Master Thesis Operations Research and Quantitative Logistics

Sustainable Industrial Cluster Games

Name student: M.J.A. Stelwagen
Student ID number: 419693

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Abstract

An investment in decarbonisation options in the industrial sector in the Netherlands is needed to reach the goals set in the climate agreement in 2019. The companies within an industrial cluster need to decide on which decarbonisation option will be executed and how the costs of this decarbonisation option will be allocated over the involved companies. Cooperative game theory is used to investigate how and if a choice can be made such that all the companies agree to work together. In this research different methods are proposed to construct the transferable utility game by computing which option gains the highest utility for each coalition, while satisfying certain constraints that imply that the resulting allocation is stable and fair. We propose to use individualised utility functions to better represent the different incentives of the involved companies. Using the individualised utility functions two procedures are proposed that iteratively compute the utility value of each coalition by making an allocation of the costs and the environmental benefits for that coalition. Adjustments and extensions on the allocation model of Tan et al. (2016) are suggested to be able to allocate the costs and environmental benefits based on different definitions of a fair and stable allocation. Finally, the different methods are tested on different data instances based on one of the five industrial clusters in the Netherlands, called Chemelot.

ERASMUS UNIVERSITEIT ROTTERDAM
Erasmus School of Economics

Supervisor:
Dr. W. van den Heuvel
Second assessor:
Dr. R. Spliet

TNO
Strategic Business Analysis

Supervisors:
Dr. M. Groote Schaarsberg
Ir. P. Verstraten

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Nomenclature

General

O	Set of all coalitions
N	Set of all companies
D	Set of all decarbonisation options
G	Set of decarbonisation options that are considered to be group investments
I	Set of decarbonisation options that are considered to be individual investments
A	Set of all alternatives/strategies that can be chosen
A_S	Set of all strategies that can be chosen by coalition S
B_S	Index of a strategy of coalition S
i	Index of a company
a	Index of a decarbonisation option
S	Index of a coalition
n	Total number of companies
E_S	Sum of current CO_2 eq. emission of the companies in S
p	Percentage of current CO_2 eq. emission that has to be reduced
e_{S,B_S}	The total amount of CO_2 eq. emission that can be reduced by coalition S by choosing strategy B_S expressed in euros (by making use of the MKI value)
e_{S,i,B_S}	The amount of CO_2 eq. emission that can be reduced by company i, if strategy B_S is chosen expressed in euros (by making use of the MKI value)
c_{S,B_S}	The amount of costs that are incurred to coalition S, when strategy B_S is chosen
$c^f_{S,a}$	The amount of fixed costs that are incurred to coalition S, when strategy B_S is chosen
c^v_{S,i,B_S}	The amount of variable costs that are incurred to company i, if strategy B_S is chosen
c_{S,i,B_S}	The amount of costs that are allocated to company i, if strategy B_S is chosen

Characteristic function

u_i	Individualised utility function of company i
u_S	Joint utility function of coalition S
$v(S)$	Characteristic function value for coalition S
y_{B_S}	Decision variable indicating if strategy B_S is chosen
x^c_{S,i,B_S}	Decision variable indicating the amount of cost allocated to company i, if coalition S chooses strategy B_S

Allocation

λ^{TM}	Continuous variable in the TM model
C_i^{TM}	Marginal contribution of company i in the TM model
x_i^{TM}	Payoff of company i in the TM model
$v^{TM}(S)$	Characteristic function in the TM model
λ	Continuous variable
γ	Continuous variable
C_i	Marginal contribution vector for each plant i in our model $:= (C_i^e, C_i^c, C_i^u)$
C_i^e	Marginal contribution of company i to the environmental benefits

C_i^c Marginal contribution of company i to the costs

C_i^u Marginal contribution of company i to the total utility

x_i Payoff vector of company i in our model $:= (x_i^e, x_i^c)$

x_i^e Payoff of company i in environmental benefit

x_i^c Payoff of company i in costs

$v(S)$ Characteristics function vector in our model $:= (v^e(S), v^c(S), v^u(S))$

$v^e(S)$ Characteristic function value on environmental benefits

$v^c(S)$ Characteristic function value on the costs

$v^u(S)$ Characteristic function value on utility

Iterative procedures

R Set of requirements that have to be satisfied by a cost allocation to be stable, determined by the cooperating companies

x_i Decision variable indicating how much costs are allocated to company i

r Rules and regulations that determine how the CO_2 eq. emission reduction and costs are allocated, predetermine by an industrial cluster management $:= (r^e, r^c)$

r^e Rules and regulations on the allocation of environmental benefits

r^c Rules and regulations on the allocation of costs

b_i Parameter indicating how much the allocation of environmental benefits to company i benefit the company in terms of utility

k_i Parameter indicating how much the allocation of costs to company i set back the company in terms of utility

f_i Utility function of company i given coalition S and the chosen strategy B_S and given the predetermined allocation rules and regulations

y_{B_S} Decision variable indicating if strategy B_S is chosen by coalition S

Abbreviations

VP Valuation Problem

AP Allocation Probelm

CM Cost Minimisation

JUF Joint Utility Function

IUF Individualised Utility Function

TM Tan/Maali

DoES Degree of Environmental Satisfaction

DoFD Degree of Financial Dissatisfaction

ETM Extensive Tan/Maali

RCA Repeated Cost Allocation

PRR Predetermined Rules and Regulations

1 Introduction

Global warming is one of the biggest problems our generation is facing. Over the past 100 years, the global average temperature has increased by approximately 0.6°C and is projected to continue to rise at a rapid rate, as stated in Root et al. (2003). This rapid rate of change is a primary concern for not only wild species and their ecosystems, but also for the world as we know it. In Root et al. (2003) it is stated that the balance of evidence presented in their studies strongly suggests that a significant impact of global warming is already discernible in animal and plant populations. The combination of rapid temperature rise and other stresses, such as habitat destruction, could lead to numerous extirpations and extinctions. Furthermore, as stated in Erlandson (2008), with global warming, average sea levels are now expected to rise between 20 and 200 cm in the 21^{st} century. A rising chorus of scientific, political and media voices has warned of the growing threats global warming and climate change pose to earth's ecosystems, cultures and geopolitical stability. Warming climate and oceans, melting glaciers, rising seas and collapsing marine ecosystems are emblematic of the growing impacts of humanity on our oceans and coastlines.

The influence of greenhouse gasses on global warming has caught the attention of scientists, politicians and the general public via the well-known "greenhouse effect". In Anderson et al. (2016) this effect is explained. Solar radiations passes partially unhindered through the atmosphere, heating the Earth's surface. In turn, energy is re-emitted as infrared, much of which is absorbed by greenhouse gasses and water vapour in the atmosphere. In this way, the atmosphere acts as a blanket surrounding the Earth. The concentration of greenhouse gasses in the atmosphere highly influences the global temperature on Earth. This concentration is increasing every year, partially due to CO_2 emissions emitted by human kind. In the report of the Netherlands Environmental Assessment Agency, Olivier and Peters (2019), it is stated that the global CO_2 emissions increased with 2.0% in 2018. The six years before 2018 the growth rate was around 1.2% and in the decade before 2011 the growth rate was even higher, with an average CO_2 emission growth rate of about 2.8%, annually. Olivier and Peters (2019) also state that in 2018 the total amount of CO_2 that was emitted globally was equal to 51.8 gigatonnes of CO_2 equivalent. CO_2 equivalent is a measure that indicates how much a given amount of greenhouse gas contributes to the heating of the earth expressed in an equivalent concentration of CO_2. In this way different greenhouse gasses can be described using one unity.

To avoid climate change, a treaty, called the United Nations Framework Convention on Climate Change (UNFCCC), was founded and signed by 154 states in 1992 in Rio de Janeiro. This treaty stated that the signatory countries pledged to take measures to avoid climate change, as is stated by Gutiérrez et al. (2018). However, no specific measures were set out in this treaty. In 1997 the Kyoto Protocol was introduced by the UNFCCC, where the signatory countries committed themselves to reduce their greenhouse gas emissions to certain levels by 2020. However, no procedures that each country should follow to achieve these goals were established. In 2015 a new meeting was held by the UNFCCC in Paris. From this meeting, the Paris Agreement came into being. In this agreement the 188 signatory countries committed themselves to controlling their greenhouse gas emissions and to gradually reduce their greenhouse gas emissions in the coming years.

In June 2019, following the Paris Agreement, a climate agreement was made in the Netherlands. This agreement stated that the Netherlands will realize a reduction in CO_2 eq. emissions of 49% in 2030, with respect to the CO_2 eq. emissions in 1990. The agreement also states that the CO_2 eq. emissions will be reduced further to approximately zero in 2050. The details of this task have been discussed over five different sectors in the Netherlands, as stated in DNV GL Netherlands B.V. (2020). For each sector the task is set to reduce the amount of CO_2 eq. emissions by a certain quantity. To cumulatively accomplish the reduction of 49% by 2030, the industrial sector has to reduce its CO_2 eq. emission by 19.4 megatonnes.

In the Netherlands the industrial sector consists of five industrial clusters. Porter (1990) defines clusters as geographical concentrations of affiliated companies and institutions in a specific market. Making use of a joint infrastructure for raw materials, products, natural gas, electricity, water, industrial gasses and steam and heat networks the companies within these clusters can achieve maximum efficiency of their entire production process. Cooperation between the different companies within the industrial clusters is called industrial symbiosis (IS). Some examples are the use of an end or waste product of one plant as feed stock for another plant or the shared use of an infrastructure for the supply of natural gasses or hydrogen. This is one of the main reasons these industrial clusters exists. The five industrial clusters in the Netherlands are spread across the country.

In recent years a lot of research has been done on different options to ensure the CO_2 eq. emission reduction in the industrial sector. In the reports, van der Linden (2019) and DNV GL Netherlands B.V. (2020), the current situation of the five industrial clusters in the Netherlands are investigated. Moreover, different suggestions and recommendations on the decarbonisation of the industry are made, such as developing a hydrogen infrastructure. Also, the Manufacturing Industry Decarbonisation Data Exchange Network (MIDDEN) project was initiated by PBL and ECN part of TNO. As is stated by Batool and Wetzels (2019), the project aims to support industry, policymakers, analysts and the energy sector in their common efforts to achieve deep decarbonisation. The reports that are part of this project, Batool and

Wetzels (2019), Semeijn and Schure (2020) and Oliveira and van Dril (2020), investigate the decarbonisation options, while focusing on the Dutch fertiliser industry, PVC industry and large volume organic chemicals production. Among these reports the most popular, or even indispensable, decarbonisation options are (i) carbon capture and storage (CCS), (ii) using hydrogen as feedstock instead of natural gasses, with a lower CO_2 footprint produced on the site of the cluster itself and (iii) using hydrogen with a lower CO_2 footprint produced on another location and transported through a hydrogen infrastructure.

DNV GL Netherlands B.V. (2020) states that, to reach the goals set in the climate agreement, it is crucial that decisions will be made in the short term on what decarbonisation options will be used. Most of the decarbonisation options are based on a common infrastructure or hydrogen plant that will benefit multiple companies. Therefore, these options require cooperation and joint investments. In the five industrial clusters in the Netherlands industrial symbiosis already takes place. However, until now, no agreements have been made on the joint investments on decarbonisation options. Some of the reasons that such an agreement has not been made yet are (i) that the social support of these new technologies is still fragile, (ii) that the current laws and regulations are not always in sync with these new technologies, (iii) that the technologies themselves still have some minor issues that have to be resolved, (iv) increasing sunk costs as firms continue to invest in incremental improvements in incumbent installations, (v) system integration in chemical clusters, (vi) the outcome of a decision of one company depends on the decisions of the other companies and (vii) the risks involved with choosing a certain decarbonisation option, as is mentioned in van der Linden (2019) and Janipour et al. (2020). Also, one of the main question that arises is, how the costs will be divided over the investing companies. In our research we will try to give answer to the latter question and in this way give a guideline for the companies in their negotiations.

We will solve this question using cooperative game theory. Game theory is a mathematical field that describes strategic conflict or cooperative situations. As stated in Gedai et al. (2012), the characteristics of these situations are (i) the parties are selfish, meaning they want to maximise their own profit and (ii) the outcome depends on the parties' actions. We call this conflict or cooperative situation a game and the involved parties are called the players. Each player will form a strategy, which determines their actions for every possible game scenario. Given the strategies of the players, a game can be played and the outcome can be determined. The outcome in general is described as the payoffs for each player. The difference between cooperative and non-cooperative game theory is that in cooperative game theory the players are able to make binding agreements, whereas in non-cooperative game theory they are not. In a cooperative game, multiple players gain benefit from working together in a coalition. Then, the total benefits of the coalition is divided among the players in the coalition. Multiple methods have been developed to compute such a division. To gain more insight in the basic ideas of cooperative game theory and cost or benefit allocation we refer to Ferguson (2020), Gedai et al. (2012) and Gedai et al. (2015). In our case, the companies within the industrial cluster are about to make strategic decisions on how to realise the energy transition if they are willing to live up to the agreements made in the climate agreement. They have multiple options in doing so and for some options, working together could reduce their costs. Therefore it seems reasonable to describe this situation using cooperative game theory. TNO, the knowledge organisation for which this research will be done, are interested in finding out if this mathematical field of cooperative game theory can provide new and necessary insights that could help the energy transition within the industrial clusters. Some applications and uses of cooperative game theory will be summarized in Section 2.1.

We will investigate solution methods to a transferable utility (TU) cooperative game that are applicable to the decision making within an industrial cluster. In a TU-game the players are able to make monetary payments to other players to convince them to work together. In our case this could be possible in the way that one company takes over some of the costs of another company, or it would even be possible to pay another company to join the coalition. A TU-game consists of a set of players and a certain characteristic function that assigns a certain value to every possible coalition that can be formed by the players. A more detailed description and mathematical formulation of a TU-game is given in Section 3.

Our research focuses both on the formulation of the characteristic function as well as on the allocation of the benefits and costs among the participating companies within a coalition. This allocation can be made after a characteristic function is defined and a certain value to every possible coalition is given. In the defining of the characteristic function we will propose different models that represent different real life situations. These models will be further explained in Section 4.1. A linear programming model that is used in Tan et al. (2016) on the designing of a new industrial cluster will form the basis of our allocation solution method. The model in Tan et al. (2016) is based on a solution method proposed by Maali (2009), which we will further explain in Sections 2.3 and 4.2.

Our research will contribute to answering the question: what can the use of game theory contribute to the energy transition within the industrial cluster? The main research questions of this research and their sub questions will be stated in Section 3.

The cluster we will focus on the most is the industrial cluster in Limburg, called "Chemelot". We will develop a general model that could be implemented on all the clusters, but test it on data that is based on the Chemelot cluster.

The remaining of this thesis will be organized as follows. In Section 2, we will give a brief literature review on applications of TU games, the research done on the defining of the characteristic function and different allocation methods. In Section 3, we will describe the problem that we will investigate formally and in mathematical notation and we will state our research questions. In Section 4, we will describe the methods we will use for the definition of the characteristic function as well as the methods we will use to allocate the benefits and the costs among the participating companies within a coalition. In Section 5, we will explain on what kind of instances we will test the different models and how we obtained these data instances. Section 6 will show and analyse the results of implementing the proposed models and solution methods on the different data instances. Furthermore, the different solution concepts will be compared and a recommendation will be made on when each solution method is best applicable. Finally, in Section 7 a discussion on the research will be given as well as a conclusion will be stated, giving answer to the research questions stated in Section 3. Furthermore, in Section 7 some ideas for future research that might be done on the subject are given.
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2 Literature review

The purpose of this literature review is to provide an overview on the past research that has been done on the subject. Combining this with the practical problem we are facing, our contribution to the research field will come to light. We will give an overview on the applications and uses of TU games. Furthermore, we will give an overview on the past research that has been done that might help answering our research question. As our research question is twofold, we have divided this collected literature into two main subjects.
Therefore, the remaining of this Section will be structured as follows. In Section 2.1 an overview will be given on applications and uses of TU games and in particular on TU games for sustainable group decision support. In Section 2.2 we will focus on the defining of the characteristic function that assigns a certain value to coalition S. Finally, in Section 2.3 we will dive deeper into the allocation of the benefits gained from the coalition as well as the allocation of the costs needed to assert the sustainability option that is used by the coalition.

2.1 Applications and uses of TU games

The use of TU cooperative game theory has been useful in multiple applications. We will start by reviewing some different applications.
van den Brink et al. (2012) use TU games to divide water from a river among the agents located along that river in such a way that the total utility that is gained from this allocation is maximised and such that every agent's utility is higher than when working alone.
In other applications, TU cooperative game theory is used to minimise costs in economic problems. For example, Fiestras-Janeiro et al. (2011) gives a review on the applications of cooperative game theory in the management of centralized inventory systems. In these applications the cooperation between suppliers, manufacturers, distributors, retailers and customers is investigated using cooperative game theory. The centralization of inventory management and coordination of actions leads to a reduction of the costs and an improvement of the customer service level. van den Heuvel et al. (2007) investigate another example in which game theory is used to minimise the cost of an economic problem. In this paper the cooperation among retailers, facing an economic lot-sizing (ELS) problem, is investigated. By placing joint orders instead of individual orders, the costs of the retailers can be reduced and a cooperative game arises. It is shown that the ELS games are balanced, meaning that the core of the ELS games is non-empty. The core is the set of stable cost divisions of the total cost in which no player or subset of player has a direct incentive to leave the grand coalition. In another example, van Zon et al. (2020) investigates the possibility of collaborative transportation in the joint network vehicle routing game, which can reduce transportation costs as well as greenhouse gas emissions. By pooling all the customers of different companies, facing a Capacitated Vehicle Routing Problem (CVRP), it is possible to reduce the costs and greenhouse gas emission significantly. The cost allocation problem that arises from this cooperation is solved using TU cooperative game theory.
Cooperative game theory is also used to support sustainable group decision. For example, Jin et al. (2018) uses cooperative game theory to allocate the energy savings among the cooperating plants of the design of the heat exchanger network (HEN). This HEN is designed such that the heat recovery among multiple plants is maximised. Another example is given in Soltani et al. (2016). Soltani et al. (2016) propose a decision framework that models the stakeholder's conflicting priorities over the sustainability criteria, when selecting a municipal solid waste treatment option. It then uses game theory to fairly distribute the costs and the benefits among the stakeholders. The framework is demonstrated by applying it to select a waste-to-energy technology for Vancouver, Canada.
Finally, the cooperative game theory approach is used in industrial symbiosis applications, which can also lead to

greater sustainability gains. Tan et al. (2016) use game theory to divide the benefits of cooperation between different companies within an eco-industrial park. Within these clusters, industrial symbiosis is used to promote sustainable exchange of materials and energy streams among different plants and companies. In this case, cooperative game theory is used to develop a rational and defensible scheme for sharing the pooled benefits among all the cooperating partners.

2.2 Characteristic function

As described before, the characteristic function in a TU-game assigns a value to every possible coalition $S \subseteq N$. For many applications, different solution methods exist. Fiestras-Janeiro et al. (2011) give a review on solution methods for defining the characteristic function, when retailers try to cooperate by centralizing their inventory management and coordination of their actions. Their review splits the solution methods for defining this characteristic function into two categories: (i) the characteristic function is given by an explicit formula or (ii) the characteristic function is given by the optimal value of an optimization problem. In the first category it is assumed that all the players in the coalition agree on working together and that there is only one way of working together. Therefore, the cost savings of every coalition can be determined by an explicit formula. In the second case, multiple ways of working together exist and an optimization method is needed to determine which way is the most preferred. As in our case there are multiple decarbonisation options we are more interested in the latter.

Guardiola et al. (2009) introduce a new class of cooperative games, the class of Production-Inventory (PI) problems. In these games the cooperation between agents by sharing production processes as well as warehouse facilities is investigated. Guardiola et al. (2009) define the characteristic function as the optimal value obtained from the linear production inventory (LPI) problem for the coalition S. This LPI problem decides on how the agents should work together to minimise the total cost. This LPI is solved for each coalition S to determine the values of the characteristic function.

van Zon et al. (2020) and van den Heuvel et al. (2007) also define the characteristic function as the solution to an optimization problem. In van den Heuvel et al. (2007) the value of the characteristic function is the solution to the combined economic lot-sizing problem of the retailers in each coalition. In the economic lot-sizing problem a retailer tries to minimise its ordering, holding and production cost when ordering a single item at a manufacturer. Now consider multiple retailers ordering the same item at the same manufacturer. If they combine their orders they could reduce their ordering cost. In this case, the values of the characteristic function are the solutions to the minimisation of the total costs of the retailers in each coalition.

van Zon et al. (2020) compute the values of the characteristic function by solving the Capacitated Vehicle Routing Problem (CVRP) on the combined graph of the companies in each coalition. In the CVRP multiple customers are served from a central depot using trucks with a certain capacity. This CVRP is defined as a complete directed graph G containing the central depot, all the customers and the arcs on which the trucks can travel. If the companies work together and the graphs are combined into one graph a solution can be found that reduces the total cost and an allocation of the costs can be made such that the costs are reduced for all the involved companies.

A similar approach is used by Jin et al. (2018) for a different application. Jin et al. (2018) design a Heat Exchanger Network (HEN) between multiple plants to maximise heat recovery. Jin et al. (2018) formulate a conventional Mixed-Integer Nonlinear Programming (MINLP) model to determine the minimum total annual cost of each coalition. The optimal value obtained from this MINLP for each coalition is used as the value of the characteristic function. Some other examples of characteristic functions given by the optimal value of an optimization problem are found in Lozano et al. (2013) and Chen and Zhang (2008). Lozano et al. (2013) investigate the cost savings that different companies may achieve from merging their transportation requirements and Chen and Zhang (2008) investigate the cost savings that multiple retailers may achieve from placing joint orders to a single supplier.

In van den Brink et al. (2012) a water sharing problem among agents located along a river is investigated. The characteristic function values are computed by maximising the utilities of all agents in each coalition. This utility function differs per agent and is described by $u(x,t) = b(x) + t$, where x is the amount of water allocated to the agent, t is a monetary compensation to the agent and $b(\cdot)$ is a strictly increasing and strictly concave continuous function yielding the benefit to the agent. In this way the individual goals of agents are incorporated in the optimization problem, as some agents might attach different value to water consumption than others.

In Kleppe et al. (2012) the situation, where multiple players would like to cooperate and have multiple options in doing so, is described as a cooperative situation. The multiple options do not only depend on how these players work together but also on the composition of the players working together. Therefore, in the cooperative situation all possible coalitions of involved players will be examined. A cooperative situation is defined by (N, A, K), where N is the set of players, A the set of alternatives and $K : A \to \mathbb{R}$ a cost function that assigns to each alternative $a \in A$ a certain cost $K(a)$. It is stated that to get the definition of the characteristic function it is needed to solve the cost minimisation problem of a cooperative situation for each coalition. Meaning that for each coalition S, the option $a \in A$ is found, which minimises the costs $K(a)$. Furthermore, an Alternative Problem Representation (APR) of a

cooperative situation is formulated by (N, A, k). In the APR the cost function $k : A \to \mathbb{R}^N$ is individualised, denoting for each alternative $a \in A$ a corresponding cost $k^i(a)$ for every player $i \in N$. Solving the cost minimisation problem again depends on its application.
In Section 3 we will give an explanation on how we will use this past research in our own research.

2.3 Benefit and cost allocation

The problem of allocating the costs as well as the benefits of the investment in a decarbonisation option by a certain coalition S can be formulated as a TU-game. In a TU-game there exists a mechanism for the transfer of utility between the players besides the game itself, as is stated in Ferguson (2020). In our case, this transfer will be in the form of money. A solution to such a game is given in the form of a payoff vector $\mathbf{x} = (x_1, x_2, ..., x_n)$, where x_i denotes the amount of costs/benefits allocated to player i. Assuming that all players of the TU-game are rational, the set of solutions called the core are believed to be stable solutions. A solution lies within the core if it satisfies the coalitional rationality constraint and the efficiency constraint. A solution satisfies the coalitional rationality constraint if the benefits allocated to a group of players in the solution are higher than the benefits that group of players could gain by leaving the coalition. The solution satisfies the efficiency constraint if the sum of the benefits allocated to the players is equal to the total benefits obtained by the grand coalition ,$S = N$. Some solution concepts, mentioned in Ferguson (2020), Gedai et al. (2012) and Gedai et al. (2015), are the Shapley value and the Nucleolus. The allocation of the Shapley value, which is introduced by Shapley (1953), is based on the contribution and the bargaining power a player has to the coalition. The Nucleolus computes an allocation while trying to minimise the worst inequity.
In Lozano et al. (2013), the Shapley value, Nucleolus and some other cooperative game solution concepts are tested on several instances and compared. Extensive numerical experiments have been carried out to gain insight into the behavior of the different solution concepts.
Another solution method, proposed by Maali (2009), is also based on the contribution of each player to the coalition. In Tan et al. (2016) a linear programming cooperative game model to allocate the benefits of a certain coalition is used on the designing of an industrial cluster, based on the model in Maali (2009). The model in Maali (2009) is based on the idea of the core, but instead of requiring rationality for all groups, a multiobjective approach is proposed. The model is based on the max-min aggregation method where the optimum solution is obtained by maximising the least satisfied constraints.
Andiappan et al. (2016) extend the work of Tan et al. (2016) by presenting an optimization-based negotiation framework for plants in an eco-industrial park. The framework combines rational allocation of the benefits with the considerations of stability and robustness of the coalition to changes in cost assumptions by analyzing its stability threshold. In Andiappan et al. (2016) a coalition is considered stable as long as the asymmetric distribution coefficient, introduced by Wang et al. (2013), falls within the bounds that are predefined by the participating plants. These plants choose their bounds individually and therefore these bounds are not mathematically substantiated. The asymmetric distribution coefficient can be interpreted as a coefficient computing whether the benefits divided by the costs allocated to a certain plant differ much from the total benefits divided by the total costs obtained in the coalition. The more these ratios differ, the more unfair the allocation seems to the participating plants.
Wu et al. (2017) introduce other methods to measure the fairness and stability of a certain coalition. To measure the fairness of a coalition, the Shapley-Shubik Power index, that is formulated to measure the powers of players in a voting game, is adopted. The index compares the gains to a player with the gains to the coalition. Based on the computation of this Power Index, a Fairness Index is computed by dividing the standard variance of this index by its mean. The greater the value of the Fairness Index, the lower the fairness of the allocation solution. For the stability of a coalition, the concept of propensity to disrupt (DP) value, introduced by Gately in Littlechild and Vaidya (1976), is employed to measure whether a coalition will be disrupt or not based on the allocation solution. The DP value of player i is defined as the loss of the members except player i in the grand coalition, $S = N$, compared to the loss of player i if i refuses to cooperate and disrupts the grand coalition. The higher the DP value for a certain player, the higher the probability that this player will disrupt the grand coalition, or claim a higher benefit allocation.
As mentioned before, another reason for a company not to cooperate in a coalition, might be the risk of investing in a certain decarbonisation option. In Melese et al. (2017) the effects of risk sharing are modeled and analysed when two agents want to work together on the development of an energy infrastructure project in an uncertain environment. It is shown that the optimal risk-sharing rule depends on the agents' risk aversions, the volatility of the common project profit, the volatilities of the agents' pre-existing businesses and the correlation of each agent's pre-existing business with the common project.
How this past research connects with our problem and how we will use some of the proposed methods will be explained in Section 3.

