y when Option 3 and Option 4 are equally costly investments

Note that in our experiments we assume that the discount rate equals 0 only to facilitate their validation. The Linny-R tool allows specification of parameters as expressions, so instead of using, for example, a constant market price of 4, we could model the time value for money by specifying the price as 4/1.05^(t-1) to represent a discount rate of 5%. This will of course affect the payoffs, and therefore the outcomes, because an option that is invested in when **r**=0 may not be invested in when **r**>0. due to gradually diminishing revenues. For example, the graph in Figure 15 shows that when looking for the cooperative strategy while all prices are discounted by 5% per year, *Actor X* will still invest in **Option 1**, but neither **Option 3** nor **Option 4** would be rational investments. This can be explained by the idea that the discount rate does not affect the investments (being made at t=1), while the (larger) profit margin on **D** erodes faster than the (smaller) profit margin on **C**.

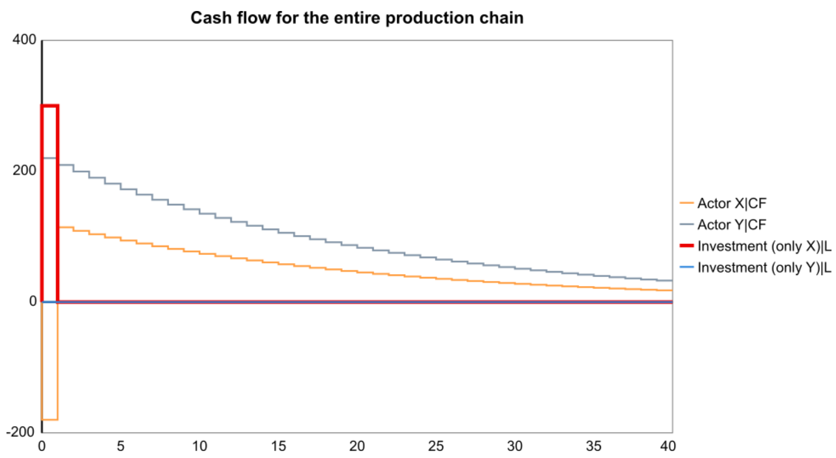

Figure 15. Competitive strategy of Y when Option 3 and Option 4 are equally costly investments

By means of these examples, we have demonstrated that alternative and potentially competing investment options in an industrial cluster can be represented using the Linny-R notation, and analysed as collaborative games as well as competitive games by executing it using the MILP solver that underlies the Linny-R tool. This means that we have essentially answered sub-questions 1 and 2 of the main research question as formulated in section 2.3.

The investment options we used in this section all involved capacity increase to resolve bottlenecks in a production chain. These do not necessarily support a transition towards sustainability. In the next section, we will elaborate a type of investment that reflects the idea of *roundput* from industrial ecology as discussed in §2.1.

3.4 Recycling Options

The diagram in Figure 16 represents a slight variation of the A-B-C production chain illustrated in Figure 2: **Process 1** and **Process 2** now both have capacity 200, and **Process 2** now outputs a main product **C** (at a rate of 80%) as well as a **Waste** product (at a rate of 20%). Product **C** has a price of **2** on the market. The waste product needs to be disposed, and the cost of this disposal is represented as a negative market price (-0.5).

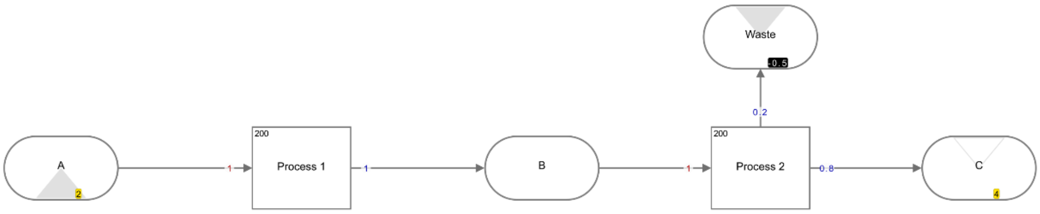

Figure 16. Simple production chain with a waste product

From these specific parameters it follows that the chain will run at full capacity of both **Process 1** and **Process 2** to generate maximum profit, consuming 200 units of feedstock **A** to produce 160 units of product **C** and 40 units of **Waste**. Assuming that the *roundput* principle from industrial ecology can be applied to this chain, we introduce **Option W** which will process this waste such that it can be fully recycled as feedstock **A**. The diagram in Figure 17 shows that this **Option W** can recycle up to 40 units, and requires an investment of 1000.

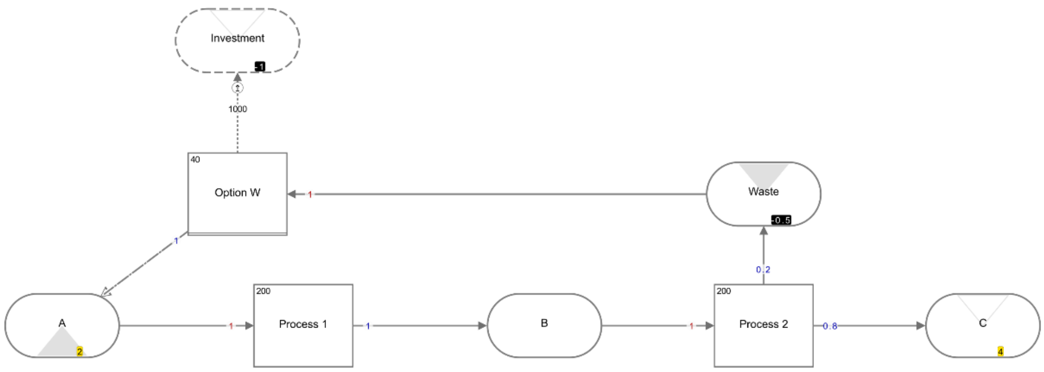

Figure 17. Simple production chain with recycle option for waste product

Like in the previous examples, we calculate the marginal contribution to the NPV for the option:

- **Option W** is used to recover **A**; the production chain will save 40 units of **A** per year and will also avoid the expense of its disposal. This means a net revenue increase of 40×1.5 = 60 per year. In 40 years, this will generate 60×40 = 2400 minus a required investment of 1000 which amounts to a marginal NPV of +1400.

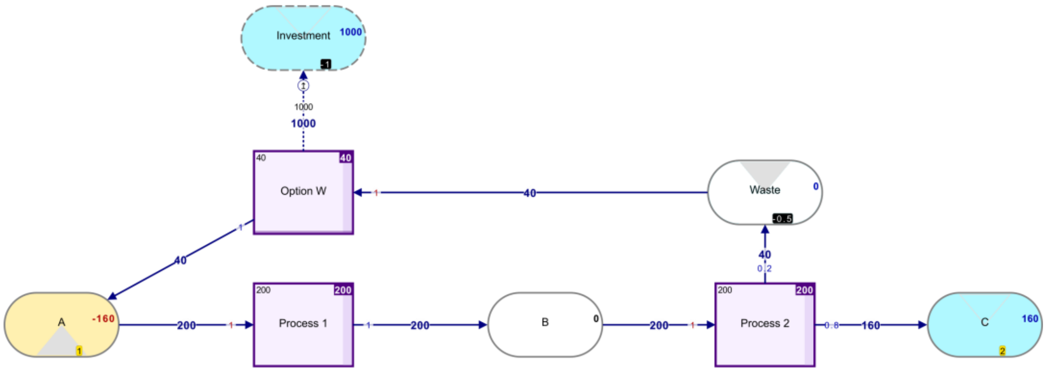

Figure 18. Executed Linny-R model with a waste recovery option (at t = 1, with N = 40 years)

The diagram in Figure 18 shows the same model after execution with a simulation period of 40 years. As expected, the investor chooses to implement **Option W**. It can also be seen that only 160 units of **A** are consumed as opposed to 200 that would have been consumed without **Option W**.

Sensitivity analysis with this particular waste recovery option model reveals that the investor will choose to implement **Option W** under various conditions.

- **Option W** is profitable as long as the investment cost is lower than 2400, since after that the marginal NPV becomes negative.
- **Option W** saves 40 units of A per year which means a net revenue increase of 1.5x40 = 60 units for 40 years. Therefore, when the investment cost is 1000 the threshold value of the units of **A** saved is 1000/60 = 16.67. Below this threshold value **Option W** is not profitable because of the negative NPV.
- If the cost of waste disposal equals *p*, the investor saves (40 + 40*p*) per year. For a period of 40 years, this amounts to 1600 + 1600*p*. This value should be greater than 1000 for the investment to be profitable, hence 1600*p* > -600, hence *p* = -0.375 is the threshold value for the cost of waste disposal.
- If we take p to be the price of **A**, the investor saves (40*p* + 20) per year, which for a period of 40 years amounts to 1600*p* + 800. For this value to be greater than the investment cost of 1000, *p* should be greater than 0.125. Below this threshold value, **Option W** is not profitable (NPV < 0). This makes sense: the more expensive product **A**, the more profitable it is to recycle it.

This example demonstrates that the idea of *roundput* can be represented quite naturally in Linny-R notation.

3.5 Storage Options

Evidently, recycling loops increase connectivity of processes in a cluster, and hence interdependence when they involve processes of multiple companies. As discussed in §2.2, such interdependencies may increase vulnerability of a cluster to disruption of processes. One way to mitigate the sensitivity of companies to (even short-period) disruptions of processes of other companies is the use of storage. By maintaining a certain stock of raw materials normally produced by company X, company Y can continue to produce (for some time) even if the production by X fails.

Storage options can also be profitable when availability of products that are imported to, or exported from, a cluster fluctuates. Assuming that such 'external' products are procured on a market, fluctuations in demand and supply will result in fluctuations in market prices. Investing in storage for such products will be profitable only if price fluctuations, production volumes and storage capacity are such that the profit margin that can be obtained by storing products when prices are low and retrieving products (to use for production, or to sell) when prices are high will cover the cost of investment in storage facilities.

In real life, price fluctuations typically have a (much) higher frequency than once per year, whereas in our examples in this thesis we use a time step of 1 year. Thus, to establish the actual change in cash flows that will result of investing in storage, we would have to run simulations with a shorter time step. To test whether this is feasible with Linny-R, we present an example with 400 time steps.

The diagram in Figure 19 represents the A-B-C production chain of Figure 5 with the addition of a storage option for product **B**. This storage has a maximum capacity of 1000. The processes **Option B** can store 150 units of **B** per time step, and the process **Option B-r** can retrieve product **B** from the storage at the same speed. As 150 > 120, this means that in this example storage and retrieval will not constraint the use of the storage.

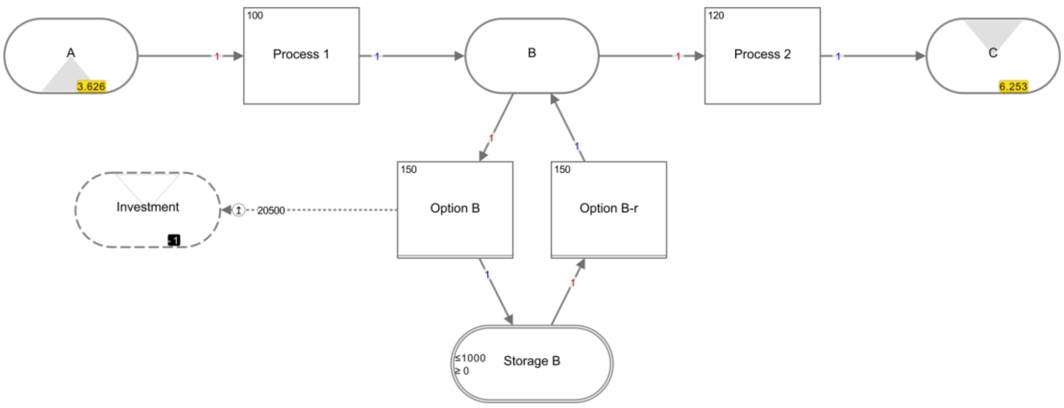

Figure 19. Investment situation with one storage option

The number 20,500 along the link from **Option B** to **Investment** is much higher than the investment cost we have used in our examples so far. This reflects that in a 10 times longer simulation period (400 time steps instead of 40) there is much more cash flow that – especially when **r**=0, so no discounting rate – accumulates the return on investment.

To simulate price volatility, we define the market price for product **A** as 3+sin(t/3)+sin(t/5)+sin(t/10), and the market price for product **C** as 5+sin(t/2)+sin(t/3)+sin(t/4)+sin(t/5). The chart in Figure 20 depicts the resulting price fluctuations over 40 time steps, the one in Figure 21 shows the quantity of product B that is in kept stock. Note that the storage capacity is at times used to its maximum of 1000.