3 Problem definition

In this Section we will provide the formal problem statement and our research questions. As mentioned in Section 1 the industrial clusters in the Netherlands face the challenge to choose in what decarbonisation options will be invested and how the costs and benefits of such a choice will be divided over the companies within the cluster. As input to the problem we will have the structure of the industrial cluster, the set N of all the companies within the cluster and the set D of all decarbonisation options. We will try to model and solve this problem using cooperative game theory.
In cooperative game theory the involved companies can form coalitions by working together in a group. For example, a coalition can be formed by the companies A, B and C, this will be denoted by: $S = (A, B, C)$. A vector describing the decarbonisation options that are chosen by each company in a coalition S is called a strategy and noted as $B_S \in A_S$, where A_S is the set of all strategies that can be chosen by coalition S. The strategy vector B_S is always given in the natural ordering of the companies in S. For example, consider coalition $S = (A, B, C)$, then $B_S = (a_1, a_1, a_4)$ indicates the strategy of coalition S in which companies "A" and "B" choose decarbonisation option a_1, whereas company "C" chooses decarbonisation option a_4. The individual utility functions $u_i(B_S)$ can be referred to as the utility company i obtains when strategy B_S is chosen by coalition S.
As mentioned in Section 1 we will try to construct TU-games that best represent the problem of the industrial clusters using the input just mentioned and we will investigate allocation methods to the constructed TU-games. A TU-game is a pair (N, v), where N denotes the set of players, in our case the companies, and $v : 2^N \to \mathbb{R}$ is the characteristic function, assigning a certain value to every possible coalition $S \subseteq N$. In the situation at hand, all the companies can choose to invest in any decarbonisation option they are interested in. However, it might not be possible for two different decarbonisation options to be executed simultaneously. For example, if the current infrastructure for natural gasses is updated and adjusted to transport hydrogen, it is not possible for any company to still make use of the natural gasses from the original infrastructure. Therefore, we will formulate the problem as a cooperative situation, assuming that, when computing the value of a coalition for choosing decarbonisation option a, this option is not infeasible due to the decisions made by the companies that are not in the coalition. Furthermore the set A_S of all possible strategies that can be chosen by coalition S will not contain a strategy in which two decarbonisation options are chosen that can not be used simultaneously.
Our research is divided into to main research questions. In the first part we will try to model the situation in the industrial cluster as best as possible and define the characteristic function $v(S)$ accordingly. In this way, in the first part the TU-games will be constructed by computing the $v(S)$ values for each coalition using the proposed definition. From now on, this will be called the Valuation Problem (VP). In the second part we will make an allocation of the costs and benefits using the constructed TU-games in the first part of our research. From now on, this will be called the Allocation Problem (AP). Now we will formulate the VP and the AP and state the research questions, which we will try to answer in this thesis.
Firstly, given the set N of all companies from which a coalition S can be formed, the set A of all possible strategies of every coalition, the VP is to define the characteristic function $v(S)$ in such a way that it can represent the utilities that are obtained by the companies in coalition S, when a certain strategy is chosen, considering all the different incentives of all the companies in S. The complexity of the VP lies in the fact that an investment results in two different consequences. A certain amount of CO_2 eq. emission reduction will be realised and a certain amount of costs will have to be paid. The difficulty is to express the utility company i obtains from a chosen strategy in one value using both the amount of CO_2 eq. emission reduction and the costs by defining the utility function $u_i(B_S)$ and that the definition of this utility function might differ per company.
Secondly, given the chosen strategy and corresponding $v(S)$ values for every possible coalition S, the AP is to allocate the environmental benefits and the costs obtained from the chosen strategy in such a way that the allocation is stable and fair. The complexity of the AP lies in the fact that we will be allocating both the environmental benefits as well as the costs and that the definition of a stable and fair allocation is not exact and might also differ among the different companies. For example, one company might not cooperate in a coalition if it gets allocated more costs than other companies, whereas another company might agree to this if it gets allocated more environmental benefits.
Finally, we will also investigate what happens if we assume that there exists an industrial cluster managements that determines how the costs and environmental benefits resulting from a chosen strategy are allocated over the involved companies. In this case the VP will be solved by determining for which strategy the total utility of a coalition is maximised given the predetermined rules. The AP will be solved by the rules and regulations that are determined by the management. If this is the case, we are interested in seeing if there exists rules that result in a TU-game for which a stable allocation exists. Furthermore, we will investigate by trial and error if there exist rules and regulations that can push the chosen strategy by the grand coalition towards certain desired options, for example realising more CO_2 eq. emission reduction.
The research questions corresponding to the explained problems are stated below. The first main question corresponds

to the VP, the second question corresponds to the AP and the third question corresponds to the research on the existence of an industrial cluster management.

1. How can we model the joint investment of an industrial cluster in certain decarbonisation options in terms of a characteristic function $v(S)$, assigning a value to every possible coalition S, such that it best represents reality?
   (a) What is the structure of the industrial cluster?
   (b) What are the incentives of the involved companies?
   (c) How can we quantify the incentives of the involved companies and define the utility function $u_i(B_S)$?
   (d) What kind of input do we need for our allocation problem?
   (e) How will the different formulations of the characteristic function affect the results?
2. Based on the used model in the first part of our research and the found $v(S)$ values, how can we allocate the environmental benefits and the costs, such that the allocation is stable and fair?
   (a) When is a coalition considered to be stable?
   (b) When is an allocation considered to be fairly distributed?
   (c) How can previously investigated models be adapted such that they are able to allocate both the environmental benefits and the costs?
3. If an industrial cluster management exists that determines the rules and regulations on the allocation of the costs and environmental benefits, can the management set rules such that the grand coalition is stable and a certain strategy is chosen?
   (a) How do the predetermined rules and regulations affect the feasibility of the AP after constructing the TU-game?
   (b) How do the predetermined rules and regulations affect the strategy chosen by the grand coalition?
   (c) How do the predetermined rules and regulations affect the negotiation space of the companies in the grand coalition?

In our research it has come to light that another complexity arises in some of the solution approaches we have suggested. In some of the proposed models the result of the AP is needed to solve the VP whereas the result of the VP is needed to solve the AP. Why this is the case and how we will tackle this problem is further explained in Section 4.3. Furthermore, the method that is suggested to investigate the influence an industrial cluster management could have on the decisions made by the companies, if such a management exists, is described in Section 4.3.2. This method is tested on different rules and regulations to give answer to the last research question and the results of these tests will be discussed in Section 6.5.

Now we will explain the basic set up of our methods to tackle the VP and AP. Similar to the found literature described in Section 2.2, we will define an optimization problem to find the values for our characteristic function $v(S)$. We are interested in finding the best strategy for each coalition and want to know the corresponding costs and environmental benefits as input for our allocation problem. The formulation of the optimization problem starts by formulating the cooperative situation as is mentioned in Kleppe et al. (2012). Furthermore, we will incorporate the idea, mentioned in van den Brink et al. (2012), into our formulation of the optimization problem by defining an individual utility function, which differs per company, based on the amount of CO_2 eq. reduction allocated to the company, the costs allocated to the company and a monetary compensation allocated to the company. We will formulate the cooperative situation as (N, A, u), in which $u_S(B_S)$ is the utility function assigning a value of utility to every company in coalition S for choosing strategy B_S. How we define this utility function is based on the function used in van den Brink et al. (2012) and is further explained in Section 4.1. We will also consider the fact that the use of a certain decarbonisation option might involve some fixed costs that need to be paid by all involved companies as well as some variable costs that might differ per company. For example, when investing in a new hydrogen infrastructure, the fixed costs will be the costs of developing and installing this infrastructure, while the variable cost for a certain company will be the cost of connecting this company to the hydrogen infrastructure.

For the allocation problem we choose to use the model proposed in Tan et al. (2016), from now on called the TAN/-MAALI (TM) model, as our starting point. The reason we choose this model is threefold: (i) its tractability and relative simplicity make it an excellent starting point, (ii) the model is based on the existence of linear programming optimization of an industrial site, which is the practical case for some industrial sites and (iii) the model offers enough options to make necessary adjustments and extensions. We will also further investigate the stability and fairness of this model and the obtained allocation. We will do so, making use of the fair distribution of the benefit/cost ratio introduced by Wang et al. (2013). Furthermore, we will introduce some other constraints that ensure some kind of fairness among the decisions. How this model will be used and these investigations will be done, is further explained in Section 4.2.

Further explanations of the methods we will use, drawn from literature, as well as some new ideas we propose, will be explained in Section 4.

4 Methodology

This Section will give a description of the methods we are going to use to solve the problems stated in Section 3. In the first part, 4.1, we will give an overview on the methods used to solve the VP, defining the characteristic function $v(S)$ used to construct the TU-games. In the second part, Section 4.2, we will describe the methods used to solve the AP, fairly allocating the costs and benefits among the companies within a coalition. As mentioned in Section 3 in some of the suggested solution approaches the VP and AP need to be solved simultaneously. Why this case will be explained in Section 4.3. Furthermore, in Section 4.3 two procedures, based on different structures of the industrial cluster, will be introduced to solve this problem and iteratively solve the VP and AP for each possible coalition S.

4.1 Valuation Problem

In this section we will introduce different solution methods that try to model an industrial cluster in terms of a characteristic function $v(S)$, assigning a certain value to each coalition S. First we will introduce some general notation and problem formulation. Then in Sections 4.1.1, 4.1.2 and 4.1.3 we will introduce three different solution methods that solve the VP by defining the characteristic function $v(S)$ based on different assumptions about the structure and the incentives of the companies in an industrial cluster.
As mentioned in Section 3, we will first formulate the problem as a cooperative situation (N, A, u), where N is the set of players, A is the set of all possible strategies. $u_S(e_{S,B_S}, c_{S,B_S}) : \mathbb{R}^2 \to \mathbb{R}$ is the utility function assigning a value to coalition S for each strategy $B_S \in A_S$. The input values e_{S,B_S} and c_{S,B_S} are the total CO_2 eq. emission reduction and the total costs, respectively, that are obtained if coalition S decides to go for strategy B_S. These values are computed as follows. Firstly, $e_{S,B_S} = \sum_{i \in S} e_{S,i,B_S}$, where e_{S,i,B_S} is the amount of CO_2 eq. emission that can be reduced by company i if it works together in coalition S and this coalition chooses strategy B_S expressed in euros. To express this amount in euros, we make use of the "Milieu Kosten Indicator" (MKI). This indicator keeps track of the current global value given to the reduction of a kg CO_2 eq. emission in euros. At this time the MKI value is equal to €0.05 per kg CO_2 eq. emission reduction. From now on, when we talk of e_{S,i,B_S}, this is the amount of CO_2 eq. emission that can be reduced by company i multiplied by the current MKI value and we will call it the environmental benefits obtained by company i. Secondly, $c_{S,B_S} = c^f_{B_S} + \sum_{i \in S} c^v_{S,i,B_S}$, where $c^f_{B_S}$ are the fixed costs of strategy B_S and c^v_{S,i,B_S} are the variable costs of company i when working together in coalition S choosing strategy B_S. The values e_{S,i,B_S}, $c^f_{B_S}$ and c^v_{S,i,B_S} are usually the values that can be obtained from the data instances. In this section we will introduce three methods for constructing TU-games and computing the $v(S)$ values of each coalition. In each method the $v(S)$ value of a coalition S is given in terms of the total utility obtained by coalition S, which is equal to the sum of the utilities obtained by the companies in coalition S.
Now we will summarize what methods are presented in Sections 4.1.1, 4.1.2 and 4.1.3. Furthermore, we will briefly state on which assumptions about the industrial cluster and the involved companies the methods are based.
In Section 4.1.1 we will formulate the characteristic function as the minimisation problem of the total cost of coalition S. This method is called the Cost Minimisation (CM) method and the utility of a coalition is formulated as the negative costs induced to the coalition when choosing a certain strategy. In this case, we assume that the companies are not interested in reducing their CO_2 eq. emission, but only in minimising their costs. Using this formulation, we are interested in how certain regulations and rules from the government could affect the decisions of the companies. For example, if a regulation was implemented, enforcing companies to pay a certain amount of money per kg CO_2 eq. emission, then we are interested in how high this amount must be to affect the decisions of the companies.
In Section 4.1.2 we will introduce a model that defines the utility function on the whole coalition. This method will be called the Joint Utility Function (JUF) method and this method is based on the assumption that the companies do have an incentive to reduce their CO_2 eq. emission and that we are able to express the weight of this incentive of a group of companies with a function of the weights of the incentives of the individual companies within that group. For the CM formulation as well as the formulation on the whole coalition it holds that the input values of the utility function are known, as these are the total amount of CO_2 eq. that can be reduced and the total incurred costs. The joint utility function assigns a single utility value to a whole coalition S, without assigning specific utility values to each company in the coalition. Therefore, the joint utility function is given by $u_S(e_{S,B_S}, c_{S,B_S}) : \mathbb{R}^2 \to \mathbb{R}$.
Finally, in Section 4.1.3 we will introduce a model in which the utility functions are individualised per company. This method will be called the Individualised Utility Function (IUF) method and is based on the assumption that the companies do have an incentive to reduce their CO_2 eq. emission and that we are not able to express the weight of the incentive of a group of companies with a function of the weights of the incentives of the individual companies within that group. We suspect that this is a more realistic resemblance of the real world, as different companies assign different value to reducing their CO_2 eq. emission. However, the problem will become more complex compared to defining the utility function of a coalition jointly in one function. In the case of individual utility functions we

will have $u_S(e_{S,B_S}, c_{S,B_S}) : \mathbb{R}^2 \to \mathbb{R}^{|S|}$, being the utility function assigning a value to each company in the coalition, which resembles the utility that is obtained by that company. Then we can also write this utility function as a vector of utility functions for each company within the coalition, so for example for the grand coalition it holds that $u_N(e_{N,B_N}, c_{N,B_N}) = (u_1(e_{N,1,B_N}, c_{N,1,B_N}), u_2(e_{N,2,B_N}, c_{N,2,B_N}), ..., u_n(e_{N,n,B_N}, c_{N,n,B_N}))$. These individual utility functions take as input the environmental benefits and costs that are allocated to the associated company. So to compute the utility obtained by each individual company and to obtain the total utility of a certain coalition S the cost and environmental benefits allocation already needs to be known. However, as mentioned in Section 3 an allocation of the costs and environmental benefits is made by solving the AP based on the TU-game constructed by solving the VP. So in this case, the difficulty is that the VP and the AP need to be solved simultaneously. The IUF method described in Section 4.1.3 computes the utility values of each coalition by making an allocation of the costs and environmental benefits that maximises the total utility of the coalition. This allocation, however, will not be the eventual allocation made in the AP. Instead, this allocation is only used to compute the $v(S)$ values for each coalition and to construct a TU-game, which then will be used as input for the actual AP. In Sections 4.3.1 and 4.3.2 two other methods are suggested to solve the VP and AP simultaneously.

4.1.1 Cost Minimisation

In this Section the CM method is explained. This method is based on the assumption that the companies within an industrial cluster do not have an incentive to reduce their CO_2 eq. emission and therefore the utility function of the companies will only consider the obtained costs from a certain chosen strategy. Therefore, we define the characteristic function as the minimisation problem of the costs. This is equivalent to defining the utility function of each company as $u_i(e_{S,i,B_S}, c_{S,i,B_S}) = -c_{S,i,B_S}$ and maximising the total sum of utilities of all the companies in S. Let us introduce the decision variable y_{B_S}, indicating whether strategy B_S is chosen by coalition S. In our objective function we want to maximise the total utility of coalition S, this is equivalent to maximising $\sum_{B_S \in A_S} \sum_{i \in S} y_{B_S} u_i(e_{S,i,B_S}, c_{S,i,B_S})$. As the utility function for all companies are equivalent, the objective function can also be written as $-\sum_{B_S \in A_S} \sum_{i \in S} y_{B_S} c_{S,i,B_S}$, which is equal to $-\sum_{B_S \in A_S} y_{B_S} c_{S,B_S}$. So our optimisation problem defining the characteristic function becomes the following.

$$v(S) = \max - \sum_{B_S \in A_S} y_{B_S} c_{S,B_S} \tag{1}$$

$$\sum_{B_S \in A_S} y_{B_S} = 1 \tag{2}$$

$$y_{B_S} \in \mathbb{B} \quad \forall B_S \in A_S \tag{3}$$

We will solve this problem for every possible coalition $S \subseteq N$. The objective function (1) maximises the total utility of all the companies. Constraint (2) ensures that only one strategy is chosen by coalition S. Constraint (3) ensures that the decision variables are binary. As all the individual utility functions are the same, the sum of the utilities is the negative of the sum of the total costs. Therefore solving this optimisation problem is quite straightforward. However, it is not unlikely that some companies only act on financial interest. Furthermore, this method can give some interesting insights. For example, when we allow companies to choose to not invest in anything, in this formulation, all the companies would choose to do nothing as there are no costs associated with that option. If a government would be interested in setting taxes on the emission of CO_2 eq., then an interesting investigation would be to research how high these taxes per kg of CO_2 eq. emission must be to affect the companies' decisions in such a way that they will choose an option, which reduces their emission.
Another interesting investigation would be to research what the cheapest decarbonisation options are when a certain amount of CO_2 eq. emission reduction has to be satisfied. This constraint would be formulated as follows

$$\sum_{B_S \in A_S} \sum_{i \in S} y_{B_S} e_{S,i,B_S} \geq pE_S \tag{4}$$

in which E_S is the current total CO_2 eq. emission of the companies in S. These and some other investigations will be carried out in our research on this method.
In Example 4.1 an example will be given in which the CM method is implemented on a small data instance to construct a TU-game to give an idea how the method works.

Example 4.1 *Consider the data instance "Example 1", summarized in Table 1. In this example there are three companies, $N = \{A, B, C\}$, and three decarbonisation options $D = \{a_1, a_2, a_3\}$. The information on the companies is* *given in the first tabular of Table 1, where the current emission values are given in million euros by making use of the current MKI value (0.05 €/kg CO_2 eq). The information on the decarbonisation options is given in the second tabular of Table 1, where again the amount of CO_2 eq. reduction, e, the fixed costs, c^f, and the variable costs, c^v, are given in million euros. The G/I indicate whether the decarbonisation option is a group or an individual decarbonisation investment option respectively.*

Companies	Emission	w_i	b_i	k_i
A	1000	0.6	1.2	1
B	500	0.5	1	1
C	400	0.5	1	1

			Company A		Company B		Company C	
D	G/I	c^f	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0
a_2	I	0	250	240	100	110	50	40
a_3	G	900	750	240	250	150	200	100

Table 1: Information on companies and decarbonisation options in instance "Example 1".

Solving the utility maximisation problem under constraint (4), *with* $p = 0.15$ *will result in the values of the characteristic function of each coalition summarized in Table 2. Both the strategy minimising the total costs as well as the coalition utility values are shown in the Table.*

S	u_S	Strategy
{A}	-240	(a_2)
{B}	-110	(a_2)
{C}	-1000	(a_3)
{A,B}	-240	(a_2, a_1)
{A,C}	-240	(a_2, a_1)
{B,C}	-150	(a_2, a_2)
{A,B,C}	-280	(a_2, a_1, a_2)

Table 2: Obtained $v(S)$ values using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1".

The obtained values of the characteristic function can now be used as input to solve the AP using the allocation method described in Section 4.2.

4.1.2 Joint Utility Function

In this Section the JUF method is explained. This method is based on the assumption that companies within an industrial cluster do have an incentive to reduce their CO_2 eq. emission. Moreover, we assume that we are able to express the weight of the incentive of a group of companies by defining a function based on the weights of the individual companies contained in this group. We will call this the coalition weight function.

In this method we will define the utility function on both the costs associated to a certain decarbonisation option as well as the amount of CO_2 eq. emission that is reduced. As we do not know exactly how much utility companies give to reducing their CO_2 eq. emission or to keeping the costs as low as possible we introduce the parameter w_i. This variable, w_i, represents the relative weight company i gives to reducing CO_2 eq. emission compared to the costs. Vice versa, $(1 - w_i)$, will represent the relative weight company i gives to minimising the costs compared to reducing its CO_2 eq. emission. For example, if $w_i = 0$, then the company does not care at all about reducing its CO_2 eq. emission and only cares about making no costs. Or, if the company totally agrees with the current value of €/kg CO_2 eq. set by the MKI, then w_i will be equal to 0.5. Now from this w_i, we will define the function w_S, which represents the relative weight a certain coalition S gives to reducing CO_2 eq. emission compared to minimising the cost. We will investigate different definitions of w_S, but we could for example just take the average of the weights of all the companies in coalition S, $w_S = \frac{\sum_{i \in S} w_i}{|S|}$. We could also compute the weighted average, based on the current emission of the companies. In that case the coalition weight would be $w_S = \sum_{i \in S} \left(\frac{E_i}{E_S} w_i \right)$, where E_i is the current emission of company i and E_S is the total current emission of coalition S. These definitions and other, some arbitrary, definitions will be investigated. In our research we are interested in what kind of definitions are needed for the weights to be able to make a stable and fair allocation and how the different values and definitions of the weights affect the results.

Now we will propose different definitions of the utility function, using the weight variable, that we think can represent the utility coalitions gain from reducing their CO_2 eq. emission against certain costs. One of the possible formulations of the utility function is $u_S(e_{S,B_S}, c_{S,B_S}) = \frac{w_S e_{S,B_S}}{(1-w_S)c_{S,B_S}}$. In this way the goal of the problem is to maximise the ratio of the reduction of CO_2 eq. emission per euro. Another possible way to define the utility function is $u_S(e_{S,B_S}, c_{S,B_S}) = w_S e_{S,B_S} - (1 - w_S)c_{S,B_S}$.

Once we have defined the utility function we can compute the values of the characteristic function $v(S)$. We will formulate the utility maximisation problem as a mixed integer programming (MIP) problem and solve this using a commercial solver for every possible coalition S. Using the binary decision variables y_{B_S} indicating whether strategy $B_S \in A_S$ is chosen, the MIP can be formulated as follows.

$$\max \sum_{B_S \in A_S} y_{B_S} u_S(e_{S,B_S}, c_{S,B_S}) \tag{5}$$

s.t.

$$\sum_{B_S \in A_S} y_{B_S} = 1 \tag{6}$$

$$y_{B_S} \in \mathbb{B} \quad \forall B_S \in A_S \tag{7}$$

In equation (5) the utility function for coalition S is maximised. Constraint (6) ensures that only one decarbonisation option is chosen. Constraint set (7) ensures that the decision variables are binary.

To give an idea how the JUF method works Example 4.2 shows the results of implementing the JUF method on a small data instance.

Example 4.2 *Consider the same data instance as in Example 4.1 called "Example 1" summarized in Table 1. Now, we will use the JUF method to compute the values of $v(S)$ for each possible coalition S. In this example the used definition of the joint utility functions is $u_S(e_{S,B_S}, c_{S,B_S}) = w_S e_{S,B_S} - (1 - w_S)c_{S,B_S}$ and the used definition of the coalition weight is the weighted average, $w_S = \sum_{i \in S} \left(\frac{E_i}{E_S} w_i \right)$. In Table 3 the obtained values of $v(S)$ are given as well as the strategy that maximises the total utility of coalition S.*

S	w_S	$v(S)$	strategy
{A}	0.6	54	(a_2)
{B}	0.5	0	(a_1)
{C}	0.5	5	(a_2)
{A,B}	0.567	46.67	(a_2, a_2)
{A,C}	0.571	51.43	(a_2, a_2)
{B,C}	0.5	5	(a_1, a_2)
{A,B,C}	0.553	46.58	(a_2, a_2, a_2)

Table 3: Obtained $v(S)$ values using JUF method on data instance "Example 1".

The obtained values of the characteristic function can now be used as input to solve the AP using the allocation method described in Section 4.2.

4.1.3 Individualised utility functions

In this Section the IUF method is explained. This method is based on the assumption that the companies within an industrial cluster do have an incentive to reduce their CO_2 eq. emission. However, we assume that we are not able to express the weight of the incentive of a group of companies by defining a function based on the weights of the individual companies contained in this group.