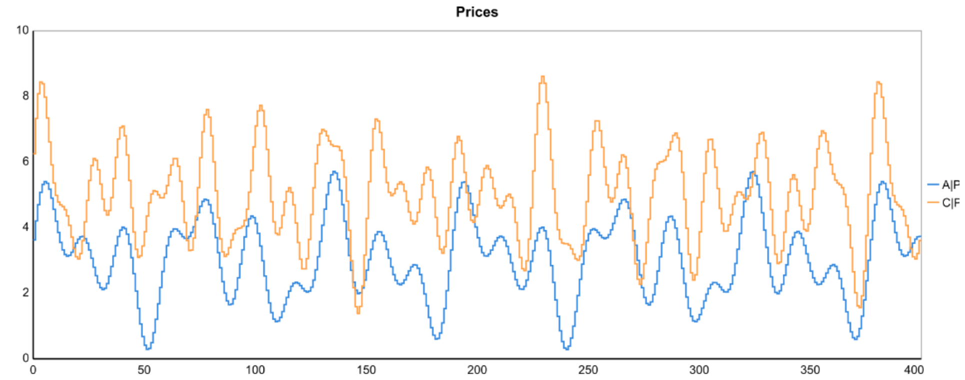

Figure 20. Market prices of products A (blue) and C (orange) over time

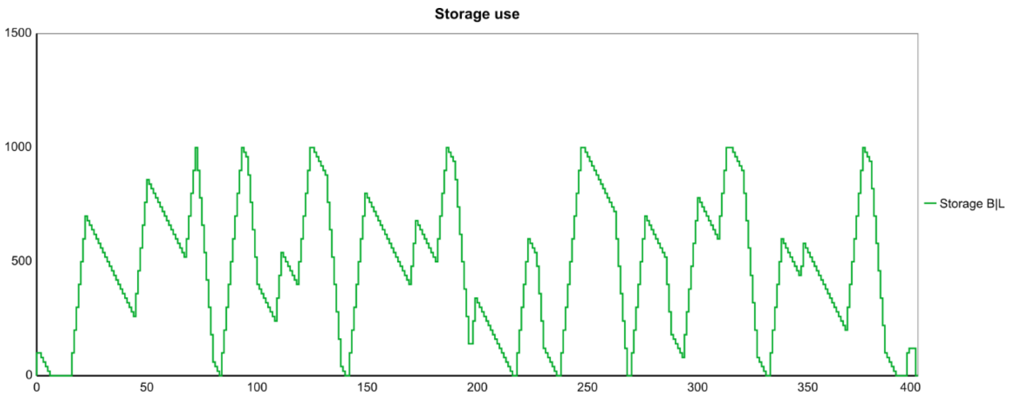

Figure 21. Quantity of stored product B over time

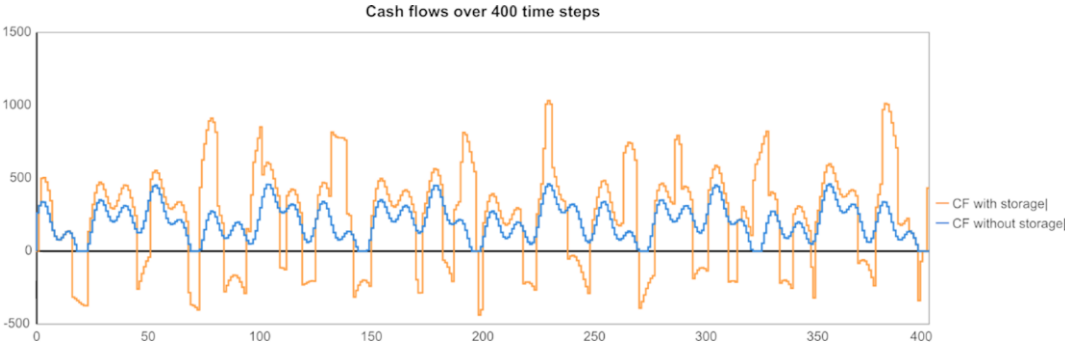

Figure 22. Net cash flow without *storage (blue) and* with *storage (orange)*

The chart in Figure 22 shows the effect for the company of having storage for product **B**. The orange line reflects that with storage, the company now purchases and processes raw material **A** when it is cheap, and only uses (stored) intermediate product **B** when the price of **C** is high. Moreover, thanks to having a stock of **B**, **Process 2** can produce at full capacity of 120 as it now is no longer constrained by the 100 capacity of **Process 1**. The negative cash flows resulting from purchasing **A** while not selling any product **C** are amply compensated by the high positive cash flows when the company *does* produce C.

Note that to better present the cash flows in Figure 22, the investment cost of storage of 20,500 is not included. When simulating 400 time steps, the total cash flow *without* storage equals 79,479 while with storage it equals 79,480, so the investment cost of 20,500 is right on the tipping point. Indeed, our experiments showed that above this cost, the investment is not selected by the solver, whereas for any lower investment cost it is.

When experimenting with longer periods and proportional investment costs, we found that, when we keep the investment cost near its tipping point, the MILP solver used by Linny-R is slowing down at a non-linear rate, taking less than 0.5 minute for simulating 400 time steps, 1.5 minute for 1000, and 5 minutes for 1500 time steps.

More experiments are needed to establish the marginal value of having more (or less) storage capacity. We mention this to emphasise that valuating storage options is tricky. Our examples merely show that storage can be profitable, but that this depends on three parameters: storage capacity, price volatility and production volumes together determine the extra cash flow that can be generated with storage. Investment decisions in storage options hence require knowledge of these parameters.

The following example demonstrates that establishing the NPV of multiple storage investments in the same production chain is even trickier because the storage decisions interact. Figure 23 shows the production chain in Figure 19 after adding storage options for products **A** and **C** as well. Note that in the shown configuration we have chosen the investment costs to allow for a final experiment.

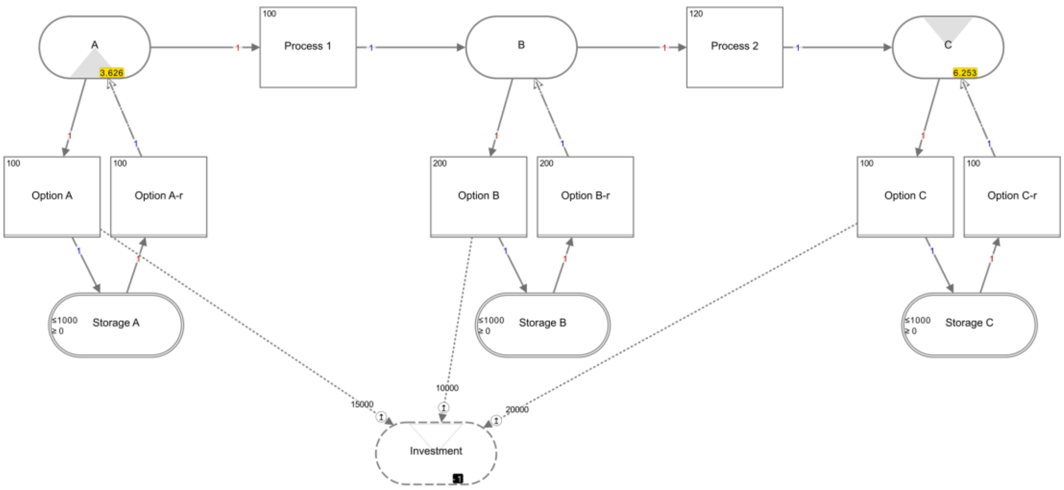

Figure 23. Net cash flow without *storage (blue) and* with *storage (orange)*

Using the same price fluctuations from our previous experiment, we first calculate the total cashflow for each storage option separately by setting the other storage capacities to 0, and also the investment cost for the option to 0. We then do the same for any combination of options (still at 0 investment cost). The results are summarised in Table 4.

Table 4. Total cash flow (x1000, ignoring investment cost) for all possible combinations of storage options

Option(s)	Total CF	Return	Synergy
None	40.0	0.0	
A	55.7	15.7	
B	49.6	9.6	
C	59.1	19.1	
A + B	62.9	22.9	-2.4
A + C	74.9	34.9	0.1
B + C	61.8	21.8	-6.8
A + B + C	77.4	37.4	-7.0

The data in column **Return** show the difference in total cash flow compared to the situation without any storage. As could be expected, having storage for all three products maximises flexibility and hence cash flow, as it allows for optimal adaptation to market prices (assuming perfect knowledge of the decision makers).

The data in column **Synergy** show the difference in total cash flow for any combination of storage options compared to the sum of the returns on the separate storage options. This reveals that only the combination of **A** + **C** leads to a very small amount of synergy. This can be explained by the fact that storage for **A** and **C** generate most of their revenue by 'rent seeking' on the fluctuating market prices of **A** and **C**, i.e., using the storage to buy and sell on the respective markets, more than to create flexibility in production. This is reflected in the chart in Figure 24 showing the stored amounts of **A**, **B** and **C**. Note that storage **B** is never used to its full capacity, but only to about 70%, and that it fluctuates mostly within a bandwidth of 300. Indeed reducing the storage capacity of option B to only 200 reduces the return with less than 2%. Table 4 shows that the added value of option B if options **A** + **C** are already in place equals 37.4 – 34.9 = 2.5 (a reduction of 7.5%).

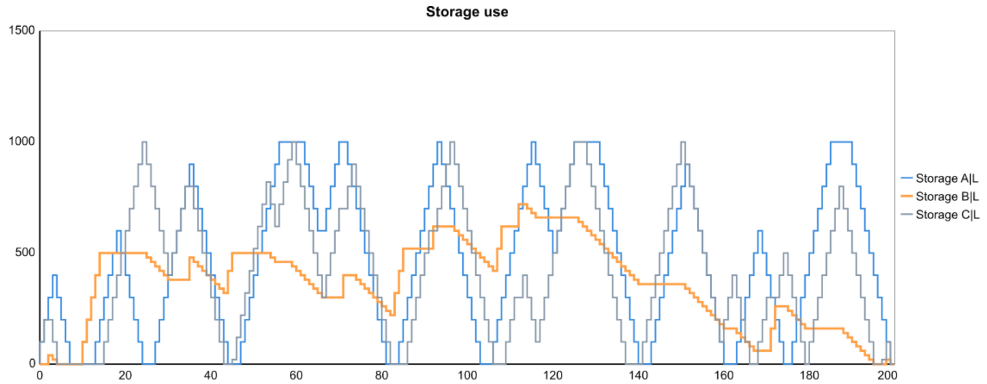

Figure 24. Quantity of stored product A, B and C over time

This explains why, if we optimise *with* the investment costs of the storage options as specified in Figure 22, only **Option A** is committed, as the return of 15.7 thousand justifies the cost of 15 thousand, whereas the return of 34.9 thousand on **A** + **C** is less than the total required investment of 35 thousand. Note that it took the MILP solver 5.5 minutes to find this optimum. If we lower the investment cost of Option A from to 14 thousand, the solver takes 4.9 minutes to find that now investment in **A** + **C** is justified.

Note that the decision to invest in **A** + **C** even though the marginal return on **Option C** is less than 20 thousand reflects that Linny-R considers the *overall* cash flow, not the return per investment option. When **Process 1** and **Process 2** would be owned and operated by different companies *X* and *Y*, then company *X* would invest 14 thousand in **Option A**, but company *Y* would not invest 20 thousand in **Option C**.

These experiments show that Linny-R also supports simulation of investment decisions on storage options, albeit that when simulating with multiple options over longer series of time steps with investment costs that are close to the profitable/not profitable tipping point becomes a computational problem.

Note that we argued earlier that in an industrial ecosystem with a variety of companies, the ecosystem principle of *roundput* could also provide justification for investment in storage options. For example, when two companies use the same product **B** for producing two different products, a storage option could allow both companies to use the raw material from the storage without being dependent on the other company. Storage can thus provide a buffer that ensures continuity in production for the two companies.

3.6 Technological Developments and Lifetime of Assets

The previous sections did not highlight the role of time involved in selection of assets for the investor. Until now, the required investment costs were constants, and all the assets had unlimited lifetime. This means that in the previous examples, all the options presented were assumed to generate the same net revenue for the entire time period (40 years in our experiments). In reality, assets typically have an economic life span. In addition, new technologies may become available in the market, rendering the old options less profitable when compared to the new technology. This may make it profitable to replace existing assets even if these assets can still be productive.

Technological developments that affect the investment cost and/or performance of assets that can be invested in can be represented in Linny-R using expressions that, similar to those we used for market prices in the previous section, are a function of the time step **t**. If we consider again the simple production chain we introduced in Figure 5, we can represent that technological developments lower the cost of the assets needed for **Process 1** by specifying the multiplier along the arrow from **Option 1** to **Investment** as, for example, `820-20*t` to indicate that at time t=1 **Option 1** requires an investment of 800, while this amount decreases linearly to 0 in 40 years.

Figure 25 shows the simple production chain with a second potential investment **Option 2**. To represent that this technology will come on the market only in t=10, we specify `t>10 ? (610-10*t) : 2500` as multiplier along the arrow from **Option 2** to **Investment**. As in Linny-R the expression `x ? y : z` denotes "**if** *x* **then** *y* **else** *z*", this expression can be read as "Until year 11, the investment cost of **Option 2** is prohibitive, but then it drops to 500 and then decreases linearly by 10 per year".

Furthermore, Figure 25 shows that the life span of an asset is modelled by adding an 'information stock' as output of the process or option that has an upper bound equal to the life span. By also specifying that its ingoing link adds 1 unit each year that the asset is in operation, and limiting the upper bound of the stock by N, this effectuates that the process thus limited can produce only for N time steps. Thus, **Process 1** has a remaining lifetime of 5 years, **Option 1** has a life time of 10, and **Option 2** has a life time of 12 years. This then leaves it up to the solver to determine when to start using them (if at all).

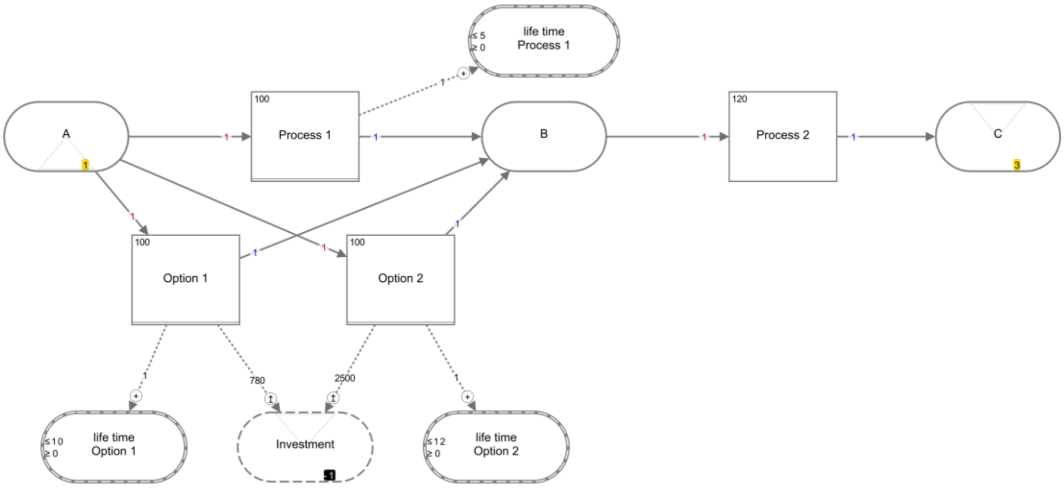

Figure 25. Simple production chain with limited lifetime for Process 1, Option 1 and Option 2

The chart in Figure 26 plots the most relevant variables over time. The blue and gray lines show the investment cost for **Option 1** and **Option 2**, respectively. For **Option 1**, these decrease as specified by the expression 820-20*t, while for **Option 2** they are prohibitively high (2500) until they drop in t=10 as specified by the conditional expression t>10 ? (610-10*t) : 2500. The orange line represents the cashflow: 200 in the first 5 time steps, as **Process 1** is then still productive. Then it is rational *not* to invest until t=8, as the cost of investing in **Option 1** is still dropping. Then investment is rational if the options generate more cash in during their lifetime than the cash out needed for the investment (green and fuchsia lines). This is the case, so the solver sequences **Option 1** and then **Option 2** as late as possible as it has perfect knowledge of the decreasing investment costs.

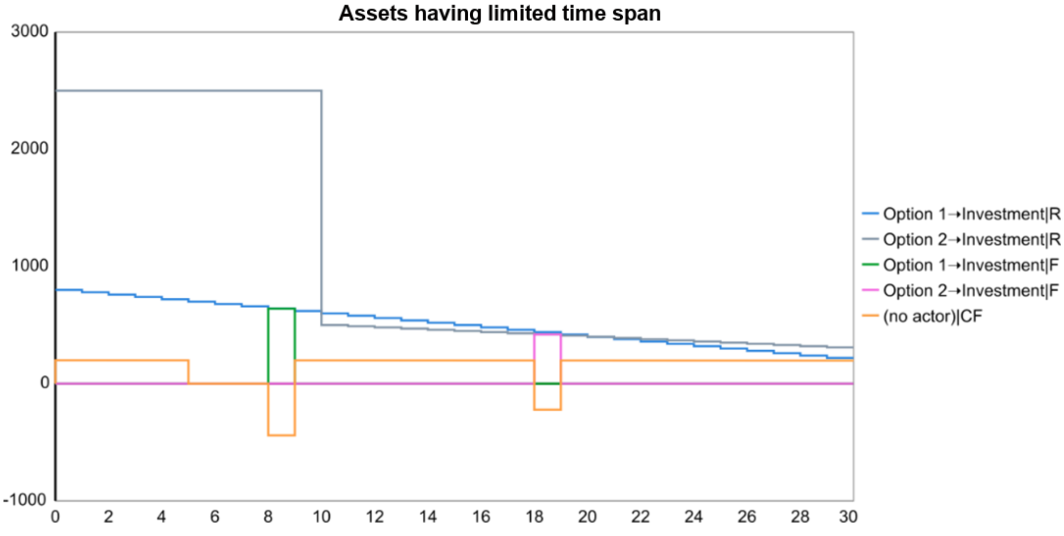

Figure 26. Lifetime of Process 1 and Option 1

With this example we have shown that the lifetime of an option can be represented using Linny-R notation, that it impacts the cashflows and hence the return on investments as expected, and that this co-determines the investment path computed by the solver. Our experiments also show that even a simple model that includes lifetime can require considerable computation time (nearly 10 minutes for only 30 years). This can be explained by the solver having to consider – for every option – committing the investment in a particular time step t, whereas with infinite lifetime the solver will always commit to invest in an option at time t=0 as this will always maximise revenue. When considering lifetime, the number of relevant binary variables in the MILP model will be much higher, requiring progressively more branch-and-bound search. We also found that using an arbitrary large number (e.g., 1.0e+6) to represent 'prohibitive investment cost' can result in a solver error that signals that the model is numerically instable. This suggests that scaling issues may also limit the scalability of using models that feature assets with limited life span.

3.7. Conclusion

Through the course of this chapter we have provided answers to sub-questions 1 and 2, and to some extent also sub-question 3 as formulated in §2.4. With our examples, we have demonstrated that Linny-R can be used to represent various types of investment options in industrial ecosystems in such a way that an investor's rational decision making can be simulated. Moreover, we have demonstrated that we can represent investments by two interdependent companies, and then simulate this investment situation as a cooperative game and also as a competitive game. This provides a basic 'proof of concept' for our approach, with the caveat that we assume that what we have demonstrated with one type of 'building block' can be generalised to all types of investments, and also to game settings with more than two players. To test these assumptions, we report in the next chapter on how we applied our approach to a more realistic example of an industrial ecosystem.

4 Case Study: Chlorine Cluster

So far, we have shown that the representation we use for investment decisions is functional in the sense that it correctly simulates rational investment behaviour for small sets of investment options in small clusters with simple production chains. In this chapter we demonstrate that this approach also works for more complex settings by applying it to a case that has more realism: an industrial cluster that comprises three companies having several interdependencies between their processes, and a variety of investment options. We introduce this cluster by first analysing the production chains of the constituent companies. We then analyse the entire cluster to compare the cooperative strategy with the optimal single-player strategies.

4.1 Case Selection

The case we have chosen is loosely based on the Chlorine cluster in the Port of Rotterdam. We chose this case because it relates to a real industrial cluster (as opposed to the abstract building blocks in Chapter 3), and also because this cluster has been used in earlier studies with Linny-R (Makker, 2013; Fayed, 2019). We have simplified the original models such that on the one hand it retains realism, multiple interdependencies between companies, and a variety of the types of investment options identified in Chapter 3, while on the other hand allowing for validation of the model results by manually calculating outcomes.

The diagram in Figure 27 shows the part of the Chlorine cluster that we have used in our study. We have selected the VCM production process because of the presence of an internal recycling loop similar to the one in the recycle option example in Chapter 3. However, there are some simplifications that are made while modelling this cluster:

- Company Y produces MDI as their primary product. The simplification here is that we do not model a separate process for distillation that produces the MDI monomer, nor the separate process for the monomer which undergoes polymerisation to produce the final product MDI. We have combined these processes into a single step and modelled it as **Produce MDI**.
- For Company Z, we have modelled the balanced process for producing VCM using direct chlorination and oxychlorination. However, we do not model a separate process for EDC purification, thermal cracking and VCM purification which are part of the balanced process. We have combined these processes into a single step and modelled it as **Produce VCM**. We also simplify the process further by modelling the torching process which has a single output of CO_2 that represents emissions in the cluster.

The capacities for processes have been chosen to provide interesting investment options. As we have mentioned before, we start by identifying potential improvements in the cluster per company. We do this to demonstrate that each company on its own makes a profit. Next, we analyse the cashflows with these improvements per company to show that the companies indeed are profitable individually. Finally, we analyse the cluster first from a cooperative perspective and the from a competitive perspective. The outcomes reveal which perspective is more profitable under which conditions for the cluster as a whole. This allows us to investigate what prices should be negotiated by the respective companies to reach what we have termed a ‘transition enabling win-win situation’.

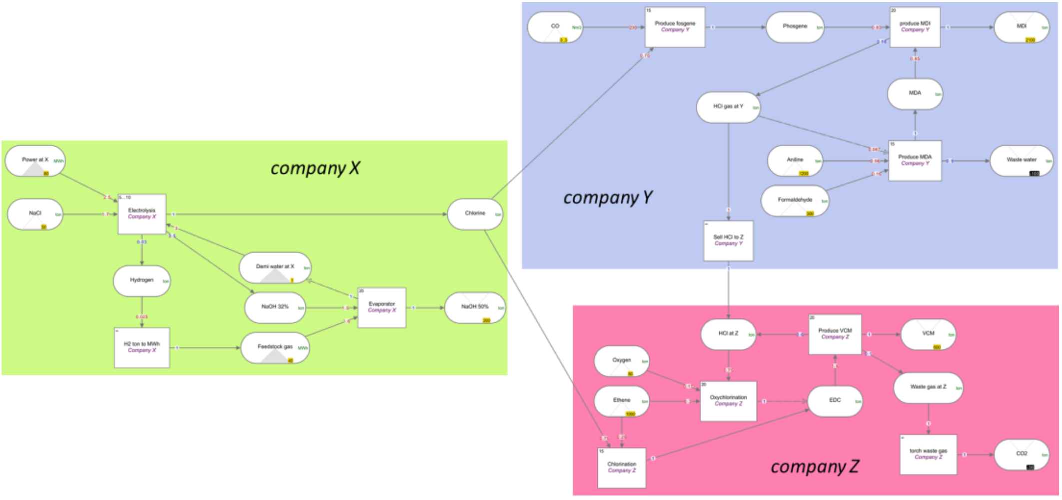

Figure 27. Chlorine cluster as a case

4.2 Current Situation

Figure 27 shows that the three companies X, Y and Z are interdependent on each other:

- Company X produces chlorine which is used by both Company Y and Z.
- Company Y has a side product HCl which is processed by Company Z as raw material.
- Chlorine is a hazardous material that is expensive to transport in large quantities; this makes Company X dependent on Y and Z, being the unique consumers.

To clarify the business case for each company separately before we analyse the cluster as a whole, we first consider each company as if it could produce for a market with infinite demand, similar to the ‘building blocks’ we analysed in Chapter 3.

4.3 Identification of improvement options

Note that the time period that we use in this chapter is 40 hours rather than 40 years as we have done previously. This is because we have set the prices of raw materials such that they are close to real market prices. Later, when we analyse whether investment options have a positive return, we scale the investment cost accordingly, assuming production 8000 production hours per year.

Company X

Figure 28 reflects the assumption that Company X is independent from the cluster. The primary product of Company X is chlorine. It is produced by electrolysis of aqueous sodium chloride (NaCl). This process yields HCl and sodium hydroxide

(NaOH). This NaOH is has a market price only when it is in a concentrated solution in water containing 50 mass % NaOH. The diagram in Figure 28 shows that Company X has an evaporator that concentrates NaOH to 50% which can then be sold on the market. The demineralised water produced during evaporation is reused in the electrolysis process.

Note that in Figure 28 the product **Chlorine** has no price (which in Linny-R defaults to 0) whereas the actual market price of chlorine is around 600-700 €/ton. We set the price for chlorine to 0 (for now) to reflect that Company X produces chlorine only for Company Y and Z, and that parties will negotiate a price that allows profit for all. Company X also produces NaOH as a side product, and this can be sold on the market for a price of 200 €/ton. Hence, NaOH is the money-making product for Company X. We assume that the chlorine is used by companies Y and Z as we will see later in this chapter.

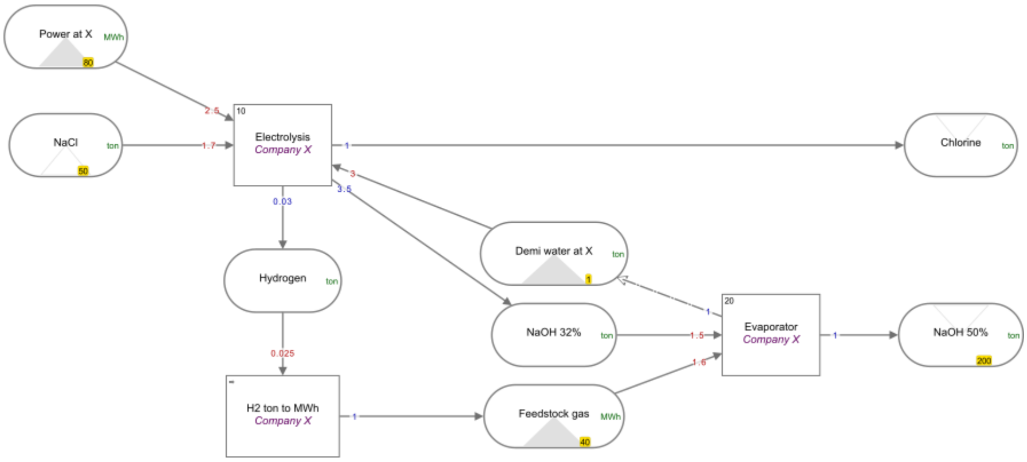

Figure 28. Company X independent from the Chlorine Cluster

Now we calculate the cost prices of the products for Company X. Thus, we calculate how much it costs for 1 ton of products to be produced. 1 ton of Chlorine requires 2.5 MWh of Power, 1.7 tons of NaCl, 0.667 tons of demi water and 2.533 MWh of feedstock gas. We assume that electric power at Company X costs 80 €/MWh, NaCl costs 50 €/ton, demi water costs 1 €/ton and feedstock gas costs 40 €/MWh.