Now we will elaborate more on defining individualised utility functions. The reason we do this is twofold. First of all, in practice different companies will assign different value to realising a certain amount of CO_2 eq. reduction. Therefore, using a coalition weight function in the computation of the utility obtained by a coalition might not be

representative of the obtained utility in reality. Secondly, when individualising the utility functions it is observed how much utility an individual company will gain from a certain coalition. Therefore, we can gain insight in whether each individual company gains more utility from working together or from working alone or in another subcoalition. In this way, we can better understand why and when a company tends to leave a coalition.
As it seems not very realistic that we can base the value of w_S on the values of w_i of all the companies in the coalition, we are also interested in investigating computing the characteristic function using individualised utility functions. In that case we can write the utility of coalition S as a vector of the utilities of all the companies in S. For example, for the grand coalition it holds that $u_N(e_{N,B_N}, c_{N,B_N}) = (u_1(e_{N,1,B_N}, c_{N,1,B_N}), u_2(e_{N,2,B_N}, c_{N,2,B_N}), ..., u_n(e_{N,n,B_N}, c_{N,n,B_N}))$. Now we will propose different definitions of the individualised utility functions, using the individual weights w_i. Just as defining the utility function for the entire coalition we propose the same kind of individual utility functions. We propose the functions $u_i(e_{S,i,B_S}, c_{S,i,B_S}) = \frac{w_i e_{S,i,B_S}}{(1-w_i)c_{S,i,B_S}}$ and $u_i(e_{S,i,B_S}, c_{S,i,B_S}) = w_i e_{S,i,B_S} - (1 - w_i)c_{S,i,B_S}$.
Note that because of the fact that the utility functions are defined per company, we actually need an allocation of the environmental benefits and costs over the companies as input. Whereas in the JUF method we could just pool all the costs and environmental benefits and use this as input for the joint utility function, in the IUF method the $v(S)$ values are computed by summating all the indivdual utility functions of each company. Therefore, an allocation of the costs and environmental benefits is needed to compute the utility values of each indivdiual company.
In the case of individualised utility functions we cannot simply compute the values, as we do not know yet which part of the costs will be allocated to each individual company. Therefore, we propose different solution methods when using individual utility functions. One of the methods we propose, is solving the maximisation problem, computing value $v(S)$ for each coalition S, by formulating it as a MIP. In this MIP an allocation of the costs is already made by allocating the costs such that the $v(S)$ value is maximised. However, this allocation is not the final allocation made after solving the AP using the allocation method explained in Section 4.2. The allocation made here is merely used to compute the potential maximum utility that can be obtained by coalition S and the found $v(S)$ values are used as input for the allocation method solving the AP described in Section 4.2. A second solution method we propose is an iterative procedure. This procedure iteratively computes the values of $v(S)$ for all possible coalitions S of size $k = 1, 2, ..., N$. This procedure combines the methods that are described in Sections 4.1 and 4.2. Why we use this iterative procedure as well as the procedure itself is further explained in Section 4.3.
For the MIP formulation on the individual utility functions we introduce the decision variables x^c_{S,i,B_S} indicating how much costs are allocated to company i when coalition S chooses strategy B_S in the maximisation problem. At first we assume that the environmental benefits are not transferable and therefore e_{S,i,B_S} is known. Later we can also investigate the possibility of transferable environmental benefits. Then, we should introduce another decision variable, x^e_{S,i,B_S}, indicating how much environmental benefits are allocated to company i. These decision variables will be the input for the individual utility functions. For each coalition, the value of $v(S)$ is computed by maximising the sum of the utilities of the companies in coalition S. By maximising the sum of utilities an allocation of the costs is made by the decision variable x^c_{S,i,B_S}. The solution of this allocation gives a value to the characteristic function $v(S)$ which are later used as input in the allocation methods solving the AP and allocating the costs and the benefits over the participating companies. This maximisation problem is formulated as follows.

$$\max \sum_{B_S \in A_S} \sum_{i \in S} y_{B_S} u_i(e_{S,i,B_S}, x^c_{S,i,B_S}) \tag{8}$$

s.t.

$$\sum_{B_S \in A_S} y_{B_S} = 1 \tag{9}$$

$$\sum_{i \in S} x^c_{S,i,B_S} = y_{B_S}(c^f_{B_S} + \sum_{i \in S} c^v_{S,i,B_S}) \quad \forall B_S \in A_S \tag{10}$$

$$y_{B_S} \in \mathbb{B} \quad \forall B_S \in A_S \tag{11}$$

$$x^c_{S,i,B_S} \in \mathbb{R}_+ \quad \forall B_S \in A_S \text{ and } \forall i \in S \tag{12}$$

In this formulation (8) maximises the sum of utilities of the companies in coalition S. Constraint (9) ensures only one strategy is chosen. Constraint set (10) ensures that all the fixed and variable costs that are incurred when strategy B_S is chosen by coalition S are allocated over the participating companies. Constraints (11) ensures that the decision variables y_i are binary and constraints (12) ensure that the variables x_{S,i,B_S} are continuous and nonnegative.
To give an idea how the IUF method works Example 4.3 shows the results of implementing the IUF method on a small data instance.

Example 4.3 *Consider again the data insatnce called "Example 1" summarized in Table 1. In this example the used definition of the individual utility functions are* $u_i(e_{S,i,B_S}, c_{S,i,B_S}) = w_i e_{S,i,B_S} - (1-w_i)c_{S,i,B_S}$ *for each company* $i \in S$.

In Table 4 the obtained values of $v(S)$ are given as well as the strategy and cost allocation that maximise the total utility of coalition S.

S	$v(S)$	Strategy	Cost Allocation
{A}	54	(a_2)	(240)
{B}	0	(a_1)	(0)
{C}	5	(a_2)	(40)
{A,B}	60	(a_2, a_2)	$(350, 0)$
{A,C}	63	(a_2, a_2)	$(280, 0)$
{B,C}	5	(a_1, a_2)	$(20, 20)$
{A,B,C}	119	(a_3, a_3, a_3)	$(1390, 0, 0)$

Table 4: Obtained $v(S)$ values using the IUF method on data instance "Example 1"

The obtained values of the characteristic function can now be used as input to solve the AP using the allocation method described in Section 4.2.

Some problems that arise with this formulation are that when using the fractional definition of the individual utility functions in the objective function the problem becomes nonlinear and therefore non solvable by a commercial solver. Furthermore, for larger instances this problem computationally takes a bit more time. We also need to solve this problem for every possible coalition, which means that we need to solve it 2^n times, with n the number of companies in the instance. Fortunately, in the cases we will study, the number of companies will remain relatively small, ranging from 4 to 8 companies.

The three above mentioned methods for computing the characteristic function $v(S)$, for each coalition S, will be tested on different data instances and compared in Section 6.

4.2 Allocation Problem

Once we have determined the characteristic function $v(S)$, we can start computing a fair and stable allocation of the benefits and the costs for a certain coalition S. For this allocation we use the model in Tan et al. (2016), which is based on the model in Maali (2009), as our starting point. The difficulty of the AP lies within the fact that we are allocating both costs and environmental benefits simultaneously, whereas the model suggested by Tan et al. (2016) only allocates benefits. Moreover, the definition of a stable and fair allocation is not exact and why companies might leave a certain coalition is unknown. Therefore, we will introduce some constraints that could be added to the model suggested by Tan et al. (2016) when they are thought to be necessary for a fair and stable allocation. First, in Section 4.2.1 we will explain the model that is stated in Tan et al. (2016) and later, in Section 4.2.2 we will explain the adjustments and further extensions that we can possibly make to the model such that it can comprehend with allocating both the costs and benefits and make the allocation more stable and fair.

4.2.1 TAN/MAALI model

For the explanation of the model in Tan et al. (2016) we assume that the model is made for the allocation of benefits only. Therefore the characteristic function $v^{TM}(S)$ only returns the benefits gained from coalition S and not the costs that are associated with this coalition. Furthermore, the variable x_i^{TM}, representing the payoff for company i, will only contain the benefits allocated to company i. In Maali (2009) a mathematical programming-based approach to the problem of allocating the benefits or costs of a certain coalition is proposed. This cooperative game model is based on max-min aggregation method where the least satisfied constraints are maximised. To ensure that the solution is Pareto optimal, the allocation of the benefits are based on the marginal contributions C_i^{TM} of each company i. The marginal contribution of a company is computed as follows.

$$C_i^{TM} = \sum_{S \subseteq N} \frac{[v^{TM}(S) - v^{TM}(S - \{i\})]}{v^{TM}(N)} \tag{13}$$

The marginal contribution of company i can be interpreted as the average value company i adds to a coalition, when company i is added to this coalition, over all possible coalitions that company i could join. Now let us introduce our decision variables x_i^{TM} representing the amount of benefits that are allocated to company i. Then $\frac{x_i^{TM}}{C_i^{TM}}$ is called the degree of satisfaction of company i, as it describes the amount of benefits allocated to company i in proportion with its marginal contribution. As we would like to maximise the lowest degree of satisfaction, we introduce the continuous variable λ^{TM}. Now we can formulate our allocation problem as follows.

$$\max \lambda^{TM} \tag{14}$$

s.t.

$$\frac{x_i^{TM}}{C_i^{TM}} \geq \lambda \quad \forall i \in N \tag{15}$$

$$x_i^{TM} \geq v^{TM}(\{i\}) \quad \forall i \in N \tag{16}$$

$$\sum_i x_i^{TM} = v^{TM}(N) \tag{17}$$

$$\lambda, x_i^{TM} \in \mathbb{R} \quad \forall i \in N \tag{18}$$

Equations (14) and (15) ensure that the lowest degree of satisfaction is maximised. Constraint set (16) ensures individual rationality in this cooperative game. This means that it is not possible that the allocation of benefits x_i^{TM} is lower than the benefits company i can get from working alone. Constraint set (17) ensures efficiency, meaning that the total amount of benefits that is allocated among the companies is equal to the benefits gained from the grand coalition.

To demonstrate the approach of the TM model Example 4.4 will show the allocation that is made when the TM model is implemented on a TU-game.

Example 4.4 *Consider the game created by obtaining the values of $v(S)$ using the IUF method explained in Section 4.1.3. For completeness, the inputted $v(S)$ values for each coalition S are stated in Table 5.*

S	$v(S)$
{A}	54
{B}	0
{C}	5
{A,B}	60
{A,C}	63
{B,C}	5
{A,B,C}	119

Table 5: Used $v(S)$ values to demonstrate TM model on data instance "Example 1".

Now, we will compute the amount of utility that will be allocated to each company by making use of the TM model. The values of $v(S)$ for the different coalitions are used to compute the marginal contributions, C_i, of each company i. The marginal contributions are computed by equation (13) and are given in Table 6.

Company	C_i
A	2.403
B	0.521
C	0.655

Table 6: Marginal contributions of each company to the $v(S)$ values in demonstration of TM model on data instance "Example 1".

Now using the found marginal contributions the allocation problem is solved, maximising the the lowest degree of satisfaction. The amount of utility and corresponding degree of satisfaction of each company are given in Table 7.

Company	Utility allocation	Degree of satisfaction
A	79.892	33.242
B	17.319	33.242
C	21.789	33.242

Table 7: Amount of utility allocated to each company and corresponding degree of satisfaction demonstrating the TM model on data instance "Example 1".

It is observed that in Example 4.4 the resulting degree of satisfaction from the allocation is exactly the same for each company, which is the aim of the TM model approach. In practice, exactly the same degree of satisfaction can often not be obtained due to individual rationality constraints or other constraints that might be added in the following Section. However, the aim is to push the lowest degree of satisfaction as far as possible towards the other degrees of satisfaction such that the least satisfied company is still as satisfied as possible.
In this example we allocated the utility value of the grand coalition over the companies. However, in practice the utility companies give to decreasing their CO_2 eq. emission against certain costs, differs per company. Therefore, in the next Section we will focus on allocating the costs and the environmental benefits over the companies. Furthermore, in the next Section we will introduce some adjustments and possible extensions we will make based on the idea of fairness and stability.

4.2.2 Extensive TM model

In this Section the possible adjustments and extensions that can be made to the TM model will be explained. As the definition of a stable and fair allocation is not exact the suggested adjustments and extensions will be examined and tested in Section 6. Meaning that the proposed extensions and adjustments are not always included in the model and do not by definition improve the TM model. The purpose of the suggested extensions and adjustments is to explore relevant constraints and analyse their effect on the allocation model. Different combinations of the suggested extensions and adjustments will be tested on different data instances and the results will be analysed in Section 6.
In our case we will not only allocate the benefits or utility gained from a coalition, but also the costs that are associated with this coalition. As we aim to invest in a energy transition the benefits will be noted as the amount of reduction in CO_2 eq. emission a certain coalition can achieve. Furthermore, the characteristic function $v(S)$ will not return a single value but three values, the benefits, the costs and the gained utility of coalition S. We will denote the characteristic function as $v(S) = (v^e(S), v^c(S), v^u(S))$, where $v^e(S)$ denotes the environmental benefits gained from coalition S, $v^c(S)$ denotes the costs associated with coalition S and $v^u(S)$ denotes the total utility gained from coalition S. Using the methods computing the values of $v(S)$ as mentioned in Section 4.1 we have information on all three values of $v(S)$. Furthermore, the variables x_i will be denoted as $x_i = (x_i^e, x_i^c)$, where x_i^e indicates the amount of environmental benefits allocated to company i and x_i^c the costs allocated to company i. In the same manner we denote the marginal contributions of company i as $C_i = (C_i^e, C_i^c, C_i^u)$, where C_i^e indicates the marginal contribution of company i to the environmental benefits, C_i^c the marginal contribution to the costs and C_i^u the marginal contribution to the utility.
Now, similar to the basic TM model, $\frac{x_i^e}{C_i^e}$ is called the degree of environmental satisfaction (DoES) of company i. Now let us introduce the degree $\frac{x_i^c}{C_i^c}$. In this case, this degree describes the amount of costs allocated to company i in proportion with its marginal contribution. When this degree increases, the company will be less satisfied, as more cost are allocated to the company. Therefore, we will call the degree, $\frac{x_i^c}{C_i^c}$, the degree of financial dissatisfaction (DoFD) of company i. As we would like to maximise the lowest DoES in terms of the allocation of the benefits as well as minimise the highest DoFD in terms of the allocation of the costs, we introduce another continuous variable γ. In contrast to the lowest DoES for the benefits, the highest DoFD for the costs is reached for the player with the highest costs compared to its contribution to the costs. Therefore, we maximise the negative of the new variable, $-\gamma$, while constraining the DoFD of each company to be less or equal to γ, which is equivalent to minimising the highest DoFD.
The allocation mechanism can be further developed by not only basing the allocation of the costs on the marginal contribution of each company to the costs, but also on the marginal contribution to the environmental benefits and the marginal contribution to the total utility of coalition S. We will base both the allocation of the environmental benefits and the allocation of the costs on a linear combination of the three marginal contribution values, (C_i^e, C_i^c, C_i^u). Therefore, we introduce the parameters $\beta = (\beta^e, \beta^c)$ and $\delta = (\delta^e, \delta^c)$, which indicate the weight that is given to the marginal contribution to environmental benefits and the weight given to the marginal contribution to the costs respectively. In the allocation of the environmental benefits we will use β^e and δ^e and in the allocation of the costs we will use β^c and δ^c. The remaining weight, $(1 - \beta - \delta)$ will be assigned to the marginal contribution of the company to the utility value of $v(S)$. Different values of β and δ will be investigated. We adjust the constraint set defining the DoES and DoFD values of each company in terms of the allocation of the cost and the benefits in the following way.

$$\frac{x_i^e}{\beta^e C_i^e + \delta^e C_i^c + (1 - \beta^e - \delta^e) C_i^u} \geq \lambda \quad \forall i \in N \tag{19}$$

$$\frac{x_i^c}{\beta^c C_i^e + \delta^c C_i^c + (1 - \beta^c - \delta^c) C_i^u} \leq \gamma \quad \forall i \in N \tag{20}$$

Note that the DoES and DoFD value of each company in this way also depend on the chosen values of β and δ. Intuitively, the DoES value of a company will be mainly based on its marginal contribution to the environmental benefits and the DoFS value of a company on its marginal contribution to the costs. However, we will try different values of β and δ to analyse their influence. Also a company might for example claim a larger part of the environmental benefits based on a large marginal contribution to the total utility. This is a reason why different values of β and δ are tested.

In practice we see that superadditivity holds for the characteristic function value of the environmental benefits of a coalition, $v^e(S)$. This is explained by the fact that, when for example company A can realise a certain amount of CO_2 eq. emission reduction on its own or in a coalition by for example investing in decarbonisation option a_1, then when another company joins the coalition, company A can still realise the same amount of reduction by investing in option a_1 or even more when they decide to cooperatively invest in another option. This means that for the allocation of the benefits we can use the same individual rationality constraints as in the basic TM model.

However, superadditivity does not always hold for the characteristic function value of the costs of a coalition, $v^c(S)$. Contrarily, it is observed that sometimes the costs are lower for larger coalitions. This is mainly caused by the fixed costs of some decarbonisation options, which make them relatively cheaper when more companies are in the coalition. Therefore, it might occur that for example for two coalitions, A and B, for which it holds that $A \cap B = \emptyset$, it does not hold that $v^c(A \cup B) \geq v^c(A) + v^c(B)$. Also, working together is preferred, when this means the companies will reduce their costs. Therefore, we rewrite the individual rationality constraint of the costs to $x_i^c \leq v^c(\{i\})$, for each company $i \in N$. Intuitively, a company would prefer to pay lower costs. However, also shown in practice, when the size of the coalition grows, often more expensive decarbonisation options are chosen, increasing the total costs and potentially the costs that are allocated to a single company. This is caused by the fact that the increased amount of CO_2 eq. emission reduction outweighs the increased amount of costs as the fixed costs are divided over the participating companies. So in general, the individual rationality constraint on the costs will not be satisfied and therefore we will not always include this restriction in our model. However, we assume that, when the environmental benefits are greater whilst joining the coalition than whilst working alone, a company might still be interested in joining the coalition.

To ensure that the company should be more interested in joining the coalition rather than working alone, we add the individual rationality constraint associated with the utility gained from a coalition.

$$u_i(x_i^c, x_i^e) \geq v^u(\{i\}) \quad \forall i \in N \tag{21}$$

Constraint set 21 ensures that the utility gained from the allocation of the environmental benefits and the costs are greater or equal to the utility company i could gain by working alone. This is computed by using the same definition of the utility function as was used in the VP to construct the TU-game.

Now that we have introduced three kinds of individual rationality constraints, namely on environmental benefits, costs and utility, we will also introduce three kinds of rationality constraints based on subgroups of companies. These constraints are based on the definition of the core of a cooperative game. Gedai et al. (2012) describe the core as the set of allocations of profit for which all the companies find the allocation to be reasonable and they cannot justifiably demand an increase of its allocated profits. A formal definition of the core is stated below.

Definition 4.1 (The Core) *The core of a TU game (N, v) is the set of feasible payoff vectors x where $\sum_{i \in S} x_i \geq v(S)$ for every coalition $S \subseteq N$. Where a payoff vector x is said to be feasible if $\sum_{i \in N} x_i = v(N)$.*

In other words, the payoff vector is such that no group of companies is able to gain higher profits by working in that particular group and therefore there exists no group of companies with a rational incentive to leave the grand coalition. Based on the definition of the core we introduce, what we will call coalitional rationality constraints on environmental benefits, the costs and utility. Those constraints are given in the equations below.

$$\sum_{i \in S} x_i^e \geq v^e(S) \quad \forall S \subseteq N \tag{22}$$

$$\sum_{i \in S} x_i^c \leq v^c(S) \quad \forall S \subseteq N \tag{23}$$

$$\sum_{i \in S} x_i^u \geq v^u(S) \quad \forall S \subseteq N \tag{24}$$

Again, coalitional rationality on costs might cause infeasibility in many cases, so therefore is seldom included in configurations. Note that in these constraints the coalition S can consist of only one company. Therefore the individual rationality constraints are contained within the coalitional constraints and become redundant when adding the coalitional constraints. However, as mentioned before, we will include different combinations of constraints and in some

configurations individual rationality constraints will be used whereas the coalitional rationality constraints will not. Therefore, both sets of constraints are given and will optionally be included in the allocation model.
Another constraint ensuring that the company should be more interested in joining the coalition rather than working alone is based on the benefit/cost ratio allocated to a company and given below.

$$\frac{x_i^e}{x_i^c} \geq \frac{v^e(\{i\})}{v^c(\{i\})} \quad \forall i \in N \tag{25}$$

Constraints (25) ensure that the amount of CO_2 eq. emission reduction per cost unit, allocated to company i, is greater than the amount of CO_2 eq. emission reduction per cost unit, company i would obtain if it would work alone. We will call this constraint set the individual benefit/cost ratio rationality constraint.
Again, we can also ensure that this constraint is satisfied for every group of companies, similarly to the idea of the coalitional rationality constraints. This is done by including the following constraints.

$$\frac{\sum_{i \in S} x_i^e}{\sum_{i \in S} x_i^c} \geq \frac{v^e(S)}{v^c(S)} \tag{26}$$

We will call this constraint set the coalitional benefit/cost ratio rationality constraint.
Another way to make the allocation of the benefits and the costs more fair is to ensure that the benefit/cost ratio is more or less the same for each company. We do this by introducing the parameter α, indicating how much the benefit/cost ratio of a company can differ from the average benefit/cost ratio, and adding the following constraint sets.

$$\frac{x_i^e}{x_i^c} \geq (1-\alpha)\frac{v^e(N)}{v^c(N)} \quad \forall i \in N \tag{27}$$

$$\frac{x_i^e}{x_i^c} \leq (1+\alpha)\frac{v^e(N)}{v^c(N)} \quad \forall i \in N \tag{28}$$

Constraint set (27) ensures that the benefit/cost ratio of each company is greater than $(1-\alpha)$ times the average benefit/cost ratio and constraint set (28) ensures that it is less than $(1+\alpha)$ times the average benefit/cost ratio. We will investigate the effect different values of α will have on the results.
Finally, it might be realistic that the environmental benefits are not transferable. In this case we will not allocate the environmental benefits over the cooperating companies. As we want to investigate both the possibility of transferable and non transferable environmental benefits we introduce the following constraint.

$$x_i^e = e_{N,i,B_N} \quad \forall i \in N \tag{29}$$

If constraint (29) is added to the model, the obtained environmental benefits will stay at the company that realises the CO_2 eq. emission reduction. If all the suggested adjustments and extensions were added to the TM model the problem will be as given below.

$$\max \lambda - \gamma \tag{30}$$

$$\frac{x_i^e}{\beta^e C_i^e + \delta^e C_i^c + (1-\beta^e-\delta^e)C_i^u} \geq \lambda \quad \forall i \in N \tag{31}$$

$$\frac{x_i^c}{\beta^c C_i^e + \delta^c C_i^c + (1-\beta^c-\delta^c)C_i^u} \leq \gamma \quad \forall i \in N \tag{32}$$

$$x_i^e \geq v^e(\{i\}) \quad \forall i \in N \tag{33}$$

$$u(x_i^c, x_i^e) \geq v^u(\{i\}) \quad \forall i \in N \tag{34}$$

$$x_i^c \leq v^c(\{i\}) \quad \forall i \in N \tag{35}$$

$$\frac{x_i^e}{x_i^c} \geq \frac{v^e(\{i\})}{v^c(\{i\})} \quad \forall i \in N \tag{36}$$

$$\sum_{i \in S} x_i^e \geq v^e(S) \quad \forall S \subseteq N \tag{37}$$

$$\sum_{i \in S} x_i^u \geq v^u(S) \quad \forall S \subseteq N \tag{38}$$

$$\sum_{i \in S} x_i^c \leq v^c(S) \quad \forall S \subseteq N \tag{39}$$

$$\sum_{i \in S} \frac{x_i^e}{x_i^c} \geq \frac{v^e(S)}{v^c(S)} \tag{40}$$

$$\sum_{i} x_i^e = v^e(N) \tag{41}$$

$$\sum_{i} x_i^c = v^c(N) \tag{42}$$

$$\frac{x_i^e}{x_i^c} \leq (1+\alpha)\frac{v^e(N)}{v^c(N)} \quad \forall i \in N \tag{43}$$

$$\frac{x_i^e}{x_i^c} \geq (1-\alpha)\frac{v^e(N)}{v^c(N)} \quad \forall i \in N \tag{44}$$

$$x_i^e = e_{N,i,B_N} \quad \forall i \in N \tag{45}$$

$$\lambda, \gamma, x_i^e, x_i^c \in \mathbb{R} \quad \forall i \in N \tag{46}$$

From now on, this model will be called the Extensive TM (ETM) model.
As mentioned before, we will test different combinations of constraints and parameter values in our configurations. Therefore, in Table 8 all the possible constraints are summarized and are given a number. In Section 6, the numbers of the constraints that are included in each configuration will be given.

Name constraint set	Equations in ETM model	Number
Individual environmental rationality constraints	(33)	1
Individual utility rationality constraints	(34)	2
Individual cost rationality constraints	(35)	3
Individual benefit/cost ratio rationality constraints	(36)	4
Coalitional environmental rationality constraints	(37)	5
Coalitional utility rationality constraints	(38)	6
Coalitional cost rationality constraints	(39)	7
Coalitional benefit/cost ratio rationality constraints	(40)	8
Benefit/cost ratio deviation constraints	(43) (44)	9
Minimise highest DoFD	(30) (32)	10
Maximise lowest DoES	(30) (31)	11
Environmental benefits non transferable constraints	(45)	12

Table 8: Summary of the constraints that can be included in the ETM model.

Note that the constraints (41), (42) and (46) are always included in the ETM model. Furthermore, if only one of the constraints (31) or (32) is included, the objective function changes such that it maximises λ or $-\gamma$, respectively. The set of constraints that are included in a configuration will be called the set of requirements, denoted by R. The outcomes of the different configurations on different data instances will be discussed in Section 6.
To demonstrate some of the suggested extensions and adjustments in the ETM model Example 4.5 will show the cost and environmental benefits allocation that is made when the ETM model is implemented on a TU-game including some of the suggested extensions and adjustments.

Example 4.5 *Consider again the TU-game created by obtaining the values of $v(S)$ using the IUF method explained in Section 4.1.3 similar to Example 4.4. As we know what strategy is chosen by each coalition S we also know the values of $v^e(S)$ and $v^c(S)$. The values are summarized in Table 9.*

S	Strategy	$v^e(S)$	$v^c(S)$	$v^u(S)$
{A}	(a_2)	250	240	54
{B}	(a_1)	0	0	0
{C}	(a_2)	50	40	5
{A,B}	(a_2, a_2)	350	350	60
{A,C}	(a_2, a_2)	300	280	63
{B,C}	(a_1, a_2)	50	40	5
{A,B,C}	(a_3, a_3, a_3)	1200	1390	119

Table 9: Used $v(S)$ values to demonstrate TM model on data instance "Example 1".

Now, the three kinds of marginal contributions will be computed for each company. The computed values are given in Table 10.

Company	C_i^e	C_i^c	C_i^u
A	1.667	1.568	2.403
B	0.833	0.878	0.521
C	0.833	0.835	0.655

Table 10: Marginal contributions of each company to the three different kind of $v(S)$ values in demonstration of the ETM model on data instance "Example 1".

Now an allocation of the environmental benefits and costs will be computed using the ETM model. In this configuration the set of requirements is defined as $R = \{1, 2, 5, 6, 10, 11\}$*. Furthermore, the parameters are set to:* $\beta = (1, 0)$ $\delta = (0, 1)$*. The found allocation of the environmental benefits, the costs, the resulting utility and the DoES and DoFD values obtained by each company are given in Table 11.*

Company	x_i^e	x_i^c	$u_i(x_i^e, x_i^c)$	DoES	DoFD
A	900	700	60	573.85	420.00
B	250	250	0	284.84	300.00
C	240	250	5	287.59	300.00

Table 11: Allocation of the environmental benefits and the costs and the resulting obtained utility, DoES and DoFD values of each company in the demonstration of the ETM model on data instance "Example 1".

In Example 4.5 it is observed that the DoES and DoFD values are a bit further apart than was shown in Example 4.4 of the basic TM model. This is caused by the definition of the set of requirements R. Due to the new constraints, the possible allocations of costs and environmental benefits are reduced. For example, from the coalitional utility rationality constraints, we can observe that another constraint is added that ensures that the sum of utilities of company A and B is larger than 60 due to the obtained total utility of 60 by the coalition $\{A, B\}$.
In preliminary tests we have seen that the ETM model does not perform well when implemented on a TU-game for which at least one of the marginal contribution values is negative. In Section 4.2.3 we will explain why this is the case and how this is solved.
The ETM model is tested on different data instances with different definitions of the set R and different parameter settings. The results will be further explained and analysed in Section 6.