This makes that the cost price for producing 1 ton of chlorine is 387 € (2.5×80 + 1.7×50 + 0.667×1 + 2.533×40). In addition, during the production of 1 ton of Chlorine 2.333 tons of NaOH (50%) are also produced. The selling price of 2.333 tons of NaOH is 466.6 € (200×2.333). This value must be greater than the cost price of Chlorine for Company X to make a profit. The marginal profit in this case is 466.6 – 387 = 79.6 €.

Assuming these market prices, Company X makes profit on production and hence will try to maximise production by running at full capacity. In our model, the full capacity of production is limited by the **Evaporator** process because when it operates at maximum, the **Electrolysis** process will only produce 8.57 tons of **Chlorine**. Given our assumption that the plant runs for 8000 operating hours per year, the annual profit is then 8000×8.57×79.6 = 5.4M€.

The fact that Company X could use its other assets better if the evaporator had more capacity indicates that expanding the capacity of the evaporator could be an interesting investment option. This would be the investment option type that we described earlier in §3.2.

Company Y

Figure 29 reflects the assumption that Company Y is independent from the cluster because raw materials can be obtained, and products can be sold, on markets with infinite volumes. The primary product of Company Y is **MDI**. It is produced from phosgene and MDA, which both are produced on-site by Company Y. The MDI production results in HCl as a by-product. Some part of this is used by the MDA production process, but a major part is superfluous and hence exported.

Note that in Figure 29 again the price of Chlorine is unspecified (assumed 0), and that we have done likewise for the price of HCl. Similar to chlorine, HCl gas is a corrosive substance which makes it difficult to handle, and hence has to be processed on-site. So for Company Y we assume that the HCl gas is not sold, but processed by company Z (as can be seen in Figure 27).

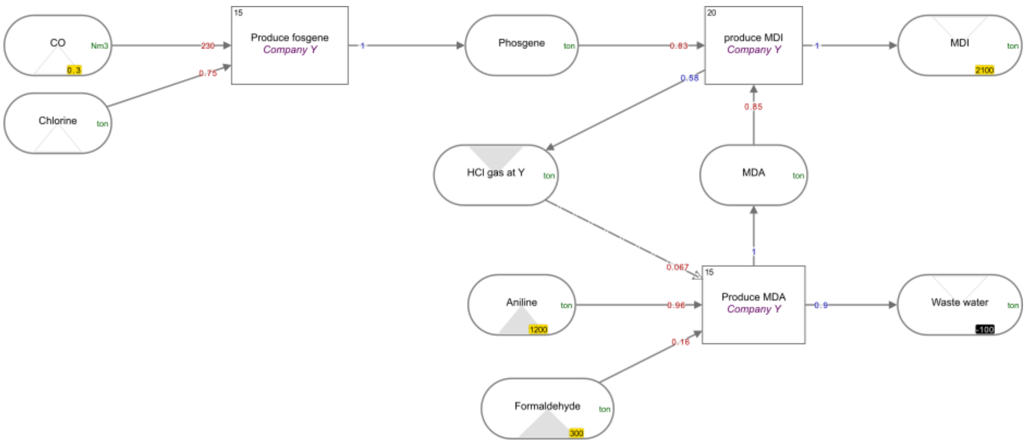

Figure 29. Company Y independent from the Chlorine Cluster

Now we calculate the cost prices of the products for Company Y. Thus, we calculate how much it costs for 1 ton of products to be produced. 1 ton of MDI requires 190.9 Nm^3 of Carbon Monoxide (CO) and 0.62 tons of Chlorine. We assume that CO costs 0.3 €/ Nm^3. Therefore, the cost price for producing 1 ton of MDI is 57.3 € (190.9×0.3). In addition, 0.85 tons of MDA are also required for producing 1 ton of MDI. The cost price of 0.85 ton of MDA is 1020 € (0.816×1200 + 0.136×300). In addition, Company Y has to dispose 0.765 tons of wastewater at a cost of 100 €/ton. This amounts to 76.5 €. The total cost price of 1 ton of MDI is 1154 € (1020 + 57.3 + 76.5).

Assuming that MDI can be sold on the market, the selling price of MDI must be greater than the total cost price of MDI for Company Y to make a profit. The marginal profit in this case is 2100 – 1154 = 946 €. Given these market prices, Company Y makes a profit and hence will try to maximise production by running at full capacity. In our model, the full capacity of production is limited by the MDA production process because when it operates at maximum, it only produces 17.65

tons of MDI. Assuming again that the plant runs for 8000 operating hours per year, the annual profit would be 8000×17.65×946 = 133.6 M€.

Thus, for Company Y it may be an interesting investment option to expand the capacity of the MDA process.

Company Z

Figure 30 reflects the assumption that Company Z is independent from the cluster because raw materials can be obtained, and products can be sold, on markets with infinite volumes. The primary product of Company Z is vinyl chloride monomer (VCM) which is a precursor to polyvinyl chloride (PVC). It is produced from ethylene dichloride (EDC), and this production yields HCl as a by-product. This HCl is used in the oxychlorination process and thus forms a recycle loop with the VCM process. EDC can be produced by using chlorination as well as oxychlorination.

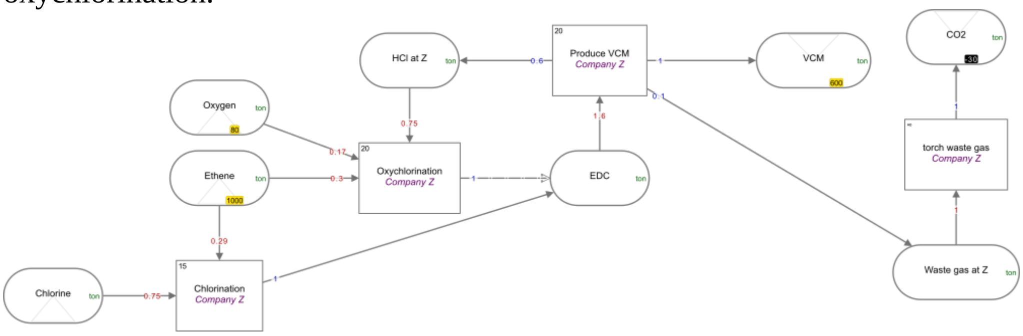

Figure 30. Company Z independent from the Chlorine Cluster

Now we calculate the cost prices of the products for Company Z. 1 ton of VCM requires 1.6 tons of EDC. EDC is produced both by chlorination and oxychlorination. EDC requires 0.136 ton of oxygen and 0.24 tons of ethene for the oxychlorination process. EDC is also produced by chlorination which requires 0.6 tons of Chlorine and 0.232 tons of Ethene. We assume that oxygen costs 80 €/ton. The total cost price is the combination of the cost prices for the chlorination and oxychlorination processes. Therefore, the cost price for producing 1 ton of VCM is 483 € (0.136×80 + 0.24×1000 + 0.232×1000). In addition, Company Z has to dispose 0.1 tons of waste gas at a cost of 30 €/ton. This amounts to 3 €. The total cost price of 1 ton of VCM then is 486 €.

Assuming that VCM can be sold on the market, the selling price of VCM must be greater than the total cost price of VCM for Company Z to make a profit. The marginal profit in this case is 600 – 486 = 114 €. Assuming that these market prices hold good, Company Z makes a profit and hence will try to maximise production by running at full capacity. In our model, the full capacity of production is restricted by the chlorination production process because when it operates at maximum, it only produces 18.75 tons of VCM. Assuming again that the plant runs for 8000 operating hours per year, the annual profit would be 8000×18.75×114.12 = 17.1 M€.

Thus, for company Z an interesting investment option could be to expand the capacity of the VCM process. Note that because of the recycle loop in the process of company Z the expansion of the chlorination process will also lead to increased roundput and locality as described in chapter 2.

4.4 Analysis of improvements

We now look at investment options for each company based on the bottlenecks identified in the previous section. Note that the values of annual profits especially for X and Y are unrealistically high because we have not considered all the variable costs. For the purpose of this thesis, however, the exact figures are not relevant.

Company X

In case of Company X, the obvious option would be to invest in the expansion of the evaporator. This will allow the **Electrolysis** process to produce a larger quantity of chlorine and in the same proportion a larger quantity of NaOH. We know that 2.333 tons of NaOH yields a marginal profit of 79.6 €. Therefore, 1 ton of NaOH would give a marginal profit of 34.14 €. Given the present capacity of 10 tons, if the electrolysis process would run at its maximum capacity, it would produce 35 tons of NaOH 32%. Since the evaporator uses 1.5 ton of **NaOH 32%** to produce 1 ton of concentrated NaOH, the required capacity of the evaporator should at least 23.333 tons.

Since we now use 1 hour as simulation time step, we must calibrate the investment costs of options to reflect this, or the solver will never select an option. For the additional capacity of 3.333 tons we can calculate the threshold investment price, i.e., the maximum price below which making the investment is economically rational, as the evaluation period (now 40 *hours*) times the *additional* production volume times the *marginal* profit on the product. So in this case: 40×34.14×3.333 = 4551 €. This would mean that when the required investment is lower than this number, the solver will commit to option

The diagram in Figure 31 shows that indeed the investment is made when the rate of the '1 on start-up, 0 otherwise' link (highlighted in red) is set to 4550 (or any lower value) while the option is not committed at rates above 4551.

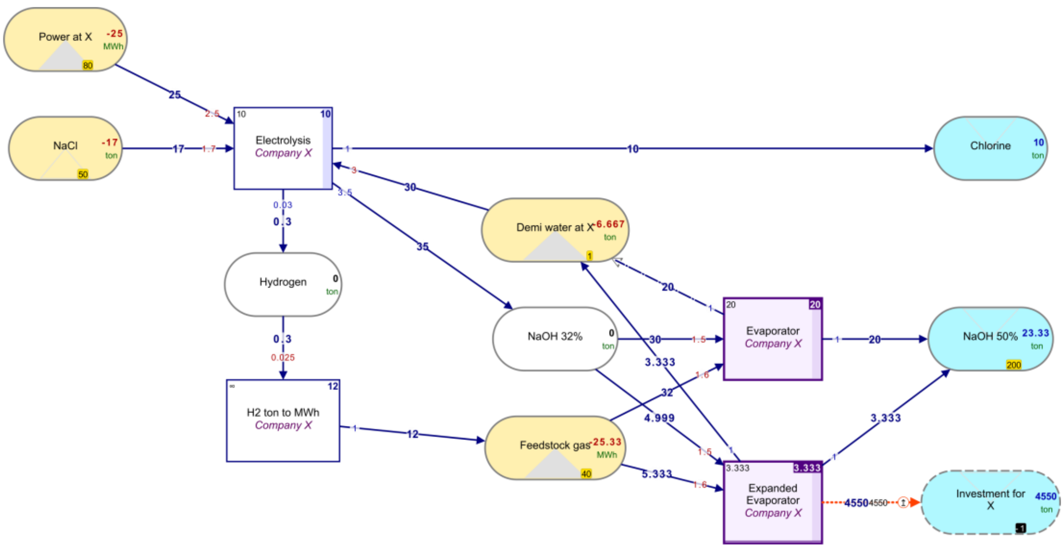

Figure 31. Company X with expansion option for the evaporator

Company Y

For Company Y, the MDA production constitutes the bottleneck. Therefore, the logical option for Company Y is to expand the MDA process. We know that 0.85 tons of MDA yields a marginal profit of 946 €. Therefore, 1 ton of MDA would give a marginal profit of 1113 €. For the additional capacity of some 0.361 tons for the MDA production we can calculate the threshold investment cost using the same method we used for Company X. The evaluation period times the additional production volume times the marginal profit on the product now gives 40×1113×0.361 which is just below 16.1 k€/h. This would mean that when the required investment is lower than this number, the solver will commit to option

The diagram in Figure 32 shows that Company Y indeed makes this investment when the rate of the ‘1 on start-up, 0 otherwise’ link (highlighted in red) is set to 16090 (or any lower value) while the option is not committed at a rate of 16100.