4.2.3 Potential savings game

In this Section we will explain why the ETM model and allocation methods based on marginal contributions in general perform poorly when implemented on negative marginal contribution values. Furthermore, we will suggest that in such cases the constructed TU-game should be transformed to a potential savings game and we will show how this is done. After transformation to a potential savings game the marginal contributions of each company are positive, meaning that the ETM model will perform as desired.
In preliminary tests we have seen that the ETM model does not perform well when computing an allocation of a TU-game for which at least one of the marginal contribution values is negative. This is caused by the fact that in these cases it may occur that the marginal contributions of different companies are different from sign. Meaning that for

example for one company the marginal contribution to the $v(S)$ values might be positive, whereas for another company the marginal contribution to the $v(S)$ values might be negative. This will yield allocations that are on the edge of the feasible region and that seem to be unfair or illogical. In Example 4.6 it is shown what kind of undesired allocation will result from using the TM model on a TU-game for which the marginal contribution signs of the companies differ.

Example 4.6 *We will allocate the costs based on the TU game constructed by the CM method on data instance "Example 1" in Section 4.1.1. For completeness the game is given in Table 12.*

S	u_S	Strategy
{A}	-240	(a_2)
{B}	-110	(a_2)
{C}	-1000	(a_3)
{A,B}	-240	(a_2, a_1)
{A,C}	-240	(a_2, a_1)
{B,C}	-150	(a_2, a_2)
{A,B,C}	-280	(a_2, a_1, a_2)

Table 12: Obtained $v(S)$ values using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1".

Computing the cost allocation using the ETM model, where $R = \{2, 10, 12\}$*, which is equivalent to the basic TM model, we obtain the following cost allocation:* $(240, 110, -70)$.

The cost allocation made in Example 4.6 suggests that side payments are made by companies A and B to convince company C to join the coalition. This allocation does indeed satisfy the individual rationality constraint however it does not seem logical that A and B would be willing to pay C this much to join the coalition, especially as C would have an utility value of -1000 if it left the coalition. This is caused by the fact that in this case the marginal contributions of companies A and B are negative, -0.93 and -2.5 respectively, whereas the marginal contribution of company C is positive, 3.86. This causes the model to minimise the costs that are allocated to C. As only the individual rationality constraints are considered, the model allocates as little costs as possible to C, while satisfying the individual rationality constraint, ensuring companies A and B obtain at least the same amount of utility as they would, when working alone. This seems unreasonable as in real life the companies A and B would have a large bargaining advantage by stating that company C would obtain a utility value of -1000, if it would work alone.
Furthermore, we have seen in literature, that positive values for the characteristic function $v(S)$ are used when describing a cooperative TU-game. Liu (2020) states that in cooperative game theory, the marginal contribution of each contributor to each coalition is a non-negative value. In Hiete et al. (2012) we have seen that the values of $v(S)$ are not described as the costs or utility that are incurred by a coalition, but by the potential savings a certain coalition could obtain.
In Lozano et al. (2013) the cost savings that different companies may achieve when they merge their transportation requirements are studied. Using a cost minimisation model, the costs of each coalition are computed. The cost savings of a coalition S are defined as the difference between the computed costs of coalition S itself and the sum of costs that would be obtained by the companies in S, if they would work alone. In the same way we will compute the potential savings of each coalition. Consider a constructed TU-game, for which the $v(S)$ values, representing the obtained utility of coalition S, are negative. Let $u_S = v(S)$ be the utility of coalition S. Now we will transform the values of $v(S)$ to a potential savings game by computing new $v(S)$ values for every coalition by the following equation.

$$v(S) = u_S - \sum_{i \in S} u_{\{i\}} \tag{47}$$

The values of $v(S)$ will be equal to zero for every coalition consisting of one company. For the larger coalitions the $v(S)$ value will be the increase in utility value that results from working together.
This transformation will be performed on every constructed TU-game that results in negative marginal contributions values for any of the participating companies.
The newly obtained $v(S)$ values will be used in the ETM model to make a cost savings allocation among the companies. Afterwards the savings allocated to a company are transformed back to costs. This is done by the following equation, where x_i will be the costs allocated to company i and y_i are the savings allocated to company i in the potential savings game.

$$x_i = u_{\{i\}} - y_i \tag{48}$$

In this way an allocation of the costs is made by making use of a potential savings game.
In Example 4.7, the TU-game of Example 4.6 is transformed to a potential savings game and a savings allocation is made.

Example 4.7 *The transformation on the TU-game, computed by equation* (47)*, will lead to the potential savings game as is stated in Table 13.*

S	u_S	Strategy
{A}	0	(a_2)
{B}	0	(a_2)
{C}	0	(a_3)
{A,B}	110	(a_2, a_1)
{A,C}	1000	(a_2, a_1)
{B,C}	960	(a_2, a_2)
{A,B,C}	1070	(a_2, a_1, a_2)

Table 13: $v(S)$ values after transforming the TU-game, found by using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance “Example 1”, to a potential savings game.

The chosen strategy will remain the same for each coalition. Using the obtained $v(S)$ values the marginal contribution of each company will be as stated in Table 14.

Company	C_i
A	1.14
B	1.07
C	2.73

Table 14: Marginal contributions of each company to the $v(S)$ values after transformation to potential savings game of data instance “Example 1”, computed by CM method.

Computing the cost allocation using the ETM model, where $R = \{2, 10, 12\}$, will now result in the following cost savings allocation: $(247.24, 231.02, 591.74)$*. Using equation* (48)*, we obtain a cost allocation of* $(-7.23, -121.02, 408.26)$.

This allocation seems more realistic, as company C is taking over the costs of companies A and B to be able to join the coalition, but is hereby reducing its own cost from 1000 to approximately 408.

4.3 Iterative procedures

In Section 4.1.3, we have stated that we are also interested in computing the values of the characteristic functions, $v(S)$, by making use of the individualised utility functions. We have seen that the use of the IUF method leads to one complication. Namely, the utility values of each company depend on the amount of costs allocated to that company. Therefore, we already need to make a cost allocation to determine the values of $v(S)$, whereas the values of $v(S)$ were meant to be used to compute a fair and stable allocation. In Section 4.1.3, we proposed a method that simply allocates the costs in such a way that the $v(S)$ values are maximised. Later, the obtained values of $v(S)$ are used to compute a fair and stable cost allocation for the grand coalition. The disadvantage of this method is that when maximising the values of $v(S)$, a cost allocation is made that might not be stable and fair. Therefore, the values of $v(S)$ for some coalitions might never be achieved in reality as some companies might have an incentive to leave the coalition and work in a subcoalition or on its own.
To give an idea what we mean, we will give an example showing why some values of $v(S)$ might never be attained in reality. Consider again “Example 1”, which data instance is summarized in Table 1. The used utility functions for all companies are equal to $u_i(e_{S,i,a}, c_{S,i,a}) = w_i e_{S,i,a} - (1 - w_i) c_{S,i,a}$. Also, we assume that the obtained CO_2 eq. emission reduction is allocated to the company that actually realises this reduction.
The values that would be obtained, if we compute the values of $v(S)$ in the way that is proposed in Section 4.1.3, are given in Table 15 as well as the chosen strategy and the made cost allocation in the determination of the values of $v(S)$. Now we will focus on the obtained value of $v(S)$ for $S = \{A, B\}$. As shown in Table 15, this value is equal to 60, computed by $v(\{A, B\}) = u_A(e_{\{A,B\},A,(a_2,a_2)}, x_A) + u_B(e_{\{A,B\},B,(a_2,a_2)}, x_B) = 0.6*250 - 0.4*350 + 0.5*100 - 0.5*0 = 60$, and is obtained by the cost allocation of $(x_A, x_B) = (350, 0)$. Now, if we look at the individual utilities gained from this allocation we see that the utility of company A equals $u_A = 250 \cdot 0.6 - 350 \cdot 0.4 = 10$ and the utility of company B equals $u_B = 100 \cdot 0.5 = 50$. From Table 15, we also observe that by working alone the gained utility of company A

would be equal to $u_A = 54$. Therefore, it seems very unlikely that company A would agree on working together with company B, whilst paying all the cost.

S	$v(S)$	Strategy	Cost Allocation
{A}	54	(a_2)	(240)
{B}	0	(a_1)	(0)
{C}	5	(a_2)	(40)
{A,B}	60	(a_2, a_2)	$(350, 0)$
{A,C}	63	(a_2, a_2)	$(280, 0)$
{B,C}	5	(a_1, a_2)	$(20, 20)$
{A,B,C}	119	(a_3, a_3, a_3)	$(1390, 0, 0)$

Table 15: $v(S)$ values using MIP formulation of maximisation problem

This example shows that the found values of $v(S)$ by solving the maximisation problem as it is stated in Section 4.1.3 could sometimes be unrealistic and unattainable in real life. Therefore, we suggest an iterative procedure that computes for each coalition the total utility that can be gained given that the allocation of the costs is made in such a way that the coalition is stable and all the companies should agree on working together.

Specifying when an allocation is thought to be stable and fair remains a challenge. In the following Sections we propose two different methods to tackle this problem in two different ways. In the first method it is assumed that the cooperating companies agree on the definition of a stable and fair allocation of the costs prior to the computations of the $v(S)$ values. From this agreement certain requirements for the cost allocation arise. Then the values of $v(S)$ are computed given that the cost allocation satisfies these requirements. The aim of this method is to find the highest possible $v(S)$ value in terms of utility for each coalition S, while satisfying all the constraints that were agreed upon by the companies. As this method repeatedly updates the value of $v(S)$ for a certain coalition and bases the cost allocation for this coalition on these updated values until the method converges, we will call this method the Repeated Cost Allocation (RCA) method. This method is further explained in Section 4.3.1.

The second approach is based on the assumption that the industrial cluster has an entirely different structure. In this approach we assume that there exists an industrial cluster management and that this management determines the rules and regulations on the allocation of the costs and the CO_2 eq. emission reduction prior to the computation of the $v(S)$ values. Therefore we will call this method the Predetermined Rules and Regulations (PRR) method. In this method, it becomes interesting to see how the rules and regulations set by the industrial cluster management will affect the choices and the negotiation space of the cooperating companies. This method gives answer to the third research question in Section 3 and is further explained in Section 4.3.2.

4.3.1 Repeated Cost Allocation

As mentioned before, we introduce an iterative procedure, such that the found $v(S)$ values for each coalition S are more realistic values and are possible to be attained in practice by coalition S. To accomplish this, the cooperating companies must agree on a set of requirements, R, that have to be satisfied by a cost allocation such that it is thought to be stable and fair. For example, the companies could agree that the cost allocation should minimise the highest DoFD, just as is done in the TM model, explained in Section 4.2. Furthermore, the companies could agree that the gained utility of a group of companies in a coalition should be higher than they could have achieved when working together in a subcoalition, or when working alone. More examples of restrictions the companies could agree on are the other restrictions suggested in 4.2.2.

The idea of this iterative procedure is to start by looking at coalitions containing only one company. At this stage, the determination of $v(S)$ is quite straightforward. The decarbonisation option that maximises the utility of the company is chosen and all the costs are evidently allocated to the company itself. This is similar to solving the maximisation problem stated in Section 4.1.3 for a coalition of only one company. Then we will move on to the coalitions containing two companies. We will act like this coalition is the grand coalition, denoted by N'. As we have already computed the values of $v(S)$ for all coalitions containing only one company, we know the values of $v(S)$ for each subcoalition of this grand coalition, N'. Next, we will determine a temporary value of $v(N')$ by solving the maximisation problem stated in Section 4.1.3. However, this will give an allocation of the costs that might not be stable, as mentioned before, so therefore we will repeatedly perform the following actions. Using the obtained values of $v(S)$ for each subcoalition of N' and the temporary value of $v(N')$ we will make a cost allocation that satisfies the set of requirements, R, set by the cooperating companies using the ETM model as it is stated in 4.2. Then, using the found cost allocation a new temporary value of $v(N')$ is computed, as the value of $v(N')$ depends on the allocation of the costs and therefore will alter when reallocating the costs. This procedure is repeated until the value of $v(N')$ is no longer adjusted, or until the problem becomes infeasible, meaning an allocation of the costs that satisfies all the requirements does not exist. This determination of temporary values of $v(N')$ is done for each possible strategy of the grand coalition N'. Then the strategy that gives the highest temporary value of $v(N')$ is chosen and the value of $v(N')$ is set equal to this value. After this is done for each coalition containing only two companies, we will perform the same actions for coalitions containing three companies. This iterative procedure is repeated until the actual grand coalition, N, is reached. In this way, realistic values of $v(S)$ will be obtained for each coalition $S \subset N$ and the actual strategy choice and cost allocation of the grand coalition can be made based on these realistic values. In Figure 1 a formal statement of the algorithm is given.

Now, we will give a brief explanation of the functions used in the algorithm. "$createStrategies(N, D)$" creates the set of all possible strategies for each coalition based on the given data instance. "$maximisation(S, B_S)$" solves the following maximisation problem for the given coalition, S, and strategy, B_S.

$$v(S) = \max \sum_{i \in S} u_i(e_{S,i,B_S}, x_i) \tag{49}$$

s.t.

$$\sum_{i \in S} x_i = c_{S,B_S} \tag{50}$$

$$x_i \in \mathbb{R}_+ \quad \forall i \in S \tag{51}$$

The function "$computeContributions(k, S, v^{temp}(S))$" computes the contributions of each company given current iteration, k, the coalition S and the current temporary values of $v(S)$ for each coalition $T \subseteq S$. The contributions are computed by $C_i = \sum_{T \subseteq S} \frac{v(T) - v(T \backslash \{i\})}{v(S)}$. The function "$isFeasible(S, B_S, v^{temp}(S), R)$", checks whether the AP solved by the ETM model including the constraints in the set of requirements R is feasible given coalition S, strategy B_S and contributions C. Finally, "$allocation(S, B_S, C, v^{temp}(S), R)$" constructs a cost allocation using the ETM model on the AP given the chosen strategy, B_S, over the companies in coalition S, given their contribution C and satisfying the set of requirements R. How this allocation is made depends on the requirements in set R. If one of the requirements is that the highest DoFD is minimised, then the allocation problem will be formulated as it is stated in 4.2.2, maximising the negative of a continuous variable, which is upper bounded by the degrees of dissatisfaction of every company in S. The other requirements in R, will determine to which other constraints the MIP will be subject to. We will now state an example of an allocation problem based on the requirements in R. Consider that the set of requirements is defined by, $R = \{6, 10\}$ from Table 8 and that $\delta = 1$. In this case, the allocation problem becomes the following.

$$\max -\gamma \tag{52}$$

s.t.

$$\frac{x_i}{C_i} \leq \gamma \quad \forall i \in S \tag{53}$$

$$\sum_{i \in T} u_i(e_{S,i,B_S}, x_i) \geq v(T) \quad \forall T \subset S \tag{54}$$

$$\sum_{i \in S} x_i = c_{S,B_S} \tag{55}$$

$$x_i \in \mathbb{R}_+ \quad \forall i \in S \tag{56}$$

In this allocation problem, the decision variables x_i indicate the amount of costs allocated to company i.
However, the AP changes significantly if both constraint sets 10 and 11 of Table 8 are not included in the requirement set R. In this case none of the requirements in R states that a certain DoFD or other ratio has to be maximised or minimised and the AP will maximise the value of $v(S)$ subject to all the restrictions in the set of requirements, R. Therefore, the allocation is not based on the marginal contributions of the companies and does not depend on the $v(S)$ values. Consequently, the algorithm converges in one iteration as the same input values will be used and the same AP will be solved by the function "$allocation(S, B_S, C, v^{temp}(S), R)$". Furthermore, in this case it is certain that the algorithm finds the allocation that maximises $v(S)$ subject to the constraints in R and therefore is optimal.
An interesting property of this algorithm comes from the fact that for each coalition an allocation of the costs is made that should satisfy the same set of individual and coalitional rationality constraints. Therefore, if for two disjoint coalitions $S_1 \subset N$ and $S_2 \subset N$ the strategies B_{S_1} and B_{S_2} were found, realising utility values of $v^u(S_1)$ and $v^u(S_2)$ respectively and satisfying the set of requirements R, then for the coalition $S = S_1 \cup S_2$ the strategy $B_S = \{B_{S_1}, B_{S_2}\}$

```
Algorithm 1: Repeated Cost Allocation
input  : O the set of all coalitions, D the set of all decarbonisation options, N the grand coalition,
         R the set of requirements that has to be satisfied by a cost allocation, ϵ upper bound on
         size of improvement to set off stopping criterion.
output: v(S) ∀S ⊆ N and the corresponding chosen strategy B_S.
// Initialise coalition size k and create all possible strategies
k ← 1;
A ← createStrategies(N, D);
stop ← False;
solutionFound ← False;
// Loop over all possible coalition sizes
while k ≤ |N| do
    // Loop over all coalitions of size k
    for S ∈ O : |S| = k do
        // Loop over all possible strategies of coalition S
        for B_S ∈ A_S do
            // Get a temporary value for v(S) by solving maximisation problem
            v^temp(S) ← maximisation(S, B_S);
            // Use found characteristic function values to compute marginal
               contributions
            C ← computeContributions(k, S, v^temp(S));
            // Perform while stop criterion is not met
            while not stop do
                // If the resulting AP is feasible
                if isFeasible(S, B_S, v^temp(S), C, R) then
                    // Solve AP using ETM and update temporary v(S) and marginal
                       contribution values
                    previous ← v^temp(S);
                    v^temp(S) ← allocation(S, B_S, C, v^temp(S), R);
                    C ← computeContributions(k, S, v^temp(S));
                    // If no change in v(S) value
                    if |v^temp(S) − previous| < ϵ then
                        // Stop while loop and store that a solution for coalition S for
                           strategy B_S is found
                        stop ← True;
                        solutionFound ← True;
                // If resulting AP is not feasible
                else
                    // Stop while loop and store that no solution for coalition S for
                       strategy B_S satisfying all requirements is found
                    stop ← True;
                    solutionFound ← False;
            // If a solution is found for coalition S and it has higher utility value
               than the found solutions for other strategies
            if solutionFound and v^temp(S) ≥ v(S) then
                // Store new best solution and corresponding strategy
                v(S) ← v^temp(S);
                chosenStrategies(S) ← B_S
    // Increase coalition size k with one
    k ← k + 1;
```

Figure 1: Formal algorithm formulation of Repeated Cost Allocation algorithm

would realise a utility value of $v^u(S) = v^u(S_1) + v^u(S_2)$ and satisfy the set of requirements R. Therefore, for every coalition it holds that a strategy and cost allocation exists that realises an amount of utility for every group of companies that is at least as high as that group of companies could attain by leaving that coalition. This property does not hold per definition when the set of requirements contains other constraints than the individual and coalitional rationality constraints $\{1, 2, 3, 4, 5, 6, 7, 8\}$. For these constraints it holds that if strategy B_{S_1} and B_{S_2} satisfy these constraints then the strategy $B_S = \{B_{S_1}, B_{S_2}\}$ will also satisfy these constraints. This does not per definition hold for other constraints such as the benefit/cost ratio deviation constraints, constraint 9. We will call this the feasibility property of the RCA algorithm as it ensures that the constructed game in $v^u(S)$ values is superadditive and therefore the feasible region of the AP will be non empty.
The algorithm of Figure 1 will return the values of $v(S)$ for all coalitions $S \subseteq N$ and the corresponding chosen strategy B_S. We are interested in the affect of the set of requirements, R, on feasibility, convergence of the algorithm and the chosen strategy with corresponding utility values and cost allocation. Furthermore, using the obtained values of $v(S)$ we can find the (in-)equalities describing the vertices of the core. The boundaries of the core, interests us as it describes the negotiation space of the cooperating companies in terms of transferable utility. How we will compute the negotiation space of each company will be explained in Section 4.3.3. When analysing the results we will also be interested in the affect of the set of requirements, R, on the negotiations space of each company.

4.3.2 Predetermined Rules and Regulations

In this Section another iterative procedure is explained which is based on the assumption that an industrial cluster management exists that determines the rules and regulations on how the costs and environmental benefits are allocated. This method will try to give answer to a different research question, namely the third research question in Section 3, than the other methods as we assume a totally different structure in the industrial cluster.
Now consider that there exists an industrial cluster management. This management determines under what rules and regulations the costs and CO_2 eq. emission reduction are allocated over the companies. The goal of the management is assumed to be twofold. First of all, the management aims to set the rules and regulations in such a way that the companies will come to an agreement. Therefore we will be interested in the solution space or negotiation space of the strategies that are chosen under certain rules and regulations. Secondly, the management aims to realise as much CO_2 eq. emission reduction as possible. Therefore, we will be interested in the strategies that will be chosen under certain rules and regulations. Furthermore in future research it might also be interesting to try to maximise the solution space under the restriction that a certain amount of CO_2 eq. emission reduction is realised.
Prior to the decision making, the companies are aware of the rules and regulations set by the management. Therefore, the companies can base their decisions on the given rules. We will define the rules and regulations made by the industrial cluster management as the functions $r^e : A_S \to \mathbb{R}^{|S|}$ and $r^c : A_S \to \mathbb{R}^{|S|}$. The function $x^e = r^e(S, B_S)$ takes as input a coalition, S, and the strategy of the coalition, B_S, and returns a vector allocating the environmental benefits to the companies in coalition S. The function $x^c = r^c(S, B_S)$ works in the same way for the allocation of the costs. Some examples of rules could be: (i) the environmental benefits are allocated to the company that realises them, (ii) the costs are evenly divided over all companies, (iii) the environmental benefits are allocated proportionally to the size of the companies, (iv) the variable costs are allocated to the company to which they are incurred and the fixed costs are allocated proportionally to the size of the companies.
We introduce two new parameters. Firstly, the parameter b_i indicates how much a company benefits from the allocation of environmental benefits. Secondly, the parameter k_i indicates how much a company will be set back by the allocation of costs. It should be possible to make an educated estimation of these parameters by analysing the structure and primary activities of the companies. This estimation is not investigated in this research. We are merely interested in their influence on the results. These parameters are used to define the utility function of each company, which is defined by $f_i(S, B_S) = b_i r^e_i(S, B_S) - k_i r^c_i(S, B_S)$.
The idea of the algorithm is to compute the values of $v(S)$ by maximising the sum of utilities of the companies in coalition S subject to the constraints that are included in requirement set R in the AP. In this case, how the costs and environmental benefits are allocated are already determined, so the AP only consists of checking whether the allocation made by the set rules for the chosen strategy meets the requirements in the set R. The set R is still used to check whether a certain strategy is stable and if not, the strategy is not chosen. The constraints that we think are most important to be included in R to obtain a feasible allocation are constraint sets 2 and 6 in Table 8, the individual and coalition utility rationality constraints. Meaning that every group of companies within the coalition gains higher utility than when working in a subcoalition. The algorithm still computes the $v(S)$ values in order of increasing size such that the constraints included in the set R can be satisfied in each iteration. For example, for satisfying the coalition utility constraint when computing $v(S)$, all $v(T)$ values for $T \subset S$ are needed. In this way the algorithm should find the best strategy B_S, maximising $v(S)$, while satisfying the constraints in R, for every coalition $S \subseteq N$. In Figure 2 a formal statement of the algorithm is given.

Algorithm 2: Predetermined Rules and Regulations

input : O the set of all coalitions, D the set of all decarbonisation options, N the grand coalition, r the function describing the rules and regulations on the allocation of the realised CO_2 eq. emission reduction and the costs, R set of requirements.
output: $v(S)\ \forall S \subseteq N$ and the corresponding chosen strategy B_S.

```
// Initialise coalition size k and create all possible strategies
k ← 1;
A ← createStrategies(N, D);
// Loop over all possible coalition sizes
while k ≤ |N| do
    // Loop over all coalitions of size k
    for S ∈ O : |S| = k do
        // Compute maximum v(S) value satisfying requirements in R and store v(S)
           value and chosen strategy
        (v(S), chosenStrategies(S)) ← maximisation(S, A_S, v(S), r, R);
    // Increase coalition size k with one
    k ← k + 1;
```

Figure 2: Formal algorithm formulation of Predetermined Rules and Regulations algorithm.

Now we will explain the functions that are used in the algorithm. Just as in the algorithm in Section 4.3.1, the function "*createStrategies*(N, D)", creates the set of all possible strategies for each coalition based on the given data instance. The function "*maximisation*$(S, A_S, v(S), r, R)$" finds the strategy that maximises the total utility of coalition S given that the allocation made by the predetermined rules and regulations, when choosing this strategy, satisfies all the requirements in the set R. If for example $R = (2, 6)$, choosing the constraint sets from Table 8, then the maximisation problem that is solved by "*maximisation*$(S, A_S, v(S), r, R)$" is the following.

$$\max \sum_{B_S \in A_S} \sum_{i \in S} x_{B_S} f_i(S, B_S) \tag{57}$$

s.t.

$$\sum_{i \in T} x_{B_S} f_i(S, B_S) \geq x_{B_S} v(T) \quad \forall T \subseteq S \tag{58}$$

$$x_{B_S} \in \mathbb{B} \quad \forall B_S \in A_S \tag{59}$$

We are interested in what different allocation rules and regulations will do to the decisions of the companies, the allocation of the costs and the environmental benefits and how these affect the core/negotiation space of the companies. How we compute the negotiation space is further explained in Section 4.3.3.

4.3.3 Computation of the negotiation space

The core of a cooperative transferable utility game is defined as the set of payoffs for which no company or group of companies is able to gain a higher utility value when leaving the grand coalition. Assuming that the companies are rational this means that for all payoffs in the core, no company should have an incentive to leave the grand coalition. Now in practice, this assumption might not hold. However, using this definition, we can compute the boundaries of the core and the boundary values for which each company, assuming they are rational, should have no incentive to leave the grand coalition. The larger the area between these boundaries of each company, the more likely these companies are really cooperating in the grand coalition in practice. Therefore, we are interested in the negotiation space of each company and what happens to the decision and negotiation space of the group of companies if one company leaves the grand coalition.
Consider $y = (y_1, y_2, ..., y_n)$, the vector of payoffs, than the vertices of the core are given by the following (in-)equalities.

$$\sum_{i \in S} y_i \geq v(S) \quad \forall S \subset N \tag{60}$$

$$\sum_{i \in N} y_i = v(N) \tag{61}$$

Therefore, as mentioned before, we can compute the boundaries of the core using the found values of $v(S)$. A possible way to compute the negotiation space of each company is by solving two LP's for each company. Maximising y_i subject to equations (60) and (61) will give the upper bound of the negotiation space of company i. Similarly, minimising y_i subject to equations (60) and (61) will give the lower bound of the negotiation space of company i. A disadvantage of this method is that we would have to solve two LP's for every company in S for every coalition $S \subseteq N$, to analyse the negotiation space of each company in each coalition.
Therefore, we will also propose another method to compute an estimation of the boundaries of each company of each possible coalition, that potentially is run in less computation time. This method is based on the core cover. Quant et al. (2005) states that the utopia demand of a company i, the maximum amount company i can hope to achieve from cooperation in the grand coalition N, is equal to

$$UB_i(N) = v(N) = v(N \backslash \{i\}), \tag{62}$$

since the group of companies $N\backslash\{i\}$ will not be satisfied with a total payoff strictly less than $v(N\backslash\{i\})$. The minimum payoff a company wants to claim corresponds to the maximum payoff this company can achieve by gathering a possible subcoalition and promising any other player in this subcoalition his maximum amount of payoff. This is observed from the restrictions imposed by equation (60). Formally, the minimum payoff a player i in the grand coalition N wants to claim is defined by

$$LB_i(N) = \max_{S \in O: i \in S} \{v(S) - \sum_{j \in S \backslash \{i\}} UB_j(N)\}. \tag{63}$$

The core cover of a game consists of all efficient payoff vectors, giving each company at least his minimum claim, but no more than his utopia demand. By definition of the core all the payoff vectors that are in the core are also contained in the core cover. Therefore, if we compute the bounds as stated by equations (62) and (63), we know that the negotiation space of the companies are between the found lower and upper bounds. We have found that for the small data instances we will investigate in our results that the exact method, solving two LP's for every company in S for every coalition is computationally little time consuming. Using this method the solution space was computed within 4 seconds for every data instance. Therefore, we will use this method for computing the negotiation space of every company. For future research, if the negotiation space would need to be computed for larger data instances, it might be interesting to use the heuristic to find reasonable upper and lower bounds.

5 Data

As mentioned before, the data we will be using, will be data from the industrial cluster in Limburg, called "Chemelot". From this data we expected to gain knowledge about the following: (i) which companies are located in the cluster, (ii) the current amount of CO_2 eq. emission of each company, (iii) all the possible decarbonisation options that could be used by each company, (iv) the reduction in CO_2 eq. emission and the costs associated with each decarbonisation option for each company. Furthermore, we hope to learn a bit more about the incentives of each company. Is it their priority to reduce their CO_2 eq. emission or keeping the costs as low as possible?
Unfortunately, the exact data values are still uncertain to us. The costs and environmental benefits of each decarbonisation option for the companies are uncertain and need more research. In van der Linden (2019) and DNV GL Netherlands B.V. (2020) some estimations of costs for certain projects (decarbonisation options) are given. The estimations give a range in which the costs of the project should lie. The estimated intervals are still quite large. For example in DNV GL Netherlands B.V. (2020), the project "CCS Athos" is estimated to cost between 570 and 870 million euros. This is just a single decarbonisation project at one location. Furthermore, as our interest lies in the investigation of the presented models and not in perfecting the data, we will not make use of exact costs and CO_2 eq. emission reduction values.
However, we do know how many companies are allocated in the industrial cluster and we know approximately what their current emission of CO_2 eq. are. Therefore, we have come up with some data instances that are based on these values and can be used to test our methods and investigate the influence of certain parameters. The parameters b_i, k_i and w_i, representing the weight companies give to obtaining environmental benefits and costs, remain very uncertain and still unpredictable. Therefore, we will try different values and investigate their influence on the results. An estimation of these parameters remains for future research.
In the instances we have come up with, we have information on the companies in the cluster, including their parameters b_i, k_i and w_i and on the available decarbonisation options. We distinguish between two types of decarbonisation options, namely individual (I) and group (G) decarbonisation options. The costs of the individual options only consists of variable costs, which are specified per company. The costs of the group options also include fixed costs, which will have to be paid by the whole coalition. For both types of options the amount of CO_2 eq. emission reduction that is

realised per company is specified. To give an idea how the data instances are presented we will show Table 16 that summarizes the data instance "Example 1".

Companies	Emission	w_i	b_i	k_i
A	1000	0.6	1.2	1
B	500	0.5	1	1
C	400	0.5	1	1

			Company A		Company B		Company C	
D	G/I	c^f	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0
a_2	I	0	250	240	100	110	50	40
a_3	G	900	750	240	250	150	200	100

Table 16: Information on companies and decarbonisation options in instance "Example 1".

Now we will give an explanation of the data instances we have come up with and used to test our different solution methods.

In our first instance, called "Chemelot 1", there are three larger companies and three smaller companies. The size of the companies is expressed in their current emission values (in megatonnes CO_2 eq.). The smaller companies, produce around 5-10 times less the amount of CO_2 eq. emission than the larger companies. The parameters b_i and k_i are randomly chosen and will be altered in other instances such that we can analyse their influence. The values of b_i and k_i will be close to 1 as we expect that the value companies give to induced costs and environmental benefits will not differ a lot from each other and the value of environmental benefits is expected to be relatively close to the MKI value. The parameter w_i is chosen such that $\frac{w_i}{1-w_i} = \frac{b_i}{k_i}$ and $0 \leq w_i \leq 1$. In this way, the two different iterative procedures are better comparable, as the ratio to which each company values CO_2 eq. emission reduction compared to the costs is the same. Furthermore, there are four different decarbonisation options included in the instance. The first option represents the choice of doing nothing at all. This options induces no costs and realises no CO_2 eq. emission reduction. The second option represents an individual investment option, for example a heat pump. This option induces no fixed costs, as it is an individual option, and in general this option is cheaper and realises less CO_2 eq. emission reduction than a group decarbonisation option. Finally, two different group decarbonisation options are included. Examples of these options could be an infrastructure for the use of CCS or the use of hydrogen as feedstock for the companies. These options induce variable costs to each company investing in this option and fixed costs to the group of companies investing in this option. In general, these options realise more CO_2 eq. emission reduction than the individual options. The two group options differ in amount of variable costs, fixed costs and realised CO_2 eq. emission reduction. In our first instance, "Chemelot 1", the first group decarbonisation option has lower fixed costs, but also realises less CO_2 eq. emission reduction. All the information on the companies and decarbonisation options can be found in Table 39 in appendix A.

In the second instance, called "Chemelot 2", the costs and amount of CO_2 eq. emission reduction that is realised by the group decarbonisation options is altered with respect to the data in the instance "Chemelot 1". In the first instance, the amount of CO_2 eq. emission reduction that is realised by each company was in proportion with the size of the company. This may cause similarity in the solution space for different allocation rules and regulations in the PRR algorithm. Therefore, in the second instance, we have changed the values of the realised CO_2 eq. emission reduction of each company, such that they are less correlated with the size of the company (in terms of current emission). Of course, some correlation still exists, as it is not possible to realise more CO_2 eq. emission than a company's current emission. The information on the companies and decarbonisation options of the "Chemelot 2" instance can be found in Table 40 in appendix A.

In the third instance, called "Chemelot 3", the parameters b_i and k_i of every company are set to 1. This means, that the values of w_i are equal to 0.5 for each company. Furthermore, some alterations have been made on the company sizes, realised CO_2 eq. emission reduction per decarbonisation option per company and the costs of the decarbonisation options. In this instance, choosing a group decarbonisation option is less profitable when looking at total reduction and total costs when compared to the first two instances. Combined with the fact that the parameters b_i and k_i are also less favorable for larger investments realising more CO_2 eq. emission reduction, we are interested to see for what methods and requirements/rules and regulations a group decarbonisation option is chosen. Furthermore, it is interesting to see what this does to the negotiation space of the companies. The information on the companies and the decarbonisation options can be found in Table 41 in appendix A.

Futhermore, all instances can be adjusted by incorporating a tax value, h, assigning extra variable costs to each decarbonisation for every company. h represents a certain tax that has to be paid by the companies for every megaton

of CO_2 eq. that is still emitted after the investment in a decarbonisation option. For example, let $h = 10$ million euros per megaton CO_2 eq. If company A decides to reduce its emission from 10 to 5 megaton of CO_2 eq., than the variable costs of this option will be increased by 50 million euros. If company A decides to do nothing, while its current emission is 10 megaton of CO_2 eq., than the costs will be 100 million euros. We are interested to see what these kind of adjustment to the data instances will do to the decisions of the companies and their negotiation space. Another example is given in Table 42 in appendix A, where a tax value of $h = 20$ is incorporated in the data instance "Chemelot 3".
Next to that, two small example instances, "Example 1" and "Example 2", are introduced that are used throughout this thesis to show the different solution approaches and their advantages and disadvantages.
Lastly, we introduce two instances of different size in terms of number of companies in the cluster. The first instance, "Small Chemelot", consists of only 4 companies and the second instance, "Large Chemelot", consists of 8 companies. We are interested in the difference in solutions and computation time of these instances in comparison with the other instances and each other. The information of the instances can be found in Tables 43 and 44 in appendix A.
In Table 17 the different data instances and some of their properties are summarized. In Table 17 the number of decarbonisation options, $|D|$, the number of companies, $|N|$, the total current emission of all the companies (in million euros), E_N, the mean of the weights of the companies, μ_w, and the variance of the weights of the companies, σ_w^2 are given. The mean and variance of the weights of the companies are given to gain insight in whether the companies give similar weight to obtaining CO_2 eq. emission reduction.

Instance	$\lvert D\rvert$	$\lvert N\rvert$	E_N	μ_w	σ_w^2
Example 1	3	3	1900	0.5333	0.0033
Example 2	4	4	3350	0.3625	0.0856
Chemelot 1	4	6	3300	0.5288	0.0024
Chemelot 2	4	6	3300	0.5388	0.0009
Chemelot 3	4	6	5250	0.5	0
Small Chemelot	4	4	2200	0.5	0
Large Chemelot	4	8	6600	0.5	0

Table 17: Summary of used data instances.

6 Results

In this Section the results of the different methods, introduced in Section 4, tested on the data instances described in Section 5, will be discussed and compared. In Section 6.1 the values of the characteristic function are computed by using the CM method as explained in Section 4.1.1. Then a cost allocation is made, using the ETM model as described in Section 4.2 and the results are discussed. In Section 6.2 the values of the characteristic function will be computed by using joint utility functions as explained in Section 4.1.2 and then a cost and benefit allocation will be made making use of the ETM model, described in Section 4.2 and the results will be discussed. In Section 6.3, the results of the third method will be discussed. In this method the values of the characteristic function will be computed using individual utility functions and solving the maximisation problem, maximising the sum of all utilities, as explained in Section 4.1.3. Afterwards, an allocation of the costs and benefits will be made, making use of the ETM model, described in Section 4.2. In Section 6.4, the results of the RCA algorithm, described in Section 4.3.1, will be discussed. In Section 6.5, the results of the PRR algorithm, described in Section 4.3.2, will be discussed. The set of requirements that will be included in the ETM model as described in Section 4.2, will differentiate through all the configurations in Sections 6.1, 6.2, 6.3, 6.4 and 6.5. However, mainly the same allocation rules will be applied such that the suggested methods are better comparable. The set of requirements that is used in each configuration will be given. Finally, in Section 6.6, the results of the different solution methods will be compared as well as a summary will be given on the advantages and disadvantages of each solution method.

6.1 Cost Minimisation and Extensive TM allocation

In this Section the CM method, described in Section 4.1.1, will be tested on different data instances and parameter settings. First we will give an overview on the different configurations that will be used to test the CM method. Then the constructed TU-games using this CM method will be summarized and analysed. Then a cost allocation will be made making use of the ETM model described in Section 4.2. The results of this cost allocation will be discussed and finally a conclusion about the CM method will be drawn.

Configurations

First, we will give an overview on the different configurations that will be used to test the CM method. In Table 18 the different configurations are summarized. In the first column a name is given to the configuration such that we can refer to that configuration. In the second column the name of the data instance that is used is given. In the third and fourth column the used values of the parameters p and h are given. Recall that p indicates the percentage of CO_2 eq. emission reduction that has to be realised by every coalition and h indicates the tax value that is given to remaining CO_2 eq. emission in million euros. In the last column the set of requirements R is given, stating which constraints are included in the ETM model. What constraints are meant by the numbers can be found in Table 8 in Section 4.2.2.

Name	Instance	p	h	β	δ	R
CM1	Example 1	15%	0	(0,0)	(0,0)	(2,6,10,12)
CM2	Example 1	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM3	Example 2	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM4	Chemelot 1	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM5	Chemelot 1	89%	0	(0,0)	(0,0)	(2,6,10,12)
CM6	Chemelot 2	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM7	Chemelot 3	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM8	Small Chemelot	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM9	Large Chemelot	49%	0	(0,0)	(0,0)	(2,6,10,12)
CM10	Example 1	0%	10	(0,0)	(0,0)	(2,6,10,12)
CM11	Example 1	0%	40	(0,0)	(0,0)	(2,6,10,12)
CM12	Example 1	0%	50	(0,0)	(0,0)	(2,6,10,12)
CM13	Example 1	0%	70	(0,0)	(0,0)	(2,6,10,12)
CM14	Chemelot 1	0%	40	(0,0)	(0,0)	(2,6,10,12)
CM15	Chemelot 1	0%	50	(0,0)	(0,0)	(2,6,10,12)

Table 18: Configuration settings used to test the CM method.

Note that the same set of requirements R is used throughout the configurations, such that the difference in data instance and parameter settings is better observed. Furthermore, as we assume that the companies obtain no utility of reducing their CO_2 eq. emission, the environmental benefits are never allocated. Therefore, the parameters β and δ are both set to $(0, 0)$, such that the allocation of the costs fully depend on the marginal contribution to the $v^u(S)$ values. This is also the reason that no restrictions involving environmental benefits are included in the set of requirements, as the companies give no value to it. Also, as the utility function of a company is the negative of the allocated costs, including the rationality constraints on utility is equivalent to including the rationality constraints on the costs. So, including only the rationality constraints on utility suffices.
In the CM method, the utility function only consists of the costs as we assumed that the companies gain no utility from reducing their CO_2 eq. emission. Therefore, one of the parameters p and h, need to be set larger than zero, otherwise the companies would just do nothing and have utility values of zero. From now on, we will call the parameters p and h external incentives, as they are set by for example a government or management in an attempt to force the companies to invest in decarbonisation options. In other methods, the environmental benefits are incorporated into the utility functions of the companies, then we will call this the internal incentive of the companies.

Constructed TU-games

In Table 19, the results of the CM method, performed on the different configurations, are summarized. The Table includes the chosen strategy by the grand coalition, whether the constructed game was transformed to a potential savings game, the obtained characteristic function utility values for the grand coalition, $v^u(N)$, after potential transformation and the computation time in seconds of the CM method.

Name	Strategy	Transformed	$v^u(N)$	Computation time
CM1	(a_2, a_1, a_2)	True	1070	0.077
CM2	(a_3, a_1, a_3)	False	-1240	0.115
CM3	(a_3, a_3, a_2, a_1)	False	-2040	0.336
CM4	$(a_3, a_3, a_1, a_3, a_1, a_2)$	False	-1980	1.658
CM5	$(a_4, a_4, a_4, a_4, a_4, a_1)$	False	-2780	1.734
CM6	$(a_1, a_3, a_3, a_1, a_1, a_1)$	False	-1900	2.244
CM7	$(a_1, a_3, a_3, a_3, a_3, a_3)$	True	8090	1.932
CM8	(a_1, a_3, a_3, a_1)	True	2870	0.245
CM9	$(a_3, a_3, a_3, a_1, a_1, a_1, a_1, a_1)$	True	16710	67.582
CM10	(a_1, a_1, a_1)	False	-380	0.112
CM11	(a_1, a_1, a_1)	False	-1520	0.125
CM12	(a_2, a_1, a_2)	False	-1880	0.094
CM13	(a_3, a_3, a_3)	False	-2370	0.149
CM14	$(a_1, a_1, a_1, a_1, a_1, a_2)$	False	-2630	1.706
CM15	$(a_4, a_4, a_4, a_4, a_4, a_4)$	False	-3060	2.416

Table 19: Obtained $v^u(N)$ values and optimal strategies using the CM method on test instances summarized in Table 18.

Furthermore, in appendix B.1, some of the constructed TU-games are shown. In Tables 45 and 49 the found characteristic function utility values before transformation to the potential savings game of configurations "CM1" and "CM8" respectively are given. In Tables 46 and 50 the obtained utility values of the characteristic function are given after transformation to the potential savings game of configurations "CM1" and "CM8". In Tables 47, 48 and 51 the obtained characteristic function utility values of the configurations "CM2", "CM3" and "CM13" respectively, are given.
From the results in Table 19 we can observe that the CM method finds the strategy that minimises the costs within 3 seconds for all the instances containing 6 or less companies. For the larger instance of 8 companies the CM methods takes about 68 seconds to compute all the characteristic function values and the corresponding strategies. This is caused by the fact that the number of coalitions equals 2^n (if the empty coalition is included), where n is the number of companies. We expect to see the same growth in computation time for the other solution methods, which results will be presented in Sections 6.2, 6.3, 6.4 and 6.5.

Potential savings game transformation

Table 19 also shows that only some created games are transformed to a potential savings game. Recall, that this transformation is made whenever one of the companies' marginal contributions is negative. This is done, because the ETM model performs poorly when there exist negative marginal contributions. From the created games we have seen that a negative marginal contribution potentially occurs when there is a big difference in the characteristic function value between the coalitions consisting of one company. For example, when looking at the characteristic function values before transformation of "CM1" and "CM8" in Tables 45 and 49, we can observe that in both configurations there exists a big difference in $v(S)$ values for the coalitions of a single company. In Table 45 we can observe that the value of $v(\{C\})$ is significantly lower than the values of $v(\{B\})$ and $v(\{A\})$. Recall that the marginal contributions of the companies were computed by $\sum_{S\subseteq N} \frac{[v(S) - v(S-\{i\})]}{v(N)}$. Now, the computation of the marginal contribution of company B will be as follows: $C_B = \frac{-110}{-280} + \frac{-240+240}{-280} + \frac{-150+1000}{-280} + \frac{-280+240}{-280} = -2.5$. It is observed that due to the part $\frac{-150+1000}{-280}$, the marginal contribution of company B becomes negative. This part represents $\frac{v(\{B,C\})-v(\{C\})}{v(\{A,B,C\})}$, and is a big negative value due to the large negative value of $v(\{C\})$ compared to the relatively small negative value of $v(\{B,C\})$. Similarly, the marginal contribution of company A becomes negative. In Table 49 we can observe that the value of $v(\{D\})$ is significantly higher than the $v(S)$ values for the other coalitions consisting of one company. In this case, the marginal contribution of company D becomes negative.

External incentives

We can also observe that this method could be used by a government or cluster management to investigate how high the tax, h, should be to force the decision of the companies to a strategy realising more CO_2 eq. emission reduction. For example, when looking at the results of configurations "CM14" and "CM15", we observe that setting the value

of h to 50, will ensure that in fact the strategy $B_S = (a_4, a_4, a_4, a_4, a_4, a_4)$, in which all companies reduce their CO_2 eq. emission with the group decarbonisation option a_4, is the cheapest of all strategies. Whereas, setting the value of h to 40, ensures that the strategy $B_S = (a_1, a_1, a_1, a_1, a_1, a_2)$, is the cheapest of all strategies. From the data instance "Chemelot 1", summarized in Table 39, we can observe that the strategy $B_S = (a_1, a_1, a_1, a_1, a_1, a_2)$ realises 1 megaton CO_2 eq. emission reduction from the total 66 megaton CO_2 eq. that is currently being emitted. The strategy $B_S = (a_4, a_4, a_4, a_4, a_4, a_4)$ realises 61 megaton CO_2 eq. emission reduction. So increasing the value of h by 10, in this fictional data instance, results in an increase of the CO_2 eq. emission reduction from 1.5% to 92.4% of the current emission, under the assumption that the companies' decision makers are rational and only care about minimising their cost. As this is a fictional example and in reality the costs and environmental benefits of certain decarbonisation options are difficult to determine exactly, we cannot conclude something directly on how high the value of h should be to ensure a certain amount of reduction or to force decision makers towards a certain strategy. However, we can conclude that this method is suitable for a government or management to investigate how high the value of h should be, if the real data is available, to ensure that a certain desired strategy is in fact the cheapest option, which will probably result in that strategy to be chosen. Furthermore, by altering the value of p, it could be investigated what strategy is the cheapest, while realising a certain percentage of reduction. So, when a government or cluster management forces the companies within a cluster to ensure a certain percentage of CO_2 eq. emission reduction, the companies could use this method to compute which strategy is the cheapest, while realising the set percentage of emission reduction.
A disadvantage of having to use external incentives, is that in some cases setting the parameter p to a certain value, might lead to an infeasible problem for a certain subcoalition $S \subset N$, while the problem is feasible for the grand coalition N. For example, when looking at data instance "Example 1", setting the value of p to 60% will lead to an infeasible problem for the coalition $S = \{B\}$, as there does not exist a decarbonisation option that realises 60% CO_2 eq. emission reduction for company B. However, for the grand coalition, there does exist a strategy that realises 60% CO_2 eq. emission reduction. In this case, we would have a value for $v(N)$, but no value for $v(\{B\})$. Therefore, we will not be able to use the ETM model to make a cost allocation based on the characteristic function values.

Cost allocation

The found characteristic function values for each configuration are used to make an allocation using the ETM model with the parameter settings as stated in Table 18. The found allocation and the computation time of the ETM model are given in Table 20.

Name	Cost allocation	Computation time
CM1	$(165, 40, 75)$	0.013
CM2	$(457, 407, 376)$	0.012
CM3	$(476, 462, 499, 602)$	0.011
CM4	$(240, 318, 80, 650, 662, 30)$	0.033
CM5	$(675, 675, 670, 262, 262, 237)$	0.031
CM6	$(607, 414, 477, 220, 173, 8)$	0.049
CM7	$(895, 750, 780, 670, 6, -2)$	0.021
CM8	$(542, 562, 435, 0)$	0.031
CM9	$(694, 607, 669, 638, 17, 561, 504, 0)$	0.291
CM10	$(200, 100, 80)$	0.009
CM11	$(800, 400, 320)$	0.012
CM12	$(990, 500, 390)$	0.008
CM13	$(1244, 632, 494)$	0.009
CM14	$(800, 760, 720, 160, 120, 70)$	0.016
CM15	$(933, 895, 847, 178, 136, 72)$	0.048

Table 20: Obtained allocation using the ETM model on the games constructed by the CM method, with parameter settings summarized in Table 18.

From the results in Table 20 we can observe that the ETM model is able to find a cost allocation within 0.3 seconds for all tested configurations.
Another possible disadvantage of the CM method follows from the fact that there are no internal incentives incorporated in the utility functions of the companies. This leads to cost allocation that might seem unfair to the participating companies. Due to the fact that no internal incentives exists the $v(S)$ values are only based on the costs and the cost allocation made by the ETM model is completely based on the marginal contributions of the companies to the

costs. That is why it may occur that in a chosen strategy a company does not realise any of the CO_2 eq. emission reduction, but is allocated a big share of the costs. For example, in configuration “CM7”, the strategy that is chosen is $B_N = (a_1, a_3, a_3, a_3, a_3, a_3)$, whereas the cost allocation that is made is $(895, 750, 780, 670, 6, -2)$. In this case, company A’s marginal contribution to the costs is quite high and therefore gets allocated a big share of the costs. However, the chosen strategy only realises CO_2 eq. emission reduction on the site of the other companies. The chosen strategy is the cheapest for this configuration and the costs for company A are lowered as well as compared to working in smaller subcoalitions or alone. However, in practice company A might want to reduce its own CO_2 eq. emission against higher costs, or might accept the chosen strategy only for a lower cost allocation. It remains to be seen, what the real incentives are of a company, but for example due to public opinion and customer happiness a company could be interested in reducing its ecological footprint. Therefore, we will also test incorporating internal incentives in the utility functions in the coming Sections.

Conclusion

The CM method is a simplistic model with little computation times. The CM method can be used to compute the cheapest strategy under different values of the external incentive parameters p and h. However, the method does not incorporate internal incentives of the companies. If this is not the case in reality, the method can result in cost allocations made by the ETM model that are unfair and unstable in reality.

6.2 Joint Utility Function and Extensive TM allocation

In this Section the JUF method, described in Section 4.1.2, will be tested on different data instances and parameter settings. First we will give an overview on the different configurations that will be used to test the JUF method. Then the constructed TU-games using this JUF method will be summarised and analysed. Then an allocation of the costs and the environmental benefits will be made by making use of the ETM model described in Section 4.2.2. The results of this cost and environmental benefits allocation will be discussed and finally a conclusion about the JUF method will be drawn.

Configurations and constructed TU-games

First, we will give an overview on the different configurations that will be used to test the JUF method. In Table 21, the different configurations are summarized in the same manner as in Section 6.1. The Table contains the name of the configuration and data instance and the different parameter settings and the set of requirements included in the ETM model. Furthermore, the used utility function and coalition weight function are given. The numbered functions represent the following functions: $u^1_S(e_{S,B_S}, c_{S,B_S}) = w_S e_{S,B_S} - (1 - w_S)c_{S,B_S}$, $u^2_S(e_{S,B_S}, c_{S,B_S}) = \frac{w_S e_{S,B_S}}{(1-w_S)c_{S,B_S}}$, $w^1_S = \sum_{i\in S} \frac{w_i}{|S|}$ and $w^2_S = \sum_{i\in S} \frac{E_i}{E_S} w_i$.

Also, in Table 22, the results of the JUF method, performed on the different configurations, are summarized. Again, the Table includes the chosen strategy by the grand coalition, the obtained $v^u(N)$ value and the computation time in seconds of the JUF method. As we are allocating the environmental benefits as well as the costs, there is the possibility to base the DoES and DoFD value of each company on the marginal contribution to the utility, environmental and cost values of the characteristic function. Therefore in Table 21, the used values for β and δ in the ETM model are given. Unfortunately, due to time limitations we were not able to analyse if the values of $v^u(S)$, $v^e(S)$ and $v^c(S)$ imposed negative marginal contributions and therefore should be transformed to a potential savings game. This is left for future research. This may cause the ETM model to perform poorly, however the made allocation does in fact satisfy the included restrictions in the set R, so therefore the made allocation should be feasible and attainable in reality. Only, we might obtain undesired definitions of the DoES and DoFD values and therefore the made allocation could be undesired, but within the boundaries of the feasible region. In Section 7 we will discuss that in practice analysing the found feasible region in each game might be more interesting than the made allocation by the ETM model.