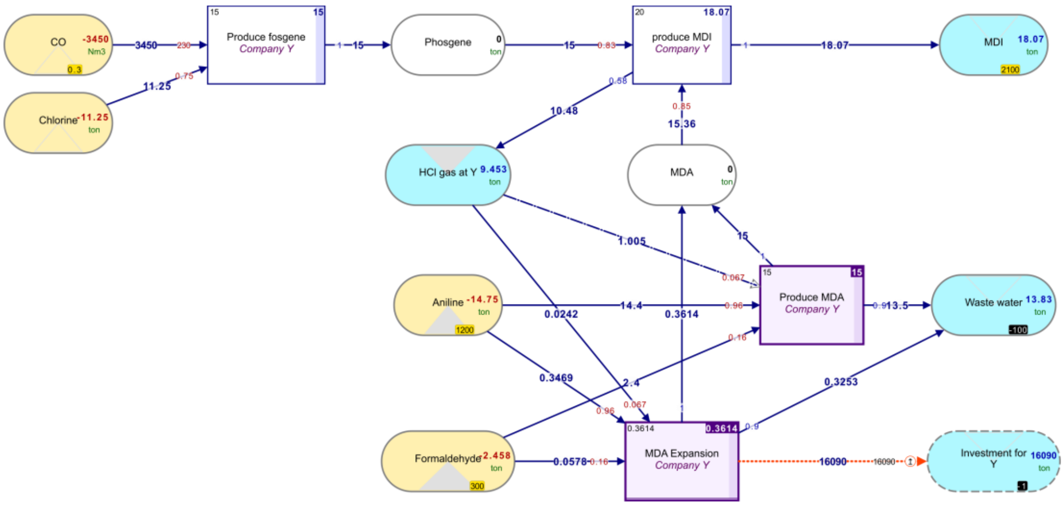

Figure 32. Company Y with the option to expand its MDA production

Company Z

Company Z has a bottleneck at the chlorination process, which means that the option of investing in a higher capacity for chlorination could be interesting. Again we follow the same approach of calculating the investment threshold. We know that 0.8 tons of EDC from chlorination yields a marginal profit of 114.12 €, and hence that 1 ton of EDC from chlorination would give a marginal profit of 142.65 €. Since VCM production uses 1.6 of EDC, the required capacity of the chlorination process should be at least 16 tons, while its actual capacity is 15 tons. For the additional capacity of 1 ton of VCM production we can calculate the threshold investment price as 40×142.65×1 = 5706 €. Figure 33 shows that – again as expected – the solver commits the investment option when the investment cost for Company Z is set to 5705, while the option is not committed when the rate on the link (again highlighted in red) is set to 5710 or any other value above the threshold value.

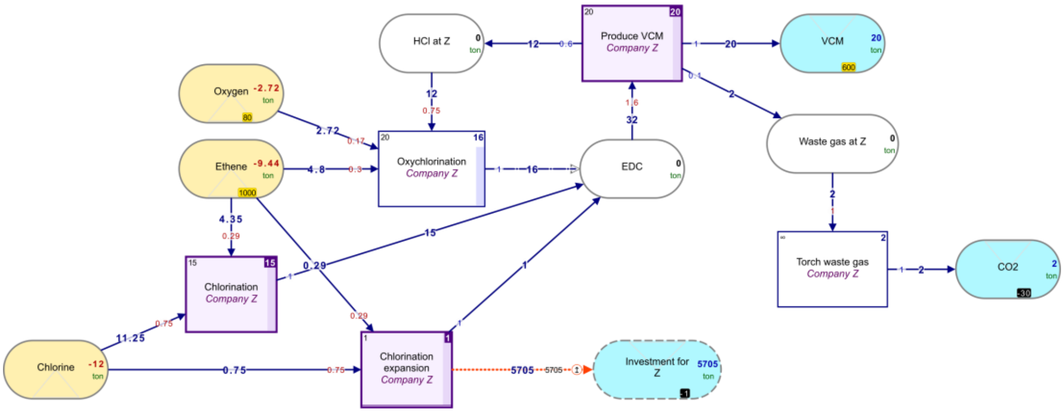

Figure 33. Company Z with the option to expand the chlorination process

Table 4 summarises the options for the three companies with their cash flows per hour before and after the investment, and the additional *annual* cash flow this would mean, assuming 8000 production hours per year. The table makes clear that each of the three investment options results in a significant increase in cash flow. Assuming a 10 year depreciation period, the evaporator expansion could justify an investment up to 63 million euro, and the expansion of the MDA process even twenty times that amount. As we mentioned earlier, our model ignores many cost factors, as we focus on testing our method rather than evaluating a real world business case. For our research, the main takeaway for now is the investments are economically realistic up to a certain threshold value.

Table 5. Summary of the results over the time period of 40 hours

Company	Investment option	Original cash flow (€/h)	Cash flow after investing (€/h)	Additional cash flow (M€/yr)
X	Evaporator	682	796	6.3
Y	MDA process	16698	17100	136.8
Z	Chlorination	2139	2282	18.2

Having analysed its constituting companies, and identified the investment options that could be interesting from their individual perspective, we now turn to the cluster as a whole.

4.5 Analysis of improvements for the cluster

We now consider the Chlorine cluster as it is represented in Figure 27, i.e., still without considering the investment options identified in the previous section. Assuming that the Chlorine cluster would be operated by a single entity (cooperative game), we use Linny-R to maximize its overall profit. The result is shown in Figure 34.

The active flows in the diagram how the HCl from Company Y is used by Company Z, and how chlorine is used by Companies Y and Z. Moreover, it shows that presently the evaporator of Company X constitutes the production bottleneck, as this is the only process that is producing at maximum capacity.

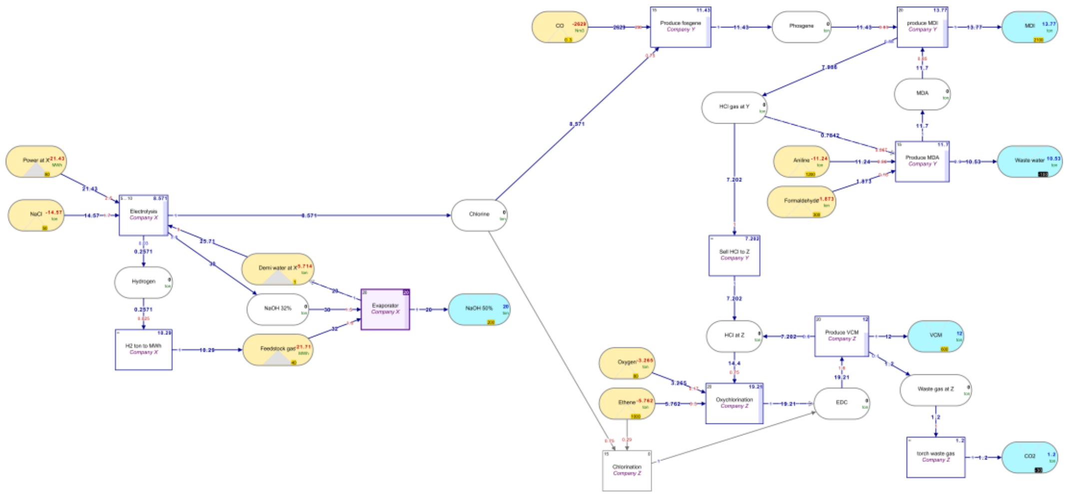

Figure 34. Executed model of the Chlorine cluster (t=1, N=40 hours)

So far we have seen how each individual actor will expand their respective processes in order to maximise their profit. Now we incorporate the investment options discussed in §4.4 into the Chlorine cluster. Figure 35 shows the result after optimising the chlorine cluster with these options, using the same investment thresholds.

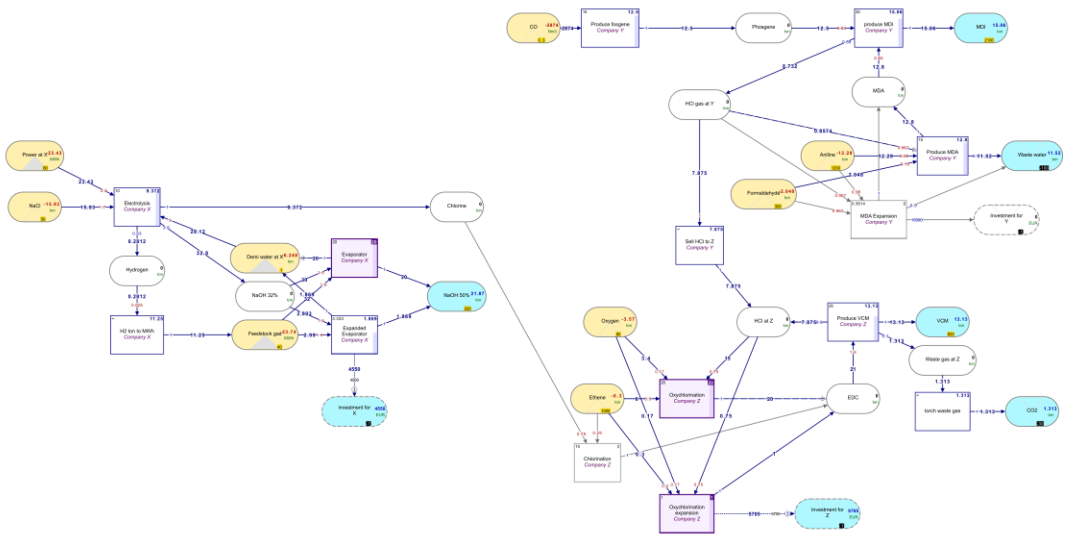

Figure 35. Executed model of the Chlorine cluster with investment options

The expanded evaporator process runs because it facilitates higher production of chlorine and NaOH by removing the bottleneck at the evaporator. Note that it does not run at its full capacity. Company X could produce more chlorine, but apparently this is not needed. Company Y does not invest in the option for expansion of MDA, which can be explained by the fact that it now does not even utilise its full existing capacity. Company Z invests in the oxychlorination, but since Company Z alone required only 1 ton to reach its maximum VCM production, the oxychlorination process now constitute the bottleneck for the entire cluster despite its expansion.

This simulation demonstrates the interdependence between the investment decisions of companies. The expansion option for Company Y has been rendered unprofitable in the combined configuration, whereas the expansion option of

Company Z turns out to be insufficient (and hence probably also inefficient, assuming that there will be economy of scale).

Assuming cooperation – and hence complete information sharing – between the companies, we can address the new bottleneck in the system by devising different investment options for the cluster.

Analysing the oxychlorination bottleneck, we see that the required capacity of oxychlorination should be at least 22.406 tons based on the input of the oxychlorination process. This would increase the production of VCM from 12.5 to 14 tons. We know that 1.6 tons of EDC from oxychlorination yields a marginal profit of 95.24 €. Therefore, 1 ton of EDC from chlorination would give a marginal profit of 59.525 €. For an additional capacity of 2.406 tons of production we can calculate the threshold investment price as follows, 40×59.525×2.406 = 5735 €.

When this bigger option is incorporated in the cluster, the simulation of the cluster as shown in Figure 36 shows that the oxychlorination expansion indeed increases the production of VCM (from 13.13 to 14) but still not to its maximum of 20. This can be explained by the fact that now Company X again constitutes the bottleneck for the cluster, as now it is producing chlorine at its full capacity, which turns out to be still constraining the production of the other companies.

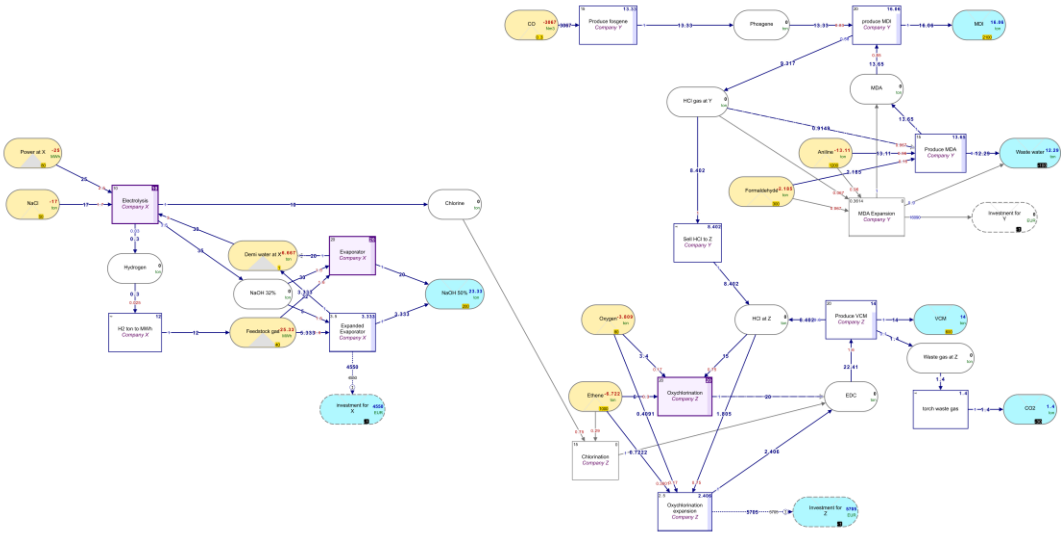

Figure 36. Executed model of the Chlorine cluster with updated Options

Evidently, we could continue this analysis until we resolve the last bottleneck. However, that is not the purpose of this case example. Instead, we want to add more diversity in our investment options.

Another interesting option is to make better use of the waste gas that is now torched by Company Z. Because of CO_2 emission tariffs, Company Z has to pay a price of 30 €/ton to dispose the waste gas. This waste gas can be converted into feedstock gas and supplied to Company X. When we calculate the threshold investment cost in the same way as in the previous cases, this threshold turns out to be 39024 €. This is shown in Figure 37.

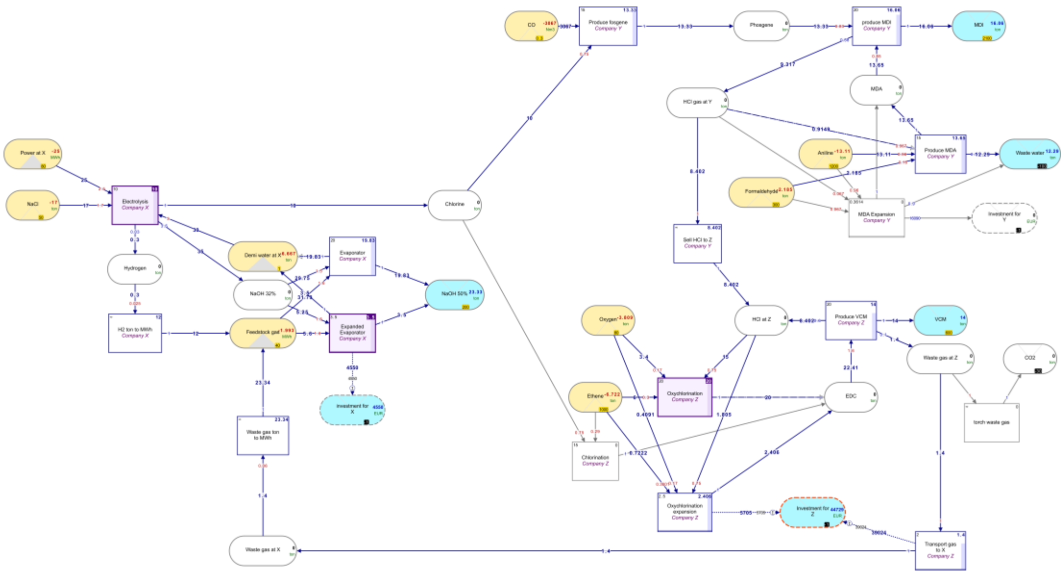

Figure 37. Executed model of the Chlorine cluster with option for waste gas recovery

We now summarise the options for the three companies with their cash flows before and after the investment for the cooperative case.

Table 6. Summary of the results for a cooperative case in the cluster

Company	Investment option	Original cash flow (€/h)	Cash flow after investing (€/h)	Additional cash flow (M€/yr)
X	Evaporator	682	1730	13.8
Y	-	13028	15200	121.6
Z	Oxychlorination	1143	1375	11
Cluster (co-op)	-	14855	18306	146.4

From Table 5 we see that the difference in the cash flows before and after the investment is large in case of the cooperative situation. Assuming 8000 operating hours in a year we calculate the cash flow per year. This will enable the calculation of the threshold investment costs for the options. The table also shows that companies X and Z make a higher profit cooperatively than when they were analysed individually, whereas Company Y is not. This can be explained by the fact that there now is no unlimited supply of raw materials, in this case: chlorine.

The simulation shown in Figure 37 reflects the cooperative strategy for the cluster as a whole. To properly analyse the investment options as a competitive game, we should now consider each company separately within the cluster. In our next series of experiments, we let the solver optimise the cash flow of each individual company while completely ignoring the cash flows of the other two companies. This means that these companies will invest at any cost as long as the new assets will enhance the one company's cash flow.

When the model shown in Figure 37 is run from the perspective of Company X, we see that Company Y does not make any profit. All the chlorine produced is used by the Company Z through chlorination. Company X invests in the expansion of its evaporator since it stands to make a profit on the high chlorine production. Company Z does not invest in the oxychlorination expansion because it will use its the chlorination process. The waste recovery option is also used by Company Z, but now it still spends on torching a small part of the waste gas. Thus Company X makes the highest profit while Company Y makes nothing. This is shown in Figure 38.

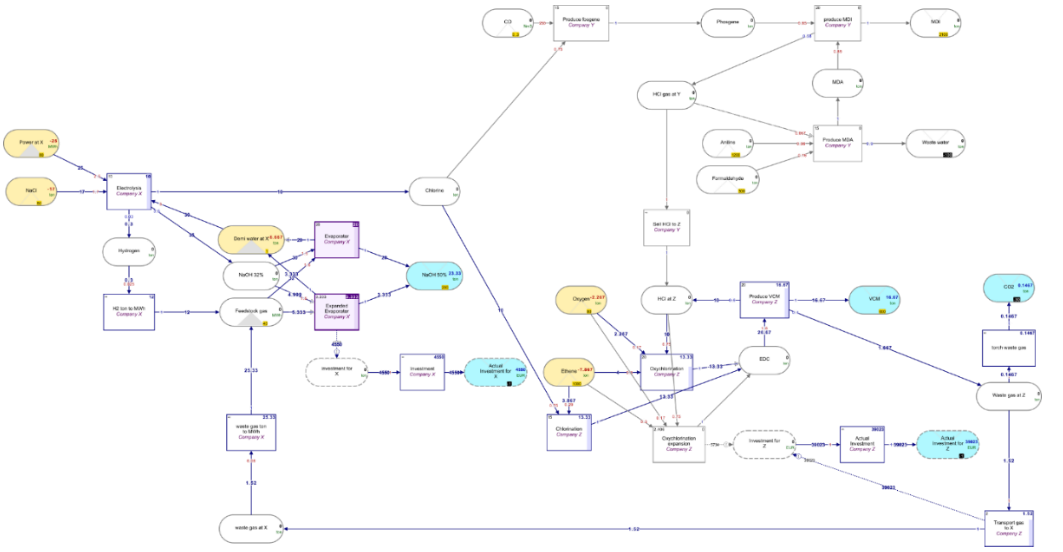

Figure 38. Executed model of the Chlorine cluster to the sole benefit of Company X

We do the same experiment and run the model from the perspective of Company Y. In this case we observe that all companies make a profit with Company X making the highest profit, followed by Y and Z. All the options for expansion and the waste recovery option are utilised in this case. This is shown in Figure 39.

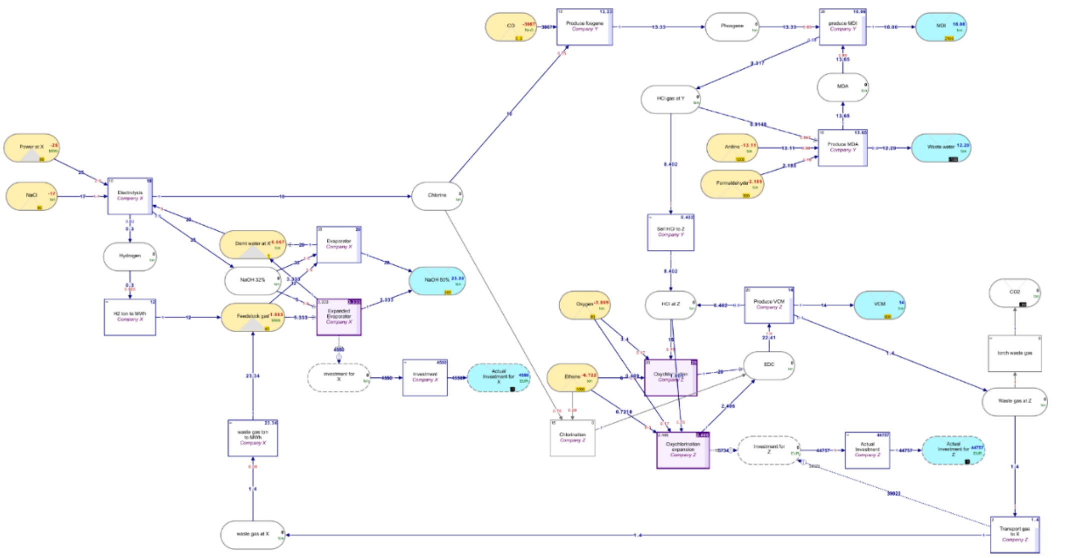

Figure 39. Executed model of the Chlorine cluster to the sole benefit of Company Y

When the above model is run from the perspective of Company Z, we see that Company Y does not make any profit. Moreover, the waste recovery option (waste gas) is not utilised by Company Z. This experiment shows that Company X in the first and Company Y in the second case compel Company Z to invest in the waste recovery option, since it does not do so when analysed in isolation. This is shown in Figure 40. Thus for the cluster to make a higher profit (overall system benefit) Company Z must invest in the waste recovery option.

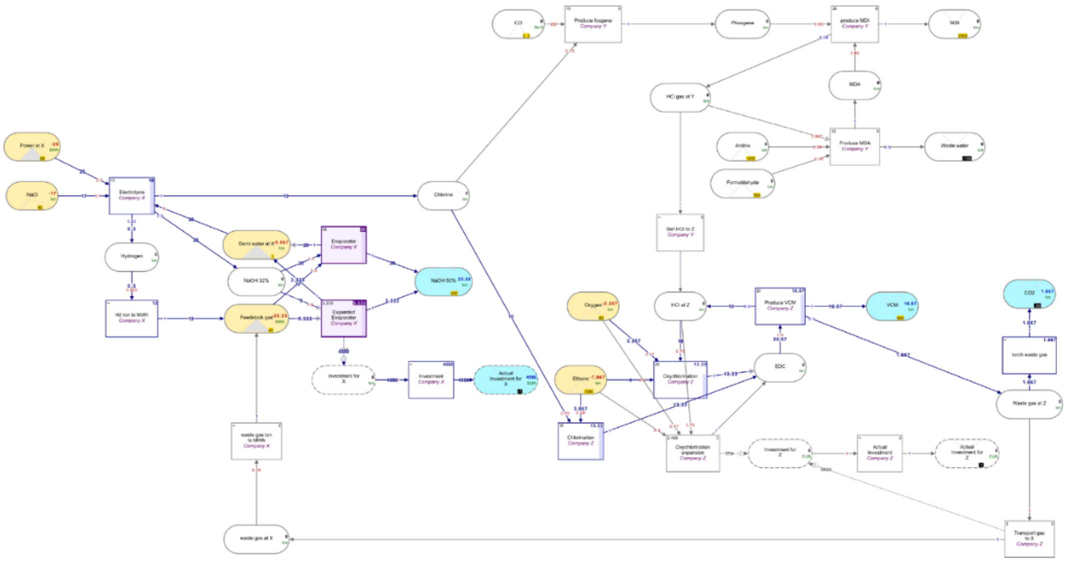

Figure 40. Executed model of the Chlorine cluster to the sole benefit of Company Z

These three experiments demonstrate the preferred single-player strategies, but evidently in a competitive setting the other companies will not make investments unless they are beneficial for themselves as well. The experiments do provide an important insight: they show that Company Z is likely to assume the role of a negotiator in the cluster. Company Z would probably demand that the price of HCl should be negative and then it would invest in the waste recovery option for the benefit of the cluster.

Although this would be a good strategy towards achieving a win-win situation, Company Y will not be happy with a negative price of HCl, as this would mean negative cash flow for Y. This creates an incentive for Company Y to look for another way of processing its side product HCl. To test this idea, we now introduce an **Absorber** as investment option for Company Y. Such an asset could convert HCl gas to a concentrated HCl solution that has market value. This asset completely changes the current situation in the cluster. Given the present assets of Company Y, this absorber can have maximum capacity of 30.77 tons. Company Y will invest in the absorber because it reduces its dependency on Company Z for processing its HCl.

Our experiments have also shown that there is a new bottleneck at the electrolysis process. Now we add an expansion process for electrolysis. This will be an expansion of 12.234 tons. We calculate the threshold investment cost for the expanded evaporator in the same way as in the previous cases. This comes up to 19827 €/hour. For the absorber, the threshold investment cost is found to be 160000 €/hour. Again we observe each Company separately within the cluster. However, the process to calculate investment costs and additional capacities becomes complex because of the non-linearity in the cluster.

When the above model is run from the perspective of Company X, we see that Company X chooses to invest in the electrolysis expansion and the evaporator expansion. This is because it stands to make a profit from the higher production of chlorine and NaOH. Since the absorber is now an option, Company Z will not invest in the oxychlorination expansion. It will now prefer a chlorination expansion. The waste gas recovery option of Company Z is again committed because the model is run from the perspective of Company X. Company Y will invest in the absorber because it can then sell processed HCL 30% on the market. This is shown in figure 41.