Name	Instance	p	h	u_S	w_S	β	δ	R
JUF1	Example 1	0%	0	u_S^1	w_S^1	(1,0)	(0,1)	(1,4,5,10,11)
JUF2	Example 1	0%	0	u_S^1	w_S^2	(1,0)	(0,1)	(1,4,5,10,11)
JUF3	Example 1	0%	0	u_S^2	w_S^1	(1,0)	(0,1)	(4,8,10,11)
JUF4	Example 1	0%	0	u_S^2	w_S^2	(1,0)	(0,1)	(4,8,10,11)
JUF5	Example 2	0%	0	u_S^1	w_S^1	(1,0)	(0,1)	(4,8,10,11)
JUF6	Example 2	15%	20	u_S^1	w_S^1	(1,0)	(0,1)	(1,2,4,5,6,8,10,11)
JUF7	Example 2	0%	0	u_S^2	w_S^2	(1,0)	(0,1)	(1,4,5,8,10,11)
JUF8	Chemelot 1	0%	0	u_S^1	w_S^2	(1,0)	(0,1)	(1,2,4,5,6,8,10,11)
JUF9	Chemelot 1	0%	0	u_S^2	w_S^2	(1,0)	(0,1)	(4,8,10,11)
JUF10	Chemelot 2	0%	0	u_S^1	w_S^2	(1,0)	(0,1)	(1,2,4,5,6,10,11)
JUF11	Chemelot 3	0%	0	u_S^1	w_S^2	(1,0)	(0,1)	(1,2,4,5,6,10,11)
JUF12	Small Chemelot	0%	0	u_S^1	w_S^2	(1,0)	(0,1)	(1,2,4,5,6,8,10,11)
JUF13	Small Chemelot	0%	0	u_S^2	w_S^2	(1,0)	(0,1)	(1,2,4,5,6,8,10,11)
JUF14	Large Chemelot	0%	0	u_S^1	w_S^1	(1,0)	(0,1)	(1,2,4,5,6,10,11)
JUF15	Large Chemelot	49%	0	u_S^1	w_S^1	(1,0)	(0,1)	(1,2,5,6,8,10,11)
JUF16	Large Chemelot	0%	10	u_S^1	w_S^1	(1,0)	(0,1)	(1,2,4,5,6,10,11)

Table 21: Configuration settings used to test the JUF method.

Name	Strategy	$v^u(N)$	Computation time
JUF1	(a_2, a_2, a_2)	31.33	0.064
JUF2	(a_2, a_2, a_2)	46.58	0.085
JUF3	(a_1, a_1, a_2)	1.43	0.101
JUF4	(a_1, a_1, a_2)	1.54	0.062
JUF5	(a_1, a_1, a_1, a_1)	0	0.155
JUF6	(a_4, a_4, a_4, a_4)	-812.25	0.151
JUF7	(a_3, a_3, a_3, a_3)	0.68	0.161
JUF8	$(a_4, a_4, a_4, a_4, a_4, a_4)$	391.18	1.218
JUF9	$(a_1, a_1, a_1, a_1, a_1, a_2)$	2.01	1.339
JUF10	$(a_4, a_4, a_4, a_4, a_4, a_4)$	354.06	1.741
JUF11	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	1.457
JUF12	(a_4, a_4, a_4, a_4)	75	0.142
JUF13	(a_4, a_4, a_4, a_4)	1.08	0.153
JUF14	$(a_4, a_4, a_4, a_4, a_4, a_4, a_4, a_4)$	300	24.094
JUF15	$(a_4, a_4, a_4, a_4, a_4, a_4, a_4, a_4)$	300	23.384
JUF16	$(a_4, a_4, a_4, a_4, a_4, a_4, a_4, a_4)$	232	23.231

Table 22: Obtained $v^u(N)$ values using the JUF method on test instances summarized in Table 21

Furthermore, in appendix B.2, some of the constructed TU-games are shown. In Tables 52, 53, 54, 55 and 56 the resulting w_S, $v^u(S)$ and chosen strategy maximising $v^u(S)$ are given for each coalition S.
From Table 22 we can observe that the JUF method finds the strategy that maximises the $v^u(S)$ value within 2 seconds for all the instances containing 6 or less companies. For the larger instance of 8 companies the JUF method takes about 24 seconds. The growth in computation time can again be explained by the exponential growth in the number of coalitions when adding a company.

Requirement set and infeasibility

In this paragraph we will explain how the requirement set R is chosen and how this influences the feasibility of the AP solved by the ETM model and what it means when adding a certain constraint to R leads to infeasibility in the AP. Note that the rationality constraints on the benefit/cost ratio are not included if the costs are equal to zero. Therefore we should inspect the constructed games to analyse what it means if these constraints are included in the set of requirements and the ETM model is still feasible. The individual and coalitional rationality constraints on the costs are not included, because including these constraints in many cases leads to an infeasible allocation problem. Also, these constraints complicate the possibility of investing in a group decarbonisation option as in general these are more expensive than individual decarbonisation options. Furthermore, in the cases that less constraints are included in the set of requirements, these constraints were left out due to the fact that they also caused infeasibility in the allocation problem. In some configurations different sets of requirements could be found to obtain a feasible allocation problem. For each configuration it is tried to add as many constraints as possible. Furthermore, the order in which the constraints are added, if possible, to R is: $2 \rightarrow 6 \rightarrow 1 \rightarrow 5 \rightarrow 4 \rightarrow 8$. The other constraints are either always included or excluded. This order is chosen, because we believe that including the rationality constraints on utility are the most important for the stability of a found allocation. If a company can obtain a higher utility value in an other coalition than the grand coalition we believe the company will leave the grand coalition.

It is observed that including rationality constraints on utility lead to infeasibility for the following configurations: "JUF1", "JUF2", "JUF3", "JUF4", "JUF5", "JUF7", "JUF9", which is quite often. This means that for those configurations there does not exist an allocation of the costs and the environmental benefits such that every company is better of than for working in a subcoalition or even than for working alone in terms of utility. This actually implies that for those configurations the grand coalition will not be stable and that the companies will not work together as a whole group. This can be caused by two different factors.

The first factor is that of choosing utility function u_S^2. In that case, the rationality constraints on utility can not be added as a division by a decision variable makes the problem non linear, which is also not allowed in the commercial solver CPLEX. Therefore, when using u_S^2 we can not guarantee that the found solution lies within the core and therefore can not guarantee that the found solution is stable. So if in reality the utility of the companies is best described by the function u_S^2 we suggest that more research is needed to investigate if it is possible to model this using cooperative game theory and how this should be done.

The second factor that can cause the obtained game to be infeasible when adding the rationality constraints on utility is the fact that we use a function for the coalition weight w_S. This leads to different utility values for certain cost and environmental benefit values among different coalitions. So for example it could occur that in a coalition consisting of only company A, a utility value of 100 is reached by an environmental benefits value of 200 and costs of 100, whereas in a coalition of companies A and B, a utility value of only 50 is reached by an environmental benefits value of 200 and costs of 100. This depends on the definition of w_S and the weights w_i of the companies in coalition S. This causes the constructed TU-game to be non superadditive and it seems like the coalition of A and B can not obtain equal or higher utility than company A could on his own, so therefore the coalition is unstable and company A would tend to leave this coalition. To give another example, we will focus on the results of configuration "JUF5" stated in Table 54. It is observed that the coalitional weight the coalitions $S = \{A\}$ equals $w_S = 0.8$. Therefore, this coalition benefits largely from environmental benefits and a strategy is chosen consisting of the most expensive and most environmental beneficial decarbonisation option. In this coalition company A obtains a utility value of 274. In the coalition $S = \{A, B\}$, the coalition weight equals $w_S = 0.5$, due to the fact that a weighted average is taken from the companies in the coalition and the weight of company B is equal to 0.2. Therefore, this coalition takes less benefits from environmental benefits and chooses a less environmental beneficial, but cheaper strategy, namely $B_S = (a_2, a_1)$. For even larger coalitions, consisting of three or more companies, including company A, the coalition weight becomes lower and lower and the chosen strategies become less environmental beneficial. It is observed that the utility obtained in all the coalitions in fact is lower than the utility obtained by company A by working on its own. Therefore, it is not possible to make a cost and environmental benefits allocation such that the utility of company A is higher in any of these coalitions than for working alone. So this means that the core of the constructed game is empty. We have seen that such games can arise when there is a difference in w_i values, the value companies assign to environmental benefits, among the companies. The example in "JUF5" might be a bit extreme, but also for smaller differences we have seen that this can be the case. For example for configurations "JUF1" and "JUF2".

Homogeneous and heterogeneous group of companies

When the group of companies have similar w_i values in the data instance, we will call this a homogeneous group of companies. When the group of companies have different w_i values, we will call it a heterogeneous group of companies. Another disadvantage might arise when implementing the JUF method on a heterogeneous group of companies. When a coalition consist of companies that have different w_i values, we try to come up with a coalition weight value w_S that represents this value the best. However, this is challenging and the found w_S can be a bit off, which will influence the correctness of the $v^u(S)$ values. For example let $w_S = w_S^1$, meaning that we take the average weight of the companies within the coalition as the coalition weight. Then if for example for coalition $S = \{A, B\}$, the strategy $B_S = (a_2, a_1)$ is chosen, in which a_2 represents some decarbonisation option and a_1 represents doing nothing. Now let $w_A = 0.7$ and $w_B = 0.3$, yielding $w_S = 0.5$. Now let the strategy yield environmental benefits value of $e_{S,B_S} = 20$ and cost value $c_{S,B_S} = 20$. Then the obtained $v^u(S) = 0.5 \cdot 20 - 0.5 \cdot 20 = 0$. However, if the (Cost, Environmental benefits) allocation made for this coalition would in fact be $((20, 20), (0, 0))$, then the real obtained utility value of the coalition would be $v^u(S) = 0.7 \cdot 20 - 0.3 \cdot 20 = 8$. So in that sense, the found $v^u(S)$ values might not represent the real utility values when implemented on a heterogeneous group of companies. Therefore, another way of modelling is proposed in the IUF method when encountering a heterogeneous group of companies. The results of the IUF method will be discussed in Section 6.3.

Coalition weight

The choice between w_S^1 and w_S^2 as the definition of the coalition weight w_S does not seem to have much effect on the feasibility of the made TU-game or on how realistic the computed $v^u(S)$ values are or on the outcome of the allocation of the constructed game itself. For example, looking at configurations "JUF1" and "JUF2" the chosen strategy and the found allocation are exactly the same, whereas there is only a small difference in the values of $v^u(S)$. As the costs and environmental benefits allocation are only based on the marginal contribution to the costs and environmental benefits respectively, the difference in $v^u(S)$ values does not lead to a difference in the found allocation. For different values of β and δ this would in fact be the case, but with small differences. Moreover, we have only tried two different definitions of the coalition weight w_S, which are much alike. Trying out different definitions that differ much from these definitions might be interesting and realise different results. Trying this remains possible for further research.

Cost and benefit allocation

The found characteristic function values for each configuration are used to make an allocation using the ETM model with the parameter settings as stated in Table 21. The found allocation and the computation time of the ETM model are given in Table 23.

Name	(Cost, Environmental benefits) allocation	Computation time
JUF1	$((295, 307), (55, 43), (40, 50))$	0.000
JUF2	$((295, 307), (55, 43), (40, 50))$	0.000
JUF3	$((0, 0), (0, 0), (40, 50))$	0.016
JUF4	$((0, 0), (0, 0), (40, 50))$	0.000
JUF5	$((0, 0), (0, 0), (0, 0), (0, 0))$	0.000
JUF6	$((1325, 950), (705, 950), (713, 900), (237, 200))$	0.000
JUF7	$((448, 466), (665, 767), (517, 517), (500, 500))$	0.010
JUF8	$((874, 931), (868, 916), (845, 886), (157, 200), (34, 50), (33, 66))$	0.031
JUF9	$((0, 0), (0, 0), (0, 0), (0, 0), (0, 0), (30, 50))$	0.006
JUF10	$((433, 584), (950, 950), (900, 900), (13, 20), (38, 50), (56, 94))$	0.031
JUF11	$((1061, 1187), (1194, 1279), (792, 792), (250, 250), (113, 141), (100, 100))$	0.041
JUF12	$((879, 965), (887, 950), (150, 150), (35, 35))$	0.016
JUF13	$((743, 900), (887, 950), (180, 150), (140, 100))$	0.021
JUF14	$((1541, 1987), (1400, 1500), (1092, 1092), (1098, 1098), (153, 191), (20, 23), (7, 14), (8, 14))$	0.064
JUF15	$((1177, 1745), (1104, 1500), (1177, 1250), (1080, 925), (160, 200), (326, 100), (273, 106), (24, 94))$	0.085
JUF16	$((1486, 2000), (1710, 1490), (921, 1250), (909, 800), (70, 100), (130, 100), (130, 100), (90, 80))$	0.098

Table 23: Obtained allocation using the ETM model on the games constructed by the JUF method, with parameter settings summarized in Table 21

From the allocation in Table 23 we can observe that the ETM model is able to find a cost and environmental benefits allocation within 0.1 seconds for all tested configurations. Note that some allocations might in reality be unstable as the requirement set R could not include the desired constraints in each configuration.

Conclusion

We have seen that the JUF method performs well, in the sense that it constructs games with a non empty core in which the $v^u(S)$ values do represent the obtained utility of the coalitions, when implemented on a homogeneous group of companies. However, the JUF method performs poorly, in the sense that empty core games arise and the fact that the obtained $v^u(S)$ values might not represent the real obtained utility values of the coalition, when implemented on a heterogeneous group of companies.

6.3 Individualised Utility Function and Extensive TM allocation

In this Section the IUF method, described in Section 4.1.3, will be tested on different data instances and parameter settings. First we will give an overview on the different configurations that will be used to test the IUF method. Then the constructed TU-games using the IUF method will be summarised and analysed. Then an allocation of the costs and the environmental benefits will be made by making use of the ETM model described in Section 4.2.2. The results of the allocation will be discussed and finally a conclusion about the IUF method will be drawn.

Configurations

First, we will give an overview on the different configurations that will be used to test the IUF method. In Table 25 the different configurations are summarized. The Table contains the names of the configurations and data instance and the different parameter settings as well as the set of requirements included in the ETM model. Furthermore, the used definition of the utility functions are given. The numbered functions represent the following functions: $u_i^1(e_{S,i,B_S}, c_{S,i,B_S}) = w_i e_{S,i,B_S} - (1-w_i)c_{S,i,B_S}$ and $u_i^2(e_{S,i,B_S}, c_{S,i,B_S}) = \frac{w_i e_{S,i,B_S}}{(1-w_i)c_{S,i,B_S}}$.
Due to time limitations we were not able to analyse if the values of $v^u(S)$, $v^e(S)$ and $v^c(S)$ needed to be transformed to potential savings games. But again, the ETM model finds an allocation if possible that lies in the core, however it might be an undesired allocation.

Table 24: Test instances, corresponding parameter values and used set of requirements R.

Name	Instance	p	h	u_i	β	δ	R
IUF1	Example 1	0%	0	u_i^1	(1,0)	(0,1)	(1,2,5,6,10,11)
IUF2	Example 2	0%	0	u_i^1	(1,0)	(0,1)	(1,2,5,10,11)
IUF3	Chemelot 1	0%	0	u_i^1	(1,0)	(0,1)	(1,2,5,6,10,11)
IUF4	Chemelot 2	0%	0	u_i^1	(1,0)	(0,1)	(1,2,6,10,11)
IUF5	Chemelot 3	0%	0	u_i^1	(1,0)	(0,1)	(1,2,4,5,6,10,11)
IUF6	Small Chemelot	0%	0	u_i^1	(1,0)	(0,1)	(1,2,4,5,6,8,10,11)

Table 25: Configuration settings used to test the IUF method.

Note that only u_i^1 is used in the configurations. As the costs are allocated in the maximisation problem as explained in Section 4.1.3, the costs become a decision variable. Therefore, the definition of u_i^2 is no longer usable as using a decision variable as denominator is not allowed, because of non linearity.
Again, similar to the configurations in Section 6.2, as many constraints as possible are added to the configuration until the ETM model became infeasible in the following order: $2 \to 6 \to 1 \to 5 \to 4 \to 8$.

Constructed TU-games

In Table 26, the results of the IUF method, performed on the different configurations, are summarized. Again, the Table includes the chosen strategy by the grand coalitions, the obtained $v^u(N)$ values and the computation time in seconds.

Name	Strategy	$v^u(N)$	Computation time
IUF1	(a_3, a_3, a_3)	119	0.115
IUF2	(a_4, a_4, a_4, a_4)	614.5	0.516
IUF3	$(a_4, a_4, a_4, a_4, a_4, a_4)$	476.32	124.457
IUF4	$(a_4, a_4, a_4, a_4, a_4, a_4)$	419.87	272.186
IUF5	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	213.36
IUF6	(a_4, a_4, a_4, a_4)	75	0.444

Table 26: Obtained $v^u(N)$ values using the IUF method on different test instances summarized in Table 25

Furthermore, in appendix B.3, the constructed TU-games of configurations “IUF1” and “IUF2” are shown in Tables 57 and 58 respectively. The Tables include the found $v^u(S)$ value, chosen strategy and made cost allocation by the maximisation problem explained in Section 4.1.3 for each coalition S.
From Table 26 we can observe that the IUF method’s computation time is increasing much faster than the previous two methods. This can be explained by the fact that the MIP that is solved for each coalition in this method has become larger and more complicated due to the fact that we are also allocating the costs of the chosen strategy in this step. This has to be done for every coalition so therefore the computation time grows faster when the number of companies increases.

Requirement set and infeasibility

From Table 25 we observe that the IUF method encounters a similar problem as the JUF method. For the configuration "IUF2" the method could not construct a TU-game that had a feasible allocation problem, when including the coalitional rationality constraints on utility. Meaning that the grand coalitions in that game is unstable and there exists a group of companies that is better off by leaving the grand coalition in terms of utility value. As we only tried one definition of the utility function this can be explained by one factor. Namely, the infeasibility of the allocation problem is caused by the unrealistic $v^u(S)$ values for each coalition S. As explained in Section 4.1.3 the $v^u(S)$ values are maximised for each coalition by choosing a certain strategy B_S and making an initial cost allocation. As in this initial cost allocation the goal is to maximise the $v^u(S)$ value, the cost allocation is made such that all the costs are allocated to the company with the highest w_i value. This results in unrealistic high values of $v^u(S)$ for subcoalitions $S \subset N$, making the coalitional rationality constraint on utility too restrictive. Again, this can occur when large differences exist between the w_i values of the companies. For a homogeneous fleet this can not occur, as the allocation of the costs in the maximisation problem, computing $v^u(S)$, will not influence the value of $v^u(S)$.

Cost and benefit allocation

The found characteristic function values for each configuration are used to make an allocation using the ETM model with the parameter settings as stated in Table 25. The found allocations and the computation time of the ETM model are given in Table 27.

Name	(Cost, Environmental benefits) allocation	Computation time
IUF1	$((900, 700), (250, 250), (240, 250))$	0.008
IUF2	$((2359, 1000), (98, 750), (283, 850), (100, 400))$	0.009
IUF3	$((1103, 1000), (435, 850), (1053, 900), (0, 93), (181, 150), (38, 57))$	0.0189
IUF4	$((594, 767), (436, 733), (1150, 900), (0, 0), (179, 150), (30, 50))$	0.022
IUF5	$((1108, 1167), (1233, 1330), (854, 854), (135, 200), (80, 100), (100, 100))$	0.024
IUF6	$((830, 900), (887, 950), (140, 150), (93, 100))$	0.011

Table 27: Obtained allocations using the ETM model on the games constructed by the IUF method with different parameter settings summarized in Table 25

From the allocations in Table 27 we can observe that the ETM model is able to find a cost and environmental benefits allocation within 0.03 seconds for all tested configurations. Note that the allocation made for configuration "IUF2" might in reality be unstable, because including the coalitional rationality constraint on utility made the allocation problem infeasible.

Conclusion

To conclude, the IUF method encounters similar problems as the JUF method when implemented on a heterogeneous group of companies. Furthermore, the method is slower and the obtained $v^u(S)$ values might not be attainable in reality, as explained in Section 4.3. As mentioned in Section 4.3, to tackle these problems two algorithms are proposed. In the following two Sections the results of these algorithms will be discussed and analysed.

6.4 Repeated Cost Allocation algorithm

To overcome the problems arising from implementing the JUF and IUF methods on a heterogeneous group of companies we have suggested to use the RCA algorithm as described in Section 4.3.1. In this Section the RCA algorithm will be tested on different data instances and parameter settings. Both the constructed TU-game and the found allocation and negotiation space will be analysed and discussed in the remainder of this Section.

Configurations

First, we will give an overview on the different configurations that will be used to test the RCA algorithm. Recall that the algorithm iteratively computes the values of $v^u(S)$ by making a cost allocation for each subcoalition that satisfies the set of requirements that have been set by the companies. So in this case, different from the previous methods, the set of requirements R is used in each iteration to compute the utility value of each coalition, whereas in previous methods it was only used in the final computation of the ETM model to come to an allocation of the costs and environmental benefits. Furthermore, as the execution of the ETM model is already performed for every coalition $S \subseteq N$ by the RCA algorithm, the algorithm already obtains an allocation and we do no longer need to execute the ETM model again for the grand coalition N. In Table 28, the different configurations are summarized. The used parameter settings and set of requirements are given.

Name	Instance	β	δ	α	p	h	R
RCA1	Example 1	0	1	-	0%	0	(1,2,4,5,6,8,10,12)
RCA2	Example 1	0	1	-	0%	0	(1,2,5,6,10,12)
RCA3	Example 2	0	1	-	0%	0	(1,2,4,5,6,8,10,12)
RCA4	Chemelot 1	0	1	-	0%	0	(1,2,4,5,6,8,10,12)
RCA5	Chemelot 1	0	1	-	0%	0	(2,6,12)
RCA6	Chemelot 2	0	1	-	0%	0	(1,2,4,5,6,8,10,12)
RCA7	Chemelot 2	0	1	0.5	0%	0	(1,2,4,5,6,8,9,10,12)
RCA8	Chemelot 3	0	1	-	0%	0	(1,2,4,5,6,8,10,12)
RCA9	Chemelot 3	0	1	-	0%	0	(2,4,6,8,10,12)
RCA10	Chemelot 3	0	1	-	0%	0	(2,6,10,12)
RCA11	Chemelot 3	0	1	-	0%	0	(2,6,12)
RCA12	Chemelot 3	0.33	0.33	-	0%	0	(1,2,4,5,6,8,10,12)
RCA13	Chemelot 3	0	1	-	0%	10	(1,2,4,5,6,8,10,12)
RCA14	Small Chemelot	0	1	-	0%	10	(1,2,4,5,6,8,10,12)
RCA15	Large Chemelot	0	1	-	0%	10	(1,2,4,5,6,8,10,12)

Table 28: Configuration settings used to test the RCA algorithm.

Note that in the RCA algorithm we assume that the environmental benefits are non transferable, therefore the given values of parameters β and δ indicate how much the DoFD of a company depends on its marginal contribution to the environmental benefits and the costs respectively. As the environmental benefits are non transferable, the DoES value is never used. Allocating the environmental benefits simultaneously with the costs in the RCA algorithm remains for future research.

Constructed TU-games and cost allocation

In Table 29 the results of the RCA algorithm on the different configurations are summarized. The found strategy, the utility value of coalition N, the made cost allocation for the grand coalition and the computation time of the repeated cost algorithm are given.

Name	Strategy	$v^u(N)$	Cost allocation	Computation time
RCA1	(a_2, a_1, a_2)	59	$(240, 0, 40)$	0.750
RCA2	(a_3, a_3, a_3)	75	$(950, 250, 190)$	0.770
RCA3	(a_3, a_1, a_1, a_1)	274	$(1630, 0, 0, 0)$	7.336
RCA4	$(a_4, a_4, a_4, a_4, a_4, a_4)$	397.76	$(840, 850, 779, 101, 180, 60)$	187.804
RCA5	$(a_4, a_4, a_4, a_4, a_4, a_4)$	433.87	$(1085, 456, 1086, 0, 183, 0)$	183.367
RCA6	$(a_4, a_4, a_4, a_4, a_4, a_4)$	358.67	$(720, 742, 679, 69, 120, 60)$	230.520
RCA7	$(a_3, a_3, a_3, a_3, a_3, a_2)$	335.28	$(480, 766, 694, 100, 180, 30)$	223.440
RCA8	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	$(950, 1027, 1243, 200, 80, 11)$	223.699
RCA9	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	$(950, 1027, 1243, 200, 80, 11)$	224.552
RCA10	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	$(990, 1080, 1060, 200, 80, 100)$	524.690
RCA11	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	$(990, 1080, 1250, 190, 0, 0)$	587.943
RCA12	$(a_4, a_4, a_4, a_4, a_4, a_4)$	120	$(950, 1027, 1188, 200, 80, 66)$	458.372
RCA13	$(a_4, a_4, a_4, a_4, a_4, a_4)$	-30	$(1259, 1224, 1108, 61, 90, 68)$	596.491
RCA14	(a_4, a_4, a_4, a_4)	65	$(930, 990, 30, 20)$	8.653
RCA15	$(a_4, a_4, a_4, a_4, a_4, a_4, a_4, a_4)$	232	$(1722, 1663, 830, 821, 61, 130, 130, 100)$	74018.01

Table 29: Obtained $v^u(N)$ values and cost allocations using the RCA algorithm on the configurations summarized in Table 28

Furthermore, in appendix B.4, the constructed TU-games of configurations "RCA1", "RCA2" and "RCA4" are

shown in Tables 59, 60 and 61 respectively. In Table 61 also the negotiation space of the companies investing in a group decarbonisation option for each coalition S are given.
From Table 29 we can observe that the RCA algorithm constructs a game and finds feasible cost allocations for all the configurations on data instances with 6 or less companies within 10 minutes. It is observed that for the instance of 8 companies the RCA algorithm takes about 20.5 hours to construct the game and find a cost allocation. This is significantly longer than the previous methods. This can be explained by the fact that at least three MIP problems have to be solved for each possible strategy for each coalition. Namely, recall that the algorithm described in Figure 1, first solves the maximisation problem, then the allocation problem and then again the allocation problem with the updated $v(S)$ values. If the stopping criterion is not met after solving these three MIP problems, the algorithm needs to solve even more MIP problems.

Requirement set and feasibility

From Table 29 we can also observe that indeed for every configuration a game is constructed, such that the core of that game is nonempty and an allocation can be found, regardless of the restrictions included in the set of requirements R and regardless of the difference in w_i values of the companies. For example, also for configuration "RCA3", consisting of the extreme example "Example 2" with large differences in w_i values, a game is constructed with a non empty core and a cost allocation within this core is found. This can be explained by the feasibility property of the RCA algorithm explained in Section 4.3.1. So assuming that the optimal $v^u(S)$ value is found for each coalition a stable and fair allocation is found for every configuration by the RCA algorithm.