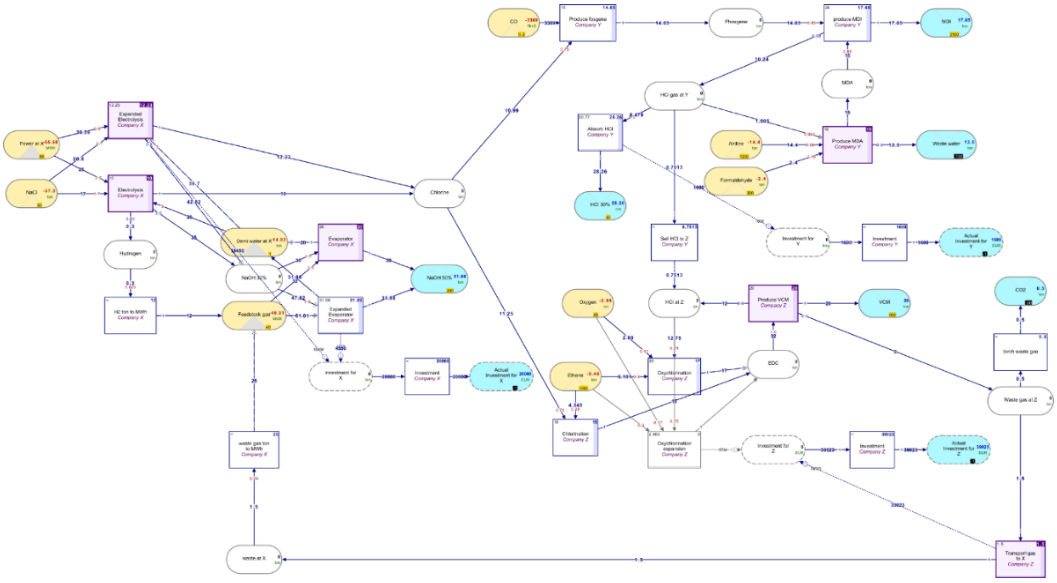

Figure 41. Executed model of the Chlorine cluster with HCl absorber from the perspective of Company X

We do the same experiment and run the model from the perspective of Company Y. In this case we observe that all companies make a profit with Company X making the highest profit, followed by Y and Z. In this case Company X still makes the two expansion investments for its electrolysis and evaporator. Company Y will now use the maximum capacity of 30.77 tons of the absorber. For Company Z, the oxychlorination expansion again is of no use because no HCl from Company Y is being sold to Company Z. This is shown in figure 42.

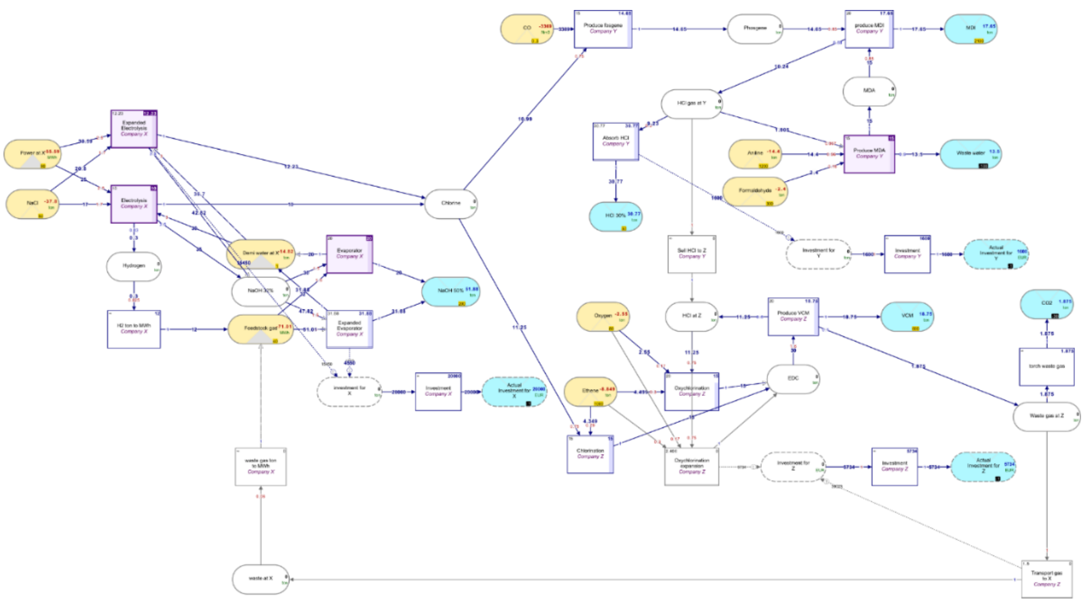

Figure 42. Executed model of the Chlorine cluster with absorber from the perspective of Company Y

When the above model is run from the perspective of Company Z, we see that Company Y does not make any profit. Moreover, the waste recovery option (waste gas) is not utilised by Company Z. This experiment shows that Company X in the first and Company Y in the second case compel Company Z to invest in the waste recovery option, since it does not do so when analysed in isolation. The absorb HCl option will also not be used in this case because the HCl produced is not enough to make profit on the investment. This is shown in figure 43.

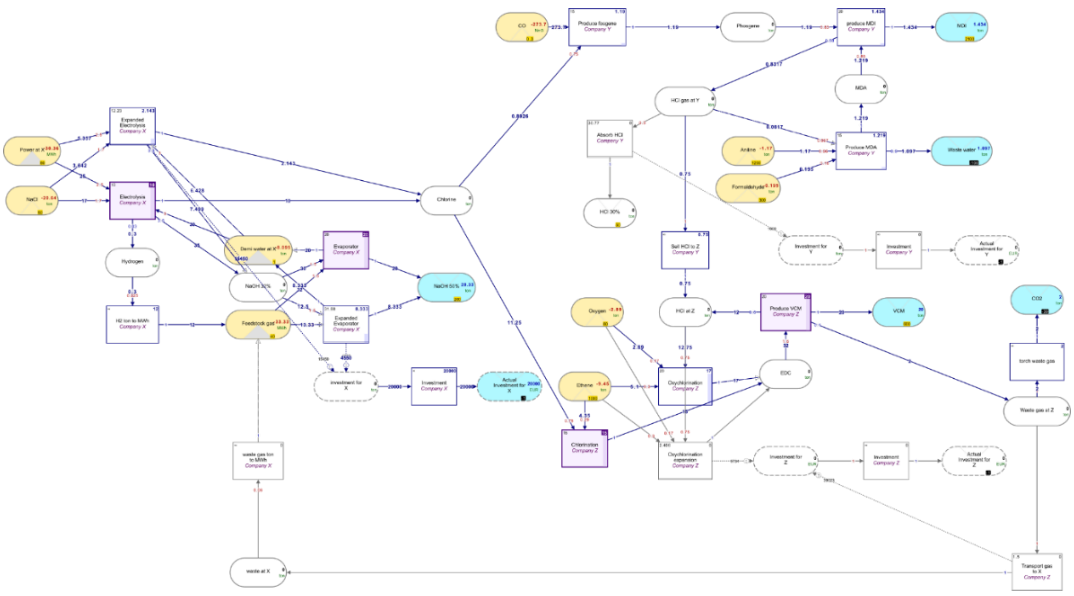

Figure 43. Executed model of the Chlorine cluster with absorber from the perspective of Company Z

We now summarise the options for the three companies with their cash flows before and after the investment for the cooperative and competitive cases.

Table 7. Summary of the results for a cooperative and competitive cases in the cluster

Company	Investment option	Original cash flow (€/h)	Cash flow after investing (€/h)	Additional cash flow (M€/yr)
X	Evaporator	682	796	6.3
Y	Absorber	13028	15350	122.8
Z	Oxychlorination	1143	1227	9.8
Cluster (co-op)	-	14855	18306	146.4
Cluster (comp)	-	14855	17337	138.7

From Table 6 we can see that the cluster performs the best in the cooperative setting in terms of overall profit. Assuming 8000 operating hours in a year we calculate the cash flow per year. This will enable the calculation of the threshold investment costs for the options. The competitive case may have higher individual profits for companies, but the cooperative case maximises the profit for the cluster as a whole.

The addition of the absorber has changed the game completely within the cluster. Now Company Z is slowly producing less VCM due to lack of HCl supply from Company Y. Although this is beneficial for Company Y, for the cluster Company

Z is important as it handles the waste from Y, produces VCM which is profitable and saves a considerable amount of feedstock gas for Company X. Company X in this case may come up with a solution where it sells chlorine to Company Z at a negative price and to Company Y at a higher price 80 €/ton. Company Y will have to comply because its production line depends on the chlorine from Company X. As we have seen before Company Z will want to invest in the expansion of the chlorination process rather than the oxychlorination process. The next section focusses on which strategies would lead companies X, Y and Z to all act cooperatively.

One strategy is reducing the price of chlorine for Company X and increasing it for Company Y will prevent Company Z from going out of business. Consider Company X strikes a deal with Companies Y and Z and sells chlorine to Y at a price of 80 €/ton. It then sells chlorine to Z at a price of -80 €/ton. Company X will lose a small amount of profit because it helps Company Z to stay afloat with the new prices of chlorine. This new experiment is shown in figure 44.

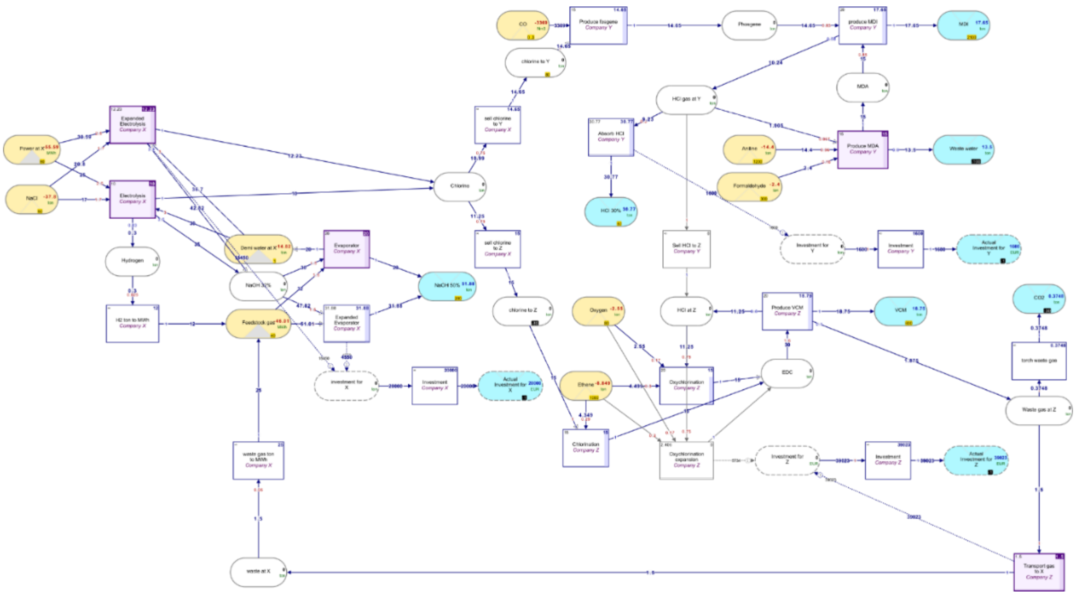

Figure 44. Different prices of chlorine for Company Z

Figure 44 shows that Company Z would invest in an expansion of the chlorination rather than the oxychlorination process. In the above case we also see that all the other investment options are being used at their maximum capacities. Thus Company X helps Company Z and in doing so makes the cluster produce at its maximum capacity. Now we introduce the chlorination expansion option as we have seen before. This is shown in figure 45.

From figure 45 we see that the chlorination expansion is indeed useful for increasing the production of VCM and thus increasing the profit for Company Z. Company Y, on the other hand has to pay a higher price for chlorine from Company X. Company Y will lose a small part of their profit, but the performance of Company Z is improved. The result is that with these prices and options each company produces their at their maximum capacity. All the options for expansion and waste recovery are used by the cluster. Company X is still making the highest profit in the cluster followed by Y and Z. However, Company X saves Y from losses by changing the price of chlorine. In doing so Company X also facilitates its own requirement of feedstock gas from the waste gas of Company Z.

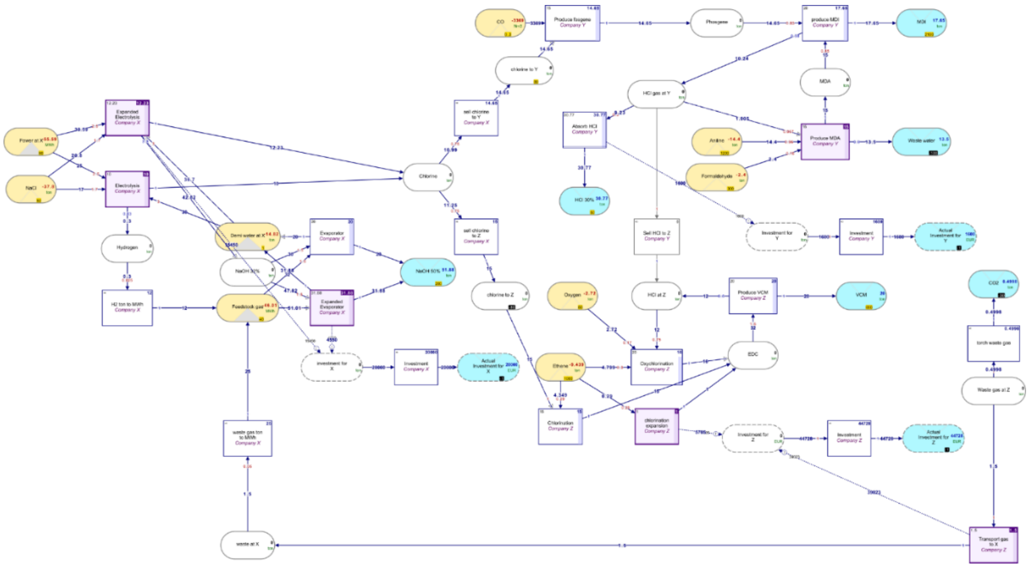

Figure 45. Different prices of chlorine for Company Z with chlorination expansion

4.6 Conclusion

In this chapter we have tested the applicability of the idea of analysing investments in an industrial cluster as multi-player games using Linny-R in a more realistic setting, compared to the more basic settings analysed in Chapter 3. We have shown that expansion options can be identified through per-company simulation, and subsequently be analysed within the cluster setting. The fact that none of our simulations took longer than a few seconds to compute suggests that the method is scalable as long as the investment options do not involve storage, or lifetime of assets. It appears to be especially the inclusion of stocks that – when combined with the binary investment decisions – make Linny-R models become computationally unfeasible.

Our experiments show that the cooperative case is more profitable for the cluster as compared to the competitive case. We also see that under certain contractual arrangement such as different prices of chlorine for Companies Y and Z, the cooperative strategy can generate benefit for all companies in the cluster. Thus, Linny-R not only optimises the cluster and shows the most optimal path but also provides analysis to support contractual arrangements between companies. This is done by changing the price of chlorine in this case.

We view our personal experience in making representations of the Chlorine cluster using the Linny-R notation, and the how we have benefited in our study from the way Linny-R visualises outcomes using colours, highlighting bottlenecks, showing material flows, and computing cash flows, as suggestive evidence that Linny-R diagrams can be used in support of communication between companies. However, it is important to note that we did not have a one-to-one discussion on communication of the models with a company. This is something that needs further research.

While we add options to the cluster such as the absorber, evaporator expansion we see that it becomes increasingly difficult to manually calculate the marginal contribution of each option. This is especially the case when a model contains feedback loops. The calculation of the investment cost and maximum capacity can then only be done through simulations, and no longer by manually doing marginal analysis.

The case study has evidently limitations in terms of applying the storage and replacement options as discussed in Chapter 3 due to computational limits.

5 Discussion

We begin this chapter by discussing the value added by this study in relation to the knowledge gap, the work performed and the significance of the research. In the next part of this chapter we discusses the Linny-R tool from the perspective of policy analysts, decision makers and researchers. Finally, the limitations of this thesis are discussed.

5.1 Relevance of the study

We reflect on the relevance of this study for three groups: policy analysts, decision makers and Industrial Ecosystem researchers. Policy analysts are experts who provide advice on the best moves regarding a policy problem. This process often involves model development with other stakeholders. Decision makers are the experts that essentially take responsibility for implementing strategic decisions. In addition, researchers who study the evolution of Industrial Ecosystems will now have access to a new dimension in terms of predicting transition pathways under various conditions

Relevance to policy analysts

This study uses the Linny-R tool to represent and analyse industrial ecosystems, adding to existing policy analysis research. It consists of examples that highlight how models can be analysed with the combination of technical knowledge and analytical thinking. In addition, it provides a practical aspects and examples to model development (chapters 3 and 4). The study demonstrates a clear and coherent use of a method of representation which enables the assessment of results for implementation of policy advice in Industrial Ecosystems. It also establishes a different way of viewing transitions in complex multi-actor ecosystems, using game theory and Mixed Integer Linear Programming. The study shows the potential of using Linny-R to handle complex information for addressing research challenges, converting this information into a relatively easy form of representation, and conducting analysis that leads to optimal strategy/s for transitions in these ecosystems.

Relevance to decision makers

According to Pruyt et al. (2011), methodologies that include model-based methods are required for companies to achieve sustainable behaviour through long term strategies. This study combines marginal analysis and optimisation techniques to analyse the consequences of decision-making. Additionally, it communicates these results through simple yet effective visualisations. The ease of calculations in terms of the marginal cumulative cash flows as well as the assumptions made, and anticipated bottlenecks offers data and support to decision-makers in order to take the best decision for the ecosystem.

This study provides a means in support of investigating possible roadmaps for emerging technologies that can be installed to accelerate and support transitions in Industrial Ecosystems. Such investigation is critical for the decision-making process because no single technology (option) is the only solution or the best solution for an effective transition. Our approach helps analysts to infer pathways for transitions in Industrial Ecosystems. After testing these pathways under various uncertainties, decision-makers can make more informed decisions to promote transitions in Industrial Ecosystems.

Relevance to researchers

Currently researchers that study Industrial ecosystems focus on the evolution of Industrial Ecosystems using agent based modelling (ABM). One of the examples we cited in Chapter 3 uses ABM for operationalising the idea of systems sustainability in the Picardie/Champagne-Ardenne oilseed crops agriculture (France) ecosystem (Bichraoui et al., 2013). The approach we have presented in thesis facilitates the *prediction* of transition pathways for industrial ecosystems under a set of preconditions, rather than studying the evolution. This research could perhaps provide an alternative method to analyse transitions in ecosystems based on the fact that Linny-R predicts the optimal investment path. This would enable researchers working on industrial ecosystems to understand investment behaviour under uncertainties such as prices of raw materials and products. Thus, the Linny-R tool could be used to carry out an exploratory analysis for investments in industrial ecosystems. This would help to identify promising configurations in ecosystems where transitions are likely to happen and where they are unlikely. In addition, the simplicity of the notation will enable effective communication to researchers and companies alike.

5.3 Limitations of the study

The approach in this thesis went through iterative changes from its inception to its final state. There are some limitations both with respect to the methods used as well as with the modelling method itself. In retrospect, these limitations will provide a strong evaluation of the findings and pave the way for recommendations for future research.

Limitations of Game Theory in the context of Industrial Ecosystems

Game theoretic concepts applied to Industrial Ecosystems function on the premise that each actor/player in the ecosystem/game aims to maximise their profit. Owing to this, policymakers must consider the reactions and behaviours of the actors while developing strategies to maximise welfare for actors. Therefore, game theory in itself cannot be used unilaterally by policymakers as a guide for their actions. However, game theory is an effective tool for policymakers to develop and refine optimal strategies which are feasible and beneficial to all the actors in the ecosystem.

Another limitation of game theory in the context of Industrial Ecosystems is the unpredictability and uncertainty of in terms of market prices, seasonal effects, availability of new technologies etc. Since transitions associated with Industrial Ecosystems will have some uncertainty attached to it, and the policymaker must change the existing strategy. This might often result in negative effects observed with respect to transitions in these ecosystems (Dubina et al., 2015). For example, changes in strategies might result in discouragement of investment in a new technology which was otherwise beneficial for the ecosystem.

Model-related Limitations

The Linny-R graphical notation has some limitations with respect to its model design and simulation. The box-and-arrow representation is clear and depicts information as described in chapter 3. However, it becomes increasingly difficult to read models with large number box and arrow connections. This can be observed already in Chapter 4, where a diagrams become more complicated (with an increasing number of crossing arrows) as investment options are added.

Another limitation to the Linny-R notation is that introducing storage options and life time of assets result in long computation times. When solver time is limited, Linny-R will produce sub-optimal solutions that – given that the investment decisions are represented by binary decision variables – are then arbitrary and hence meaningless. In addition, uncertainties such as price changes of products affect the optimisation, and many such additions lead to a slow runtime (Ruth et al.,2009, Urbanucci, 2018).

Another limitation is on the assumption that the player/investor has complete information about the prices of products. This is related to the concept of perfect knowledge that is assumed during MILP optimisation in this thesis. This means that the solver in Linny-R finds a solution for each optimisation period based on the next time steps that are provided in the time series data.

A technical limitation of the current browser-based Linny-R implementation is that it does not yet support copy/paste from one model to another. For example, if there is a part of a model that needs to be replicated in a new file, it is not possible to directly copy and paste that part of the model. The workaround solution is to save a model, reload it and remove the unwanted connections, but evidently this is inconvenient.

Another technical limitation is that Linny-R models cannot be invoked by other software tools such as Python. It is presently not possible to automatically run many experiments with a Linny-R model to test it under a variety of scenarios. A work-around for this is to design scenarios on paper and physically input the values into the Linny-R model. This of course is cumbersome when there are a lot of variables involved. A similar argument can be made for the sensitivity analysis for a Linny-R model.

6 Conclusions and Recommendations

In this concluding chapter we revisit the aim we had for this thesis. We then review our research question and sub-questions in the light of our experiences with Linny-R as modelling language and simulation tool. Finally, we provide recommendations for future research.

6.1 Conclusions

In this thesis we have investigated a way of determining optimal investment paths for industrial clusters while assuming that these investments should contribute to sustainability, provide a positive return for a cluster as a whole, and allow for a distribution of costs and benefits such that the companies that make the investment have strong incentives for cooperation.

As explained in Chapter 2, the leading idea has been to represent industrial clusters as networks of processes that are owned and operated by different companies, and interdependent via their input-output flows. We assumed that this representation would then facilitate analysis from an industrial ecosystem perspective, and identification of potential investment options that would improve the cluster's sustainability. The next step was that from a game theory perspective, these investment options can then be seen as potential moves, the companies as players, and any combination of investments within an investment horizon of one or several decades would constitute a strategy. For each company, the difference in cumulative cash flow for that company with/without these investments would constitute the players' payoffs. Analysis of such a multi-company investment game should then reveal rational strategies.

In Chapter 3, we have elaborated and tested this idea by using the Linny-R modelling language and its associated MILP optimisation tool that is being developed at TU Delft to represent and analyse a variety of simple process configurations with only one or two investment options. Conducting this first series of small-scale simulation experiments with these basic 'building blocks', and verifying their outcomes has demonstrated the feasibility of our approach.

In Chapter 4, we have applied the same approach to a realistic, albeit simplified and stylised, industrial cluster that comprises three companies. We have used the resulting Linny-R model to simulate the production processes of individual companies, and to see whether this helped to identify potential investment options. Using this initial set of investment options, we have conducted a second series of experiments to simulate a cluster-wide cooperative strategy as well as competitive strategies, and finally look for a win-win situation for all parties by evaluating various contractual arrangements.

These experiments allow us to appraise Linny-R as a tool for representation and analysis of investment decisions in industrial ecosystems such that an economically rational transition path of the ecosystem can be inferred. We have found that the

Linny-R modelling language and its underlying MILP optimisation tool effectively allow us to:

- represent processes, companies, input output flows and interdependencies in industrial clusters as diagrams that make intuitive sense;
- assess the economic performance of such clusters, and also of possible investments in such clusters, based on profit-maximising process simulation;
- identify potential investments that could contribute to a transition towards sustainability;
- represent investment decision such that they can be made in accordance with economic rationality;
- represent and analyse investment decisions as multi-actor games, both from a cooperative and competitive perspective.

Linny-R is an executable graphical model specification language that optimises the total cash flow for (a selected subset of) the companies in a cluster. This also allows assessment of environmental performance (e.g., reduction in emissions), provided that environmental impacts can be monetarised.

We found that we were able to represent different categories of potential investments: expansion of capacity, recycling, storage, and replacement of assets. Using these categories, potential transitions can be made towards sustainability in industrial ecosystems.

We found that the Linny-R specification language allows representation of investment options and associated one-time investment cost if we take a relatively long time step (1 year) and then represent investment cost as 'start-up' cost – a cost that is normally used to represent operational start-up and shut-down on a time scale of hours, rather than years. The Linny-R semantics then ensure that investment options are committed (i.e., 'start up') only when they have a positive return on investment (Net Present Value) for the cluster.

Orr experiments in Chapter 4 have demonstrated that simulations using Linny-R support finding pricing arrangements that would be economically rational for all companies concerned.

Although our case study was stylised, we contend that the findings can be generalised to any industrial ecosystem where stakeholders aim to maintain the maximum production while focussing on more sustainable practices in the ecosystem. This suggests that – despite the limitations we have discussed in Chapter 5 – the Linny-R language and tool we used in this thesis has merits because of its qualities such as representation, analysis, and optimisation of Industrial Ecosystems with respect to investment decisions. It has a few drawbacks which will be discussed in the section after the relevance to policy analysts, decision makers and researchers studying industrial ecosystems.

6.2 Recommendations for Future Research

This section focusses on the actions that can take this research forward. From the previous sections of the reflection and limitations it is clear that the use of Linny-R is well within reason. However, its effective implementation in industrial problems would require improvements in certain spheres of the research.

Firstly, we did not investigate the scalability of the method. We experimented with a relatively small and simplified cluster; upscaling to a cluster with 10 or 100 times more processes could become computationally infeasible. As a next step, we recommend applying the approach that we have taken in this thesis to a real-world cluster, gradually expanding the scope of the model as well as the set of investment options, so as to test at which point the approach becomes strenuous, and for what reason, e.g., conceptual shortcomings, loss of clarity due to cluttering of diagrams, or computational constraints.

Secondly, we did not test in practice whether models in the Linny-R notation does indeed support communication and negotiation between companies. We therefore recommend to conduct the research we recommended in the preceding paragraph in participatory fashion as much as possible. We are aware, though, that active and open involvement of multiple companies may become more difficult to the extent that these companies have competing interests.

Thirdly, the set of categories of investment options that we have identified is not exhaustive. Our recommendations for future research hence are to explore the computational limits using a state-of-the-art commercial solver, and to conduct real-world case studies, meanwhile extending and refining the categories of investment options that can be instrumental in furthering the transition towards more sustainable industrial clusters.

Although these venues for future research reflect that the current approach and tool can be improved, the key conclusion that can be drawn from this thesis is that we can indeed use Linny-R as a modelling language and simulation tool to represent and analyse investment decisions in industrial ecosystems as multi-actor games, which then allow us to infer and evaluate cooperative as well as competitive investment strategies.

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