Computational stability

However, unfortunately it is not proven that the RCA algorithm finds the optimal $v^u(S)$ values for every coalition S. When constraint 10 is included in the set of requirements R, the made cost allocation for each coalition S is made such that the highest DoFD value of the companies is minimised. This is done based on an initial $v^u(S)$ value as is explained in Section 4.3.1. This means that using another starting point of this $v^u(S)$ value might lead to another allocation of the costs with a higher $v^u(S)$ value for that particular coalition S. Therefore, in theory it might occur that in fact there does exist a group of companies that is better of by leaving the grand coalition. We, however, have not found this group of companies and have not found the strategy and cost allocation realising this. Assuming that the companies themselves are also not able to find this specific strategy and cost allocation combination we could say that the found cost allocation for the grand coalition by the RCA algorithm is computationally stable. Meaning that as long as the companies do not have the knowledge and computational skills to find a better subcoalition they should agree to work together in the grand coalition with the found strategy and that they should agree to the found cost allocation, assuming the companies' decision makers are rational and all agree on the set of requirements R.

Parameter influence

When analysing the influence of the chosen parameter settings, we see that the chosen parameter settings can influence the cost allocation and in some cases can even influence the chosen strategy by the grand coalition. For example, when looking at configurations "RCA1" and "RCA2" we see that including the individual and coalitional rationality constraints on the benefit/cost ratio affects the strategy that is chosen by the grand coalition. This means that the chosen strategy in "RCA2", $B_N = (a_3, a_3, a_3)$, yields a higher utility for all companies in the grand coalition. However using this strategy there exists no cost allocation such that the coalition benefit/cost ration rationality constraints are satisfied. Therefore, when including these constraints, another strategy, $B_N = (a_2, a_1, a_2)$, is chosen. This shows that the set of requirements that should be agreed on by the companies in advance can have a large influence on the eventual chosen strategy by the grand coalition.
However, in other cases, their might be less difference in the chosen strategy. For example, in configurations "RCA8", "RCA9", "RCA10" and "RCA11", different sets of requirements have been tested on data instance "Chemelot 3". In all the configurations the same strategy is chosen by the grand coalition. Between some of these configurations there is a small difference in cost allocations, meaning that adding some of the constraints does decrement the size of the feasible region.
When looking at configurations "RCA8" and "RCA12" we see that the change in the values of β and δ in this case do not influence the chosen strategy, but do influence the made cost allocation. This seems logical, as the change of β and δ do not affect any of the constraints. Only the computation of the DoFD value of each company are changed and therefore the cost allocation possibly changes as well.
When looking at configurations "RCA6" and "'RCA7", we observe that the addition of constraint 9 with the parameter value $\alpha = 0.5$, ensuring that the benefit/cost ratio of every company is within 50% of the average benefit/cost ratio, does

influence the chosen strategy by the grand coalition. Apparently, this constraints is not feasible or yields significantly lower utility value combined with the other constraints for the strategy that was chosen in "RCA6".

Negotiation space

Besides making a cost allocation based on the requirements in R we have also computed the negotiation space that arises from the constructed games by the RCA algorithm. The found negotiation space is expressed in an utility interval for each company as is explained in Section 4.3.3. In theory, the company should accept to work together in the grand coalition if the cost allocation is made such that the company's obtained utility falls within this interval. The upper bound of the interval indicates that if the company obtains more utility than that upper bound then there must be a company whose obtained utility is lower than its lower bound and therefore will in theory leave the coalition. In Table 30 some information about the found negotiation space for each configuration are given. It is important to note that whenever a strategy is chosen in which a company invests in a individual decarbonisation option, then that particular company will never have any negotiation room and the length of its negotiation space is 0. This is explained by the fact that the company could obtain the same utility by working alone and does not benefit any of the other companies by joining the coalition and therefore has no negotiation space. Therefore, the information given in Table 30 is only based on the companies investing in a group decarbonisation option and the other companies are left out of the computation of the given values. The Table gives the average absolute length of the negotiation space interval of the companies, the smallest absolute length and by which companies this smallest length is attained. The same is given for the length of the negotiation space interval proportional to the company's current emission and proportional to the total utility. This is done because the absolute value might be misleading. A certain negotiation space might be interpreted as small by a large company, as it is only a small percentage of the means the company can usually negotiate with, whereas a small company would interpret the same negotiation space as large, as it is relatively large compared to the means the company can usually negotiate with.

	Absolute		Proportional to current emission		Proportional to total utility	
Name	average	(argmin:min)	average	(argmin:min)	average	(argmin:min)
RCA1	-	-	-	-	-	-
RCA2	16	(A,B,C:16)	0.047	(0.016)	0.213	(A,B,C:0.213)
RCA3	0	(0)	0	(0)	0	(0)
RCA4	177	(F:16)	0.312	(F:0.16)	0.449	(F:0.041)
RCA5	199	(F:27)	0.359	(F:0.27)	0.460	(F:0.063)
RCA6	150	(F:24)	0.253	(D:0.145)	0.420	(F:0.067)
RCA7	134	(F:1)	0.201	(F:0.01)	0.376	(F:0.003)
RCA8	70	(E:15)	0.153	(0.048)	0.583	(E:0.125)
RCA9	70	(E:15)	0.153	(0.048)	0.579	(E:0.124)
RCA10	66	(E:15)	0.136	(0.048)	0.549	(E:0.125)
RCA11	66	(E:15)	0.136	(0.048)	0.549	(E:0.125)
RCA12	70	(E:15)	0.153	(0.048)	0.583	(E:0.125)
RCA13	218	(E:15)	0.255	(E:0.1)	-7.25	(A,B,C:-13)
RCA14	141	(D:50)	0.363	(0.22)	2.173	(D:0.769)
RCA15	352	(E:15)	0.356	(E:0.075)	1.512	(E:0.064)

Table 30: Summary of negotiation space of companies investing in group decarbonisation option of grand coalition corresponding to the obtained results in 29

Recall that the negotiation space is computed based on the rationality constraints on utility, meeaning that whenever a payoff vector falls within the negotiation space the companies should accept, because they can not obtain higher utility in any other subcoalition. However, the other constraints included in R are not used to compute the negotiation space.

Note that for configuration "RCA13" the total utility value is negative and relatively close to zero, therefore the values of the negotiation space proportional to the total utilitiy in this configuration do not make much sense and are neglected in our analyses of the negotiation space.

From Table 30 we can observe that excluding constraints from the set of requirements R does not seem to reduce the size of the negotiation space. We have seen that sometimes including extra constraints lead to the choice of another strategy, so therefore the negotiation space must have been affected. However, when looking at "RCA8", "RCA9", "RCA10" and "RCA11" we see that excluding some constraints does not change or decreases the size of the average length of the negotiation space of the companies. This can be explained by the fact that the negotiation space is only based on the rationality constraints on utility. Meaning that the negotiation space is not decreased by the other constraints. Furthermore, adding constraints to the requirements set R can result in lower $v^u(S)$ values for subcoalitions $S \subset N$. If this occurs, the utility constraints for the grand coalition become less restrictive for the subcoalition S and therefore it might occur that adding constraints to the requirement set R results in a larger negotiation space. One might argue that computing the negotiation space on all the constraints of the requirement set R is more reasonable as this is the set of requirements that was agreed upon by the companies. It remains for future research to compute the negotiation space on all the constraints in the requirement set of R. We do expect that in this case the negotiation space would decrease if more constraints would be added to the requirement set R.

Crucial companies

From Table 61 we can observe that analysing the negotiation space and how it evolves over the possible coalitions can be very interesting. For example, from Table 61 we can observe that the companies A, B and C are crucial for the coalition to invest in a group decarbonisation option. Furthermore, a fourth company is needed to invest in a group decarbonisation option. It is observed that this is possible by adding company E to the coalition. Another possibility is to add both companies D and F to the coalition. Furthermore it is observed that in the grand coalition, company F has the smallest negotiation space. However, if the companies in practice would not come to an agreement and company F would leave the grand coalition, we can observe that the companies A, B, C, D and E would still perform the same strategy, leaving out the choice of company F. In that case the company with the smallest negotiation space would be D. In this way, analysing the negotiation space and chosen strategy of every subcoalition, we can observe which companies are needed to come to certain strategies and which companies are the bottlenecks of the negotiations and which companies can lower the costs but are not crucial for the coalition to invest in a certain decarbonisation option.

Conclusion

To conclude, by agreeing on a set of requirements in advance the RCA algorithm is able to find realistic values for $v^u(S)$ for every coalition S and in this way is able to construct a TU-game that has a non empty core and is able to find an allocation of the costs for every game that lies within this core and satisfies the set of requirements. The found allocations are not proven to be stable as the obtained values of $v^u(S)$ for every subcoalition might not be the optimal value in theory. Assuming that the companies are not able to find the optimal value as well if these exist, we can state that the found cost allocation and strategy for the grand coalition is computationally stable. Furthermore, analysing the chosen strategy and negotiation space of the companies for every possible coalition can give useful insights in which companies are crucial for certain strategies and which are on the verge of leaving the grand coalition and how this will affect the strategy of the remaining companies.

6.5 Predetermined Rules and Regulations algorithm

Another method we have suggested to overcome the problems arising from implementing the joint and IUF methods on a heterogeneous group of companies based on a different industrial cluster structure is the PRR algorithm as described in Section 4.3.2. In this Section the PRR algorithm will be tested on different data instances and parameter settings. Both the constructed TU-game and the found allocation and negotiations space will be analysed and discussed in the remainder of this Section.

Tested rules and regulations and configurations

We will give an overview on the different configurations that will be used to test the PRR algorithm. Recall that in this algorithm an industrial management determines under which rules the costs and the environmental benefits resulting from a certain strategy are allocated among the participating companies. However, this does not mean that the companies are not allowed to make any side payments after the costs and environmental benefits have been allocated conform the rules and regulations. Therefore, it remains interesting to analyse how the negotiations space and chosen strategy are affected by the different parameter settings and rules and regulations. Before giving an overview of the different configurations we will summarize the different rules and regulations that were tested in the configurations. Firstly, the different rules and regulations defining the allocation of the environmental benefits that are realised by a certain strategy of a coalition, are given:

- $\mathbf{r_1^e}$:= The environmental benefits that are realised by a company are allocated to the company itself.

- $\mathbf{r_2^e}$:= The environmental benefits that are realised by a coalition are divided proportionally to the company's current emission among the companies investing in the same option.
- $\mathbf{r_3^e}$:= The environmental benefits that are realised by companies investing in individual decarbonisation options are allocated to the company that realises the environmental benefits. The environmental benefits that are realised by companies investing in group decarbonisation options are divided proportionally to the company's current emission among the companies investing in the same option.
- $\mathbf{r_4^e}$:= The environmental benefits that are realised by companies investing in individual decarbonisation options are allocated to the company that realises the environmental benefits. The environmental benefits that are realised by companies investing in group decarbonisation options are divided evenly among the companies investing in the same option.

Secondly, the rules and regulations defining the allocation of the costs induced to a coalition by choosing a certain strategy are given:

- $\mathbf{r_1^c}$:= The total costs are divided proportionally to the company's current emission among the companies investing in the same option.
- $\mathbf{r_2^c}$:= The variable costs are allocated to the company itself, whereas the fixed costs are divided proportionally to the company's current emission among the companies investing in the same option.
- $\mathbf{r_3^c}$:= The total costs are divided proportionally to the company's current emission among all the companies located in the industrial cluster.
- $\mathbf{r_4^c}$:= The costs that are induced to the coalition by investing in individual decarbonisation options are allocated to the company choosing that particular individual decarbonisation option. The costs that are induced to the coalition by investing in group decarbonisation options are divided proportionally to the company's current emission among the companies investing in the same option.
- $\mathbf{r_5^c}$:= The variable costs are allocated to the company itself, whereas the fixed costs are divided proportionally to the realised environmental benefits among the companies investing in the same option.
- $\mathbf{r_6^c}$:= The variable costs are allocated to the company itself, whereas the fixed costs are divided evenly over the companies investing in the same option.
- $\mathbf{r_7^c}$:= The variable costs are allocated to the company itself, whereas the fixed costs are divided proportionally to the allocated environmental benefits among the companies investing in the same option.
- $\mathbf{r_8^c}$:= The variable costs are allocated to the company itself, whereas the fixed costs are divided proportionally to the environmental benefits over all the companies.

Now, we will give an overview on the different configurations that will be used to test the PRR algorithm. In Table 31 the parameter settings and chosen rules and regulations of each configuration are given.

Name	Instance	r	h	p	R	α
PRR1	Example 1	(r_1^e, r_2^c)	0	0	(2,6)	-
PRR2	Example 1	(r_3^e, r_4^c)	0	0	(2,6)	-
PRR3	Example 2	(r_1^e, r_4^c)	0	0	(2,6)	-
PRR4	Example 2	(r_1^e, r_1^c)	0	0	(2,6)	-
PRR5	Example 2	(r_1^e, r_3^c)	0	0	(2,6)	-
PRR6	Chemelot 1	(r_3^e, r_2^c)	0	0	(2,6)	-
PRR7	Chemelot 1	(r_4^e, r_2^c)	0	0	(2,6)	-
PRR8	Chemelot 1	(r_3^e, r_7^c)	0	0	(2,6)	-
PRR9	Chemelot 1	(r_3^e, r_7^c)	0	0	(1,2,4,5,6,8,9)	0.5
PRR10	Chemelot 1	(r_3^e, r_7^c)	0	0	(1,2,4,5,6,8)	-
PRR11	Chemelot 2	(r_1^e, r_6^c)	0	0	(2,6)	-
PRR12	Chemelot 2	(r_3^e, r_2^c)	0	0	(2,6)	-
PRR13	Chemelot 3	(r_1^e, r_2^c)	0	0	(2,6)	-
PRR14	Chemelot 3	(r_3^e, r_4^c)	0	0	(2,6)	-
PRR15	Chemelot 3	(r_1^e, r_3^c)	20	0	(2,6)	-
PRR16	Chemelot 3	(r_3^e, r_6^c)	20	0	(2,6)	-
PRR17	Small Chemelot	(r_3^e, r_4^c)	0	0	(2,6)	-
PRR18	Large Chemelot	(r_3^e, r_4^c)	0	0	(2,6)	-

Table 31: Configuration settings used to test the PRR algorithm.

Recall that in the PRR algorithm the maximisation problem in each iteration tries to find the strategy that maximises the utility of coalition S under the given rules and regulations and the set of requirements R. In this algorithm we do not minimise the highest DoFD or maximise the lowest DoES. Therefore requirements 10 and 11 are never included. Also, as the rules and regulations on the allocation of the environmental benefits already have been determined the constraint set 12 is never added as well. Furthermore, note that the set of requirements in this method does not influence the made allocation, as it is made by the predetermined rules and regulations. The requirement set R only influences whether the allocation made by the rules for a certain strategy is feasible and therefore influences which strategy is chosen. The constraints 2 and 6 are always included in the set of requirements R as we think that for the grand coalition to be stable we at least need to include the rationality constraints on utility, ensuring that no group of companies is better off in terms of utility by leaving the grand coalition.
In Table 32 the results of the PRR algorithm on the different configurations are summarized. The found strategy, the utility value of coalition N, the made allocation for the grand coalition and the computation time of the PRR algorithm are given.

Name	Strategy	$v^u(N)$	(Cost, Environmental benefits) allocation	Computation time
PRR1	(a_2, a_1, a_2)	145	$((240, 250), (0, 0), (40, 50))$	0.378
PRR2	(a_2, a_1, a_2)	145	$((240, 250), (0, 0), (40, 50))$	0.317
PRR3	(a_3, a_1, a_1, a_1)	1370	$((1630, 750), (0, 0), (0, 0), (0, 0))$	0.795
PRR4	(a_3, a_1, a_1, a_1)	1370	$((1630, 750), (0, 0), (0, 0), (0, 0))$	0.795
PRR5	-	-	-	-
PRR6	$(a_4, a_4, a_4, a_1, a_4, a_2)$	772	$((900, 917), (865, 871), (830, 825), (0, 0), (145, 138), (30, 50))$	46.828
PRR7	$(a_4, a_4, a_4, a_1, a_2, a_2)$	623	$((937, 867), (900, 867), (863, 867), (0, 0), (60, 50), (30, 50))$	47.400
PRR8	$(a_4, a_4, a_4, a_1, a_4, a_2)$	772	$((900, 917), (871, 867), (830, 825), (0, 0), (145, 138), (30, 50))$	47.613
PRR9	-	-	-	-
PRR10	$(a_2, a_2, a_2, a_1, a_2, a_2)$	223	$((240, 250), (250, 250), (200, 200), (0, 0), (60, 50), (30, 50))$	104.153
PRR11	$(a_4, a_4, a_4, a_1, a_2, a_2)$	650	$((763, 750), (763, 800), (763, 750), (0, 0), (60, 50), (30, 50))$	52.637
PRR12	$(a_3, a_3, a_3, a_3, a_3, a_2)$	826	$((693, 750), (640, 713), (648, 675), (131, 150), (108, 113), (30, 50))$	61.528
PRR13	$(a_2, a_2, a_1, a_1, a_2, a_1)$	50	$((190, 200), (280, 300), (0, 0), (0, 0), (80, 100), (0, 0))$	55.028
PRR14	$(a_4, a_4, a_4, a_4, a_2, a_4)$	210	$((1357, 1431), (1018, 1074), (848, 895), (170, 179), (80, 100), (68, 72))$	59.579
PRR15	$(a_4, a_4, a_4, a_4, a_2, a_4)$	-390	$((1584, 1000), (1188, 1100), (990, 1250), (198, 200), (100, 100), (79, 100))$	52.137
PRR16	$(a_4, a_4, a_4, a_1, a_2, a_2)$	-680	$((1533, 1411), (1243, 1058), (1133, 882), (100, 0), (100, 100), (70, 100))$	61.222
PRR17	(a_4, a_4, a_4, a_4)	150	$((886, 955), (842, 907), (133, 143), (89, 95))$	0.893
PRR18	$(a_4, a_4, a_4, a_4, a_2, a_4, a_4, a_4)$	570	$((1647, 1819), (1235, 1364), (1029, 1137), (988, 1091), (80, 100), (165, 182))$	5604.847

Table 32: Obtained $v^u(N)$ values using the PRR algorithm on the configurations summarized in Table 31

Furthermore, in appendix B.5, the constructed TU-games of configurations “PRR1” and “PRR6” are shown in Tables 62 and 63 respectively. In Table 63 information on the negotiation space of each coalition of the companies investing in group decarbonisation options is given as well.
From Table 32 we can observe that the computation time of the PRR algorithm in general is less than the computation time of the RCA algorithm but more than the other solution methods. This is caused by the fact that the PRR algorithm only needs to solve one MIP problem for every coalition S. This is significantly less than the RCA algorithm. However, the MIP that has to be solved has more restrictions than the MIP problem in the CM, JUF and IUF method as it should satisfy every constraint in the requirement set R, and therefore is a bit slower than those methods.

Feasibility

From Table 32 we can observe that for the configurations “PRR5” and “PRR9” the PRR algorithm could not find a strategy for the grand coalition that satisfied the given set of requirements R using the given allocation rules and regulations. Furthermore, in other configurations that were not stated in Table 31 we have seen that for the following allocation rules the PRR algorithm was never able to find a strategy that satisfied the rationality constraints on utility: r_2^e, r_1^c, r_3^c and r_8^c. This means that for those rules and regulations there does not exist a strategy for the grand coalition or even a smaller subcoalition that satisfies the rationality constraints on utility. This can be explained by the fact that those rules do not distinguish between individual and group decarbonisation options. We will explain why this results in infeasible TU-games with a small example. Consider company A and B that would both invest in the individual decarbonisation option a_1 if they would work alone, realising some environmental benefits and costs. Then, consider the case that the companies A and B would work together in coalition S and the best strategy would be to both still invest in the individual decarbonisation option, so $B_S = (a_1, a_1)$. Then the realised environmental benefits and costs are just the sum of the realised environmental benefits and costs from the two coalitions consisting of the single company A or company B. Now, in coalition S the environmental benefits and costs are allocated to the companies A and B by applying the set rules and regulations. If in this case the environmental benefits and costs are not divided

over A and B in exactly the same distribution as would be the case if the companies worked alone, this would imply that one of the companies is better off and one of the companies is worse off in terms of utility. So therefore if the rules and regulations do not consider this situation and do not distinguish between individual and group decarbonisation options (or fixed and variable costs), the probability that no feasible strategy exists for a certain coalition is quite large, depending on the data instance.
From the results of configurations “PRR9” and “PRR10” we can observe that adding constraint 9 with parameter value $\alpha = 0.5$ is too restrictive for this data instance and rules and regulations combinations. This means that the rules and regulations implying the distibution of the environmental benefits and costs of a coalition can not satisfy constraint 9 for any of the strategies of coalition S.

Influence choice of rules and regulations

The rules and regulations that do in fact result in feasible TU-games and allocations are all quite similar. They all distinguish between individual and group decarbonisation options, allocating everything that is realised by individual decarbonisation options to the companies themselves and defining some allocation rule for the group decarbonisation options. However, we can observe that the small changes in the rules and regulations can result in big differences in the chosen strategy and therefore the amount of CO_2 eq. emission that is being reduced. For example when comparing configurations “PRR11” with “PRR12” and “PRR13” with “PRR14”. The only difference is that in configuration “PRR11” the allocation rules (r_1^e, r_6^c) are used, resulting in chosen strategy $B_N = (a_4, a_4, a_4, a_1, a_2, a_2)$, and in configuration “PRR12” the allocation rules (r_3^e, r_2^c) are used, resulting in chosen strategy $B_N = (a_3, a_3, a_3, a_3, a_3, a_2)$. In configuration “PRR11” a total amount of 48 megaton CO_2 eq. emission is being reduced and in “PRR12” a total amount of 49 megaton CO_2 eq. emission is being reduced. So in this instance the difference in strategy does not lead to big differences in environmental benefits. If the industrial management however prefers one of the decarbonisation options a_3 or a_4 it can push the choice of the companies by setting the correct allocation rules and regulations. In “PRR13” the rules (r_1^e, r_2^c) are used, strategy $B_N = (a_2, a_2, a_1, a_1, a_2, a_1)$ is chosen and a total amount of 12 megaton CO_2 eq. emission reduction is realised. In “PRR14”, implemented on the same data instance, the rules (r_3^e, r_4^c) are used, strategy $B_N = (a_4, a_4, a_4, a_4, a_2, a_4)$ is chosen and a total amount of 75 megaton CO_2 eq. emission is realised. So in this case the chosen rules and regulations of the industrial management have a big influence on the amount of CO_2 eq. emission that is being reduced.

Negotiation space

From the configurations we can not decide yet whether there exists a combination of rules that ensures more CO_2 eq. emission reduction than other combinations for every data instance. As mentioned before, we are also interested in what the different rules do to the negotiation space of the companies for similar data instances. In Table 33 information is given on the negotiation space of the companies investing in group decarbonisation options for the different configurations. Furthermore, we have implemented every combination of rules and regulations on the data instances “Chemelot 1” and “Chemelot 3”, with $R = (2, 6)$, $h = 0$ and $p = 0$. The chosen strategy by the grand coalition on data instance “Chemelot 1” is given in Table 34. Furthermore, the negotiation space of the companies investing in group decarbonisation options in the chosen strategy for the grand coalition are summarized in Table 35.

Name	Absolute average	Absolute (argmin:min)	Proportional to current emission average	Proportional to current emission (argmin:min)	Proportional to total utility average	Proportional to total utility (argmin:min)
PRR1	-	-	-	-	-	-
PRR2	-	-	-	-	-	-
PRR3	0	(A:0)	0	(A:0)	0	(A:0)
PRR4	0	(A:0)	0	(A:0)	0	(A:0)
PRR5	-	-	-	-	-	-
PRR6	451	(E:158)	35	(A:27)	0.585	(E:0.205)
PRR7	400	(A:400)	21	(A:20)	0.642	(A:0.642)
PRR8	451	(E:158)	35	(A:27)	0.585	(E:0.204)
PRR9	-	-	-	-	-	-
PRR10	-	-	-	-	-	-
PRR11	427	(A:427)	23	(A:21)	0.657	(E:0.657)
PRR12	351	(D:54)	28	(D:13)	0.424	(D:0.065)
PRR13	-	-	-	-	-	-
PRR14	138	(F:50)	15	(A:4)	0.657	(F:0.238)
PRR15	856	(F:70)	42	(A:33)	-2.195	(F:-0.179)
PRR16	1040	(A:1040)	34	(A:26)	0.424	(A:-1.529)
PRR17	110	(D:80)	23	(A:6)	0.733	(D:0.533)
PRR18	327	(F:60)	21	(A:13)	0.574	(F:0.105)

Table 33: Summary of negotiation space of companies investing in group decarbonisation option of grand coalition corresponding to the obtained results in Table 32

	r_1^e	r_2^e	r_3^e	r_4^e
r_1^c	-	-	-	-
r_2^c	$(a_4, a_4, a_4, a_1, a_4, a_2)$	-	$(a_4, a_4, a_4, a_1, a_4, a_2)$	$(a_4, a_4, a_4, a_1, a_2, a_2)$
r_3^c	-	-	-	-
r_4^c	$(a_4, a_4, a_4, a_1, a_4, a_2)$	-	$(a_4, a_4, a_4, a_1, a_4, a_2)$	$(a_4, a_4, a_4, a_1, a_2, a_2)$
r_5^c	$(a_4, a_4, a_4, a_1, a_4, a_2)$	-	$(a_4, a_4, a_4, a_1, a_4, a_2)$	$(a_4, a_4, a_4, a_1, a_2, a_2)$
r_6^c	$(a_4, a_4, a_4, a_1, a_2, a_2)$	-	$(a_4, a_4, a_4, a_1, a_2, a_2)$	$(a_4, a_4, a_4, a_1, a_2, a_2)$
r_7^c	$(a_4, a_4, a_4, a_1, a_4, a_2)$	-	$(a_4, a_4, a_4, a_1, a_4, a_2)$	$(a_4, a_4, a_4, a_1, a_2, a_2)$
r_8^c	-	-	-	-

Table 34: Chosen strategy by the grand coalition for different rules and regulation on data instance "Chemelot 1".

	r_1^e	r_2^e	r_3^e	r_4^e
r_1^c	-	-	-	-
r_2^c	min = 161, mean = 460	-	min = 158, mean = 451	min = 400, mean = 400
r_3^c	-	-	-	-
r_4^c	min = 163, mean = 463	-	min = 160, mean = 454	min = 401, mean = 401
r_5^c	min = 159, mean = 457	-	min = 156, mean = 448	min = 399, mean = 399
r_6^c	min = 395, mean = 395	-	min = 388, mean = 388	min = 397, mean = 397
r_7^c	min = 159, mean = 457	-	min = 156, mean = 451	min = 397, mean = 397
r_8^c	-	-	-	-

Table 35: Summary of negotiation space of companies, investing in group decarbonisation options, in the grand coalition for different rules and regulation on data instance "Chemelot 1" corresponding to the chosen strategies in Table 34.

From configurations “PRR6”, “PRR7” and “PRR8” in Table 33 we can observe that the average negotiation space in absolute value is higher in configurations “PRR6” and “PRR8”. In Table 32 we can observe that the difference between configurations “PRR6” and “PRR8” compared to configuration “PRR7” is that in configuration “PRR6” and “PRR8” company E also invests in group decarbonisation option a_4, whereas in configuration “PRR7” company E invests in individual decarbonisation option a_2. So the addition of company E to the group investments actually increases the average size of the negotiation space. Furthermore, we can observe that the smallest negotiation space in

configurations “PRR6” and “PRR8” is the negotiation space of company E in terms of absolute values. However, the smallest negotiation space proportional to the current emission of the companies is the negotiation space of the company with the highest current emission, company A. In fact we have seen that the negotiation space of the companies A, B and C in absolute value is exactly the same in all three configurations. Therefore, we can conclude that the different rules and regulations in configuration “PRR6” and “PRR8” actually make sure that company E also wants to invest in the group decarbonisation option, realising more CO_2 eq. emission reduction, and make sure that the negotiation space of the companies A, B and C increase. One might argue, that the coalition is less stable because company E’s negotiation space is smaller and company E might leave the coalition, however from analysing the entire constructed game for configuration “PRR6” in Table 63 in appendix B.5, we can observe that if E would leave the coalition, the companies would still invest in group decarbonisation option a_4. Therefore, we think that in this case the rules and regulation in “PRR6” and “PRR8” are preferred over the rules and regulations in “PRR7”.
The same phenomena can be observed from Tables 34 and 35. It is observed that the chosen strategies do not differ much between the different combinations of rules and regulations. Actually, the only difference is that in some combinations, company E also decides to invest in the group decarbonisation option a_4 and in other combinations invests in a_2. It is observed that for the combinations in which company E decides to invest in the group decarbonisation option as well, the average size of the negotiation space increases. Also, in those configurations the minimum length of the negotiation space decreased. However, in all the cases this is the negotiation space of company E and again the negotiation space of the companies A,B and C are all exactly the same and increase when company E also invests in the group decarbonisation option. The increase of the negotiation space of the companies A, B and C, when company E also invests in the group decarbonisation option can be explained by the fact that there is another company involved in the negotiations and therefore there is more room to rearrange the obtained utility values.
All combinations of rules and regulations were also tested on data instance “Chemelot 3”. For that instance all combinations that found a strategy for data instance “Chemelot 1” found a strategy for data instance “Chemelot 3”, namely all combinations found the strategy $B_N = (a_1, a_1, a_0, a_0, a_1, a_0)$, except rule combination (r_3^e, r_4^c) that found strategy $B_N = (a_3, a_3, a_3, a_3, a_1, a_3)$. Meaning that rule combination (r_3^e, r_4^c) is the only rule combination finding a strategy investing in a group decarbonisation option, realising negotation space values of $min = 50, mean = 138$. These results are also summarized in Tables 64 and 65 in Appendix B.5. Recall that in this instance the values of b_i and k_i were set to 1 for all companies. Note that this means that for some companies compared to data instance “Chemelot 1” the environmental benefits in proportion to the costs counts less towards the company’s utility. Meaning that the companies are less eager to invest in expensive decarbonisation options. This is probably the reason why almost none of the combinations finds a strategy that invests in a group decarbonisation option.

Crucial companies

Furthermore, from investigating the chosen strategy and negotiation space for all the possible coalitions for a certain configuration, one can observe which companies are crucial for the investment into a certain group decarbonisation option and which companies are less crucial just as was the case in Section 6.4. For example, when looking at Table 63 in appendix B.5, we can observe that for configuration “PRR6” the companies A, B, C are crucial for the investment into group decarbonisation option a_4. Company E is willing to join this investment whenever all these three companies are included in the coalition and companies D and F will never join this investment. We think that this kind of information could be useful for an industrial cluster management in trying to convince the companies to come to an agreement.

Conclusion

In the tested instances and configurations the rule combination (r_3^e, r_4^c) seems to perform the best in terms of realising the most CO_2 eq. emission reduction. However, we can not say that this will be the case by definition for every other data instance. However, when a real data instance becomes available and real parameter values are obtained, an industrial cluster management might try the different combinations on this data instance and observe which combination performs the best in terms of what is desired by the industrial cluster management.

6.6 Comparison of solution concepts

In this Section the results of the different solution concepts will be compared and the advantages and disadvantages of each concept will be summarized. Furthermore, a recommendation will be made on when to use which solution concept.
In Table 36 the advantages and disadvantages of the solution concepts are summarized.

Solution Concepts	Advantages	Disadvantages
Cost Minimisation method	Little computation times. Easy interpretable results. Can compute cheapest option to obtain certain percentage of CO_2 emission reduction. Can compute cheapest option when a tax value is set by a third party.	Does not incorporate internal incentives of companies. This might lead to cost allocations that might be seen as unfair and unstable. Some parameter values of the external incentives might result in an infeasible allocation problem.
Joint Utility Function method	Little computation times. Easy interpretable results, if definition of w_S is correct. Cost and environmental benefits allocations seems fair and stable when implemented on homogeneous group of companies and set of requirements that define a fair and stable allocation. Does incorporate internal incentives, which might be more representative of the reality.	Need a definition of coalition weight w_S and it is uncertain if the set definition is correct when implemented on heterogeneous group of companies. When implemented on a heterogeneous group of companies the constructed game might have an empty core and the computed $v^u(S)$ values might not be representative for the real obtained utility values by coalition S.
Individualised Utility Function method	Do not need a definition of coalition weight w_S. The utility functions u_i seem to represent the reality better.	Larger computation times. When implemented on a heterogeneous group of companies the constructed game might have an empty core and the cost allocations might in the computation of the $v^u(S)$ values seem unstable and unfair and therefore the $v^u(S)$ values are unattainable in reality and incorrect.
Repeated Cost Allocation algorithm	A non empty core TU-game is constructed for every possible implementation. A realistic allocation of the costs are made for each coalition S. The computed $v^u(S)$ values seem to represent the real obtained utility values by coalition S and attainable in reality.	Larger computation times. The companies need to agree on a set of requirements R defining whether a certain cost and environmental benefits allocation is considered to be stable and fair prior to the algorithm execution.
Predetermined Rules and Regulations algorithm	A non empty core TU-game can be constructed for every possible implementation if the correct rules and regulations are chosen by the industrial cluster management. A realistic allocation of the costs and environmental benefits are made for each coalition S by the set rules and regulations. The computed $v^u(S)$ values seem to represent the real obtained utility values by coalition S and attainable in reality. An industrial cluster management can push the decision of the companies in the right direction by trying different rules and regulations and analysing the results.	Larger computation times. An industrial cluster management is needed. The industrial cluster management predetermines the rules and regulations that determine how the costs and environmental benefits are allocated, resulting in less freedom for the involved companies. Some definitions of the rules and regulations might lead to an infeasible maximisation problem indicating that there exists no strategy such that the grand coalition is stable and wants to work together. Predetermining rules and regulations might lead to not maximising the total utility that can be obtained by the involved companies.

Table 36: Summary of the advantages and disadvantages of the solution methods.

From these advantages and disadvantages the following recommendations are made.
Whenever it is assumed that the companies do not care at all about reducing their CO_2 eq. emission and a method is needed by the companies to compute which strategy is the cheapest strategy realising a certain percentage of reduction set by a third party or which strategy is the cheapest strategy whenever some costs are assigned to emitting CO_2 eq. we recommend to use the CM method.
When it is assumed that the companies do care about reducing their CO_2 eq. emission, but all the companies gain similar utility value to the amount of CO_2 eq. emission that is being reduced compared to the costs, we recommend to use the JUF method to compute which option realises the highest utility for the grand coalition and to find a negotiation space which consists of allocations for which all the companies should agree to work together in the grand coalition based on the obtained utility values.
When it is assumed that the companies do care about reducing their CO_2 eq. emission, but not all the companies give similar utility value to the amount of CO_2 eq. emission that is being reduced compared to the costs and there does not exists an industrial cluster management, we recommend the companies to agree on what they think are correct requirements for a fair and stable allocation of the costs and use the RCA method to compute which strategy realises the highest utility for the grand coalition that can satisfy these requirements and to find the negotiation space of the grand coalition which consists of the allocations for which all the companies should agree to work together in the grand coalition based on the obtained utility values.
When it is assumed that there does exists an industrial cluster management that wants to force the companies within the industrial cluster to come to an agreement on what strategy should be chosen and how the costs and benefits should be allocated and wants to push this agreement in a certain direction we recommend the industrial cluster management to use the PRR algorithm to determine for which rules the desired strategy is chosen and a non empty negotiation space exists.

7 Discussion, Conclusion and Future Research

In this Section we will discuss the limitations of the proposed solution methods in Section 7.1. Furthermore, in Section 7.2, we will give answer to the research questions stated in Section 1. Finally, in Section 7.3, we will suggest some future research that could be done on the subject.

7.1 Discussion

We have encountered some limitations of the proposed methods. First of all, we have seen that acquiring the correct data instances can be difficult. In recent research the estimations of the costs and environmental benefits of certain decarbonisation are still very uncertain. Furthermore, due to new innovations and research on decarbonisation options, these values might change in the future or new decarbonisation options might be found.
Next to that, some parameters that have been used in the methods and are crucial for the obtained results, such as w_i, b_i and k_i, representing the weight companies give to reducing their CO_2 eq. emission compared to keeping their costs as low as possible, remain to be estimated. On top of that it might be the case that the amount a company is willing to pay is not linearly related the amount of CO_2 eq. emission reduction that is being realised.
Furthermore, the aversion to risk of companies that arise from certain decarbonisation options are not included in the models. Meaning that a company might be willing to pay more for a certain method than for another method.
Finally, the TM model computing the allocation of the costs and environmental might not be the best allocation method, depending on what the companies think of what the definition of a fair and stable allocation is. Therefore, computing and maximising or minimising the DoES and DoFD value for each company might not be as interesting as analysing the negotiation space. In reality, the companies will probably have long and difficult negotiations resulting in a totally different allocation than that is made by the TM model. However, observing the negotiation space of the companies we can gain insight in what kind of allocations the companies, if rational, should accept and if a certain strategy has a large probability of surviving the negotiations.

7.2 Conclusion

In this Section we will conclude our research by trying to give answer to the research questions stated in Section 3. Firstly, we will try to give answer to the first main question and its subquestions concerning the VP. Secondly, we will try to give answer to the second main question and its subquestions concerning the AP. Finally, we will try to give answer to the third main research question and its subquestions concerning the existence of an industrial cluster management and its influence.
First of all, we have seen that in order to model the joint investment of an industrial cluster in certain decarbonisation

options in terms of a characteristic function $v(S)$, assigning a value to every possible coalition S, such that it best represents reality, some assumptions about the structure of the industrial cluster and the incentives of the involved companies are needed. We have investigated two possible structures for the industrial cluster, with or without an industrial cluster management, and were able to compute the characteristic function values for both structures under certain assumptions about the utility functions of the involved companies. Namely, under the assumptions that the utility function of a company can be written as a linear function of the environmental benefits and the costs allocated to a company and the weight, describing the company's incentives, of a company. Furthermore, we assumed that the incentives of a company can be represented by a weight describing the interests in environmental benefits versus the costs and that this weight is exactly known. Furthermore, it is assumed that the definition of a stable and fair allocation can be agreed upon by the companies. The different suggested methods best describe different realities and can construct TU-games for which the AP has a non empty feasible region when applied on the correct scenario and if all assumptions hold.
Secondly, we have seen that we were able to adapt the TM model suggested by Tan et al. (2016) to comprehend with allocating both the costs and environmental benefits. Furthermore, we were able to add several constraints that might be necessary to find a stable and fair allocation. So, under the assumption that the exact definition of a stable and fair allocation is known and consists of adjustments and extensions we have suggested to the TM model, we can make a stable and fair allocation based on the found characteristic function values in the VP.
Finally, we have seen that for almost all the tested instances there exist certain rules and regulations for which a strategy for the grand coalition can be found that is stable and fair by the assumption that the set of requirements defining a stable and fair allocation is known. Furthermore, we have seen that by trying different rules and regulations the management might be able to find a combination of rules that results in a desired chosen strategy by the grand coalition. Furthermore, by observing the negotiation space of the companies the management is able to identify which companies are crucial for a certain strategy and which companies might be bottlenecks in the negotiations.

7.3 Future Research

We suggest that there should be done more research on the real data values defining the costs and environmental benefits for the decarbonisation options. Furthermore, we suggest that the incentives of the involved companies are better researched. It might be possible to make a good estimation of the needed parameters by interviewing the companies and taking questionnaires.
Next to that, more research could be done on the difference in operational costs and capital costs of the different decarbonisation options and the currently used feedstock or energy supply.
To further improve the suggested solution methods more research can be done on the definition of the utility functions u_i and u_S as well as the coalition weight w_S. Furthermore, more parameter settings could be tested, to gain more insight on their influence. New requirements could be tested and added to the requirement set R. Similarly, new rules and regulations could be tested in the PRR algorithm.
In future research it might be interesting to investigate whether the values $v^u(S)$, $v^e(S)$ and $v^c(S)$ should be reformulated to potential savings game when their exists negative marginal contribution. Furthermore, it would be interesting if this is also needed when the TM model is not used and we do not compute the marginal contributions but just analyse the resulting negotiation space.
Research could be done on the RCA algorithm expanding it to allocating not only the costs but also the environmental benefits. Furthermore, it could be investigated if it is possible to prove that the RCA algorithm always constructs a core that is nonempty due to its feasibility property for certain requirement sets R and if so for which combinations of constraints in the requirement set R.
The ETM model could be expanded by computing the degree of satisfaction on utility for each company by $u_i(x_i^e, x_i^c)/c_i^u$ and researching whether maximising the lowest degree seems as a fair and stable allocation of the costs and environmental benefits.
Other stability measurement concepts could be investigated and used to analyse the stability of the made allocations of the different solution concepts. For example, the Fairness Index and propensity to disrupt value stated in Littlechild and Vaidya (1976) could be used.

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Appendices

A Instances

Companies	Emission	w_i	b_i	k_i
A	1000	0.6	1.2	1
B	500	0.5	1	1
C	400	0.5	1	1

			Company A		Company B		Company C	
D	G/I	c^f	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0
a_2	I	0	250	240	100	110	50	40
a_3	G	900	750	240	250	150	200	100

Table 37: Information on companies and decarbonisation options in instance “Example 1”.

Companies	Emission	w_i	b_i	k_i
A	1000	0.8	4	1
B	950	0.2	1	4
C	900	0.25	1	3
D	500	0.2	1	4

			Company A		Company B		Company C		Company D	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0
a_2	I	0	250	240	250	250	200	200	200	200
a_3	G	1390	750	240	700	210	650	240	150	50
a_4	G	2200	900	200	850	200	850	200	400	40

Table 38: Information on companies and decarbonisation options in instance “Example 2”.

Companies	Emission	w_i	b_i	k_i
A	1000	0.565	1.3	1.0
B	950	0.520	1.2	1.1
C	900	0.577	1.5	1.1
D	200	0.440	1.1	1.4
E	150	0.552	1.6	1.3
F	100	0.519	1.4	1.3

			Company A		Company B		Company C		Company D		Company E		Company F	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0	0	0	0	0
a_2	I	0	250	240	250	250	200	200	-	-	50	60	50	30
a_3	G	1450	750	240	700	210	650	240	150	50	100	50	50	50
a_4	G	2100	900	200	850	200	850	200	200	40	150	40	100	30

Table 39: Information on companies and decarbonisation options in instance “Chemelot 1”.

Companies	Emission	w_i	b_i	k_i
A	1000	0.565	1.3	1.0
B	950	0.520	1.2	1.1
C	900	0.577	1.5	1.1
D	200	0.500	1.2	1.2
E	150	0.552	1.6	1.3
F	100	0.519	1.4	1.3

			Company A		Company B		Company C		Company D		Company E		Company F	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0	0	0	0	0
a_2	I	0	250	240	250	250	200	200	50	70	50	60	50	30
a_3	G	1450	500	240	800	210	850	240	100	40	150	40	50	20
a_4	G	1690	750	200	800	200	750	200	100	40	100	30	100	30

Table 40: Information on companies and decarbonisation options in instance “Chemelot 2”.

Companies	Emission	w_i	b_i	k_i
A	2000	0.5	1	1
B	1500	0.5	1	1
C	1250	0.5	1	1
D	250	0.5	1	1
E	150	0.5	1	1
F	100	0.5	1	1

			Company A		Company B		Company C		Company D		Company E		Company F	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0	0	0	0	0
a_2	I	0	200	190	300	280	200	210	50	70	100	80	50	50
a_3	G	2500	900	240	1250	210	1000	240	100	40	150	80	80	30
a_4	G	2650	1000	250	1100	250	1250	250	200	60	100	50	100	50

Table 41: Information on companies and decarbonisation options in instance “Chemelot 3”.

Companies	Emission	w_i	b_i	k_i
A	2000	0.5	1	1
B	1500	0.5	1	1
C	1250	0.5	1	1
D	250	0.5	1	1
E	150	0.5	1	1
F	100	0.5	1	1

			Company A		Company B		Company C		Company D		Company E		Company F	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	800	0	600	0	500	0	100	0	60	0	40
a_2	I	0	200	910	300	760	200	630	50	150	100	100	50	70
a_3	G	2500	900	680	1250	310	1000	340	100	100	150	80	80	38
a_4	G	2650	1000	650	1100	360	1250	250	200	80	100	70	100	50

Table 42: Example information on companies and decarbonisation options on instance “Chemelot 3”, where the tax value is set to $h = 20$.

Companies	Emission	w_i	b_i	k_i
A	1000	0.5	1	1
B	950	0.5	1	1
C	150	0.5	1	1
D	100	0.5	1	1

			Company A		Company B		Company C		Company D	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0
a_2	I	0	200	190	300	280	50	60	50	70
a_3	G	1280	750	240	950	210	150	50	100	40
a_4	G	1450	950	250	900	200	150	300	100	20

Table 43: Information on companies and decarbonisation options in instance "Small Chemelot".

Companies	Emission	w_i	b_i	k_i
A	2000	0.5	1	1
B	1500	0.5	1	1
C	1250	0.5	1	1
D	1200	0.5	1	1
E	200	0.5	1	1
F	200	0.5	1	1
G	150	0.5	1	1
H	100	0.5	1	1

			Company A		Company B		Company C		Company D		Company E		Company F		Company G		Company H	
D	G/I	c^f	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v	e	c^v
a_1	I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
a_2	I	0	250	240	300	280	200	210	50	70	100	80	50	50	50	80	50	60
a_3	G	3000	1100	240	1250	210	1000	240	700	200	150	80	80	30	100	30	80	20
a_4	G	4300	1700	250	1490	200	1250	250	1100	200	100	50	100	40	100	20	80	10

Table 44: Information on companies and decarbonisation options in instance "Large Chemelot".

B Results

B.1 Cost Minimisation

S	$v^u(S)$	strategy
{A}	-240	(a_2)
{B}	-110	(a_2)
{C}	-1000	(a_3)
{A,B}	-240	(a_2, a_1)
{A,C}	-240	(a_2, a_1)
{B,C}	-150	(a_2, a_2)
{A,B,C}	-280	(a_2, a_1, a_2)

Table 45: "CM1": Utility values of coalitions, when using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1", before transformation to potential savings game.

S	$v^u(S)$	strategy
{A}	0	(a_2)
{B}	0	(a_2)
{C}	0	(a_3)
{A,B}	110	(a_2, a_1)
{A,C}	1000	(a_2, a_1)
{B,C}	960	(a_2, a_2)
{A,B,C}	1070	(a_2, a_1, a_2)

Table 46: "CM1": $v(S)$ values of coalitions, when using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1", after transformation to potential savings game.

S	$v^u(S)$	strategy
{A}	-1140	(a_3)
{B}	-1050	(a_3)
{C}	-1000	(a_3)
{A,B}	-1140	(a_3, a_1)
{A,C}	-1140	(a_3, a_1)
{B,C}	-1150	(a_3, a_3)
{A,B,C}	-1240	(a_3, a_1, a_3)

Table 47: "CM2": Utility values of coalitions, when using CM method satisfying a minimum of $p = 49\%$ CO_2 eq. emission reduction on data instance "Example 1".

S	$v^u(S)$	strategy
{A}	-1630	(a_3)
{B}	-1600	(a_3)
{C}	-1630	(a_3)
{D}	-2240	(a_4)
{A,B}	-1840	(a_3, a_3)
{A,C}	-1830	(a_3, a_2)
{A,D}	-1630	(a_3, a_1)
{B,C}	-1840	(a_3, a_3)
{B,D}	-1650	(a_3, a_3)
{C,D}	-1680	(a_3, a_3)
{A,B,C}	-1840	(a_3, a_3, a_1)
{A,B,D}	-1840	(a_3, a_3, a_1)
{A,C,D}	-1870	(a_3, a_3, a_1)
{B,C,D}	-1840	(a_3, a_3, a_1)
{A,B,C,D}	-2040	(a_3, a_3, a_2, a_1)

Table 48: "CM3": Utility values of coalitions, when using CM method satisfying a minimum of $p = 49\%$ CO_2 eq. emission reduction on data instance "Example 2".

S	$v^u(S)$	strategy
{A}	-1520	(a_3)
{B}	-1490	(a_3)
{C}	-1330	(a_3)
{D}	-70	(a_2)
{A,B}	-1680	(a_2, a_3)
{A,C}	-1520	(a_3, a_1)
{A,C}	-1520	(a_3, a_1)
{B,C}	-1490	(a_3, a_1)
{A,C}	-1490	(a_3, a_1)
{A,C}	-1330	(a_3, a_1)
{A,B,C}	-1540	(a_1, a_3, a_3)
{A,B,D}	-1530	(a_1, a_3, a_3)
{A,C,D}	-1520	(a_3, a_1, a_1)
{B,C,D}	-1490	(a_3, a_1, a_1)
{A,B,C,D}	-1540	(a_2, a_1, a_2)

Table 49: "CM8": Utility values of coalitions, when using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1", before transformation to potential savings game.

S	$v^u(S)$	strategy
{A}	0	(a_3)
{B}	0	(a_3)
{C}	0	(a_3)
{D}	0	(a_2)
{A,B}	1330	(a_2, a_3)
{A,C}	1330	(a_3, a_1)
{A,C}	70	(a_3, a_1)
{B,C}	1330	(a_3, a_1)
{A,C}	70	(a_3, a_1)
{A,C}	70	(a_3, a_1)
{A,B,C}	2800	(a_1, a_3, a_3)
{A,B,D}	1550	(a_1, a_3, a_3)
{A,C,D}	1400	(a_3, a_1, a_1)
{B,C,D}	1400	(a_3, a_1, a_1)
{A,B,C,D}	2870	(a_2, a_1, a_2)

Table 50: "CM8": $v(S)$ values of coalitions, when using CM method satisfying a minimum of $p = 15\%$ CO_2 eq. emission reduction on data instance "Example 1", after transformation to potential savings game.

S	$v^u(S)$	strategy
{A}	-1290	(a_2)
{B}	-670	(a_2)
{C}	-530	(a_2)
{A,B}	-1960	(a_2, a_2)
{A,C}	-1820	(a_2, a_2)
{B,C}	-1200	(a_2, a_2)
{A,B,C}	-2370	(a_3, a_3, a_3)

Table 51: "CM13": Utility values of coalitions, when using CM method with a tax value of $h = 70$ million euros per kg CO_2 eq. ($p = 0\%$) on data instance "Example 1".

B.2 Joint Utility Function

S	w_S	$v^u(S)$	strategy
{A}	0.6	54	(a_2)
{B}	0.5	0	(a_1)
{C}	0.5	5	(a_2)
{A,B}	0.567	46.67	(a_2, a_2)
{A,C}	0.571	51.43	(a_2, a_2)
{B,C}	0.5	5	(a_1, a_2)
{A,B,C}	0.553	46.58	(a_2, a_2, a_2)

Table 52: "JUF2": Utility values of coalitions, when using JUF method, with $p = 0$, $h = 0$, $u_S = u_S^1$ and $w_S = w_S^2$ on data instance "Example 1".

S	w_S	$v^u(S)$	strategy
{A}	0.6	1.56	(a_2)
{B}	0.5	0.91	(a_2)
{C}	0.5	1.25	(a_2)
{A,B}	0.55	1.27	(a_2, a_1)
{A,C}	0.55	1.53	(a_1, a_2)
{B,C}	0.5	1.25	(a_1, a_2)
{A,B,C}	0.533	1.43	(a_1, a_1, a_2)

Table 53: "JUF3": Utility values of coalitions, when using JUF method, with $p = 0$, $h = 0$, $u_S = u_S^2$ and $w_S = w_S^1$ on data instance "Example 1".

S	w_S	$v^u(S)$	strategy
{A}	0.8	274	(a_3)
{B}	0.2	-0	(a_1)
{C}	0.25	0	(a_1)
{D}	0.2	0	$(a_2 1$
{A,B}	0.5	5	(a_2, a_1)
{A,C}	0.525	27.25	(a_2, a_2)
{A,D}	0.5	5	(a_2, a_1)
{B,C}	0.225	0	(a_1, a_1)
{B,D}	0.2	0	(a_1, a_1)
{C,D}	0.225	0	(a_1, a_1)
{A,B,C}	0.417	0	(a_1, a_1, a_1)
{A,B,D}	0.4	0	(a_1, a_1, a_1)
{A,C,D}	0.417	0	(a_1, a_1, a_1)
{B,C,D}	0.217	0	(a_1, a_1, a_1)
{A,B,C,D}	0.363	0	(a_1, a_1, a_1, a_1)

Table 54: "JUF5": Utility values of coalitions, when using JUF method, with $p = 15\%$, $h = 20$, $u_S = u_S^1$ and $w_S = w_S^1$ on data instance "Example 2".

S	w_S	$v^u(S)$	strategy
{A}	0.8	254	(a_3)
{B}	0.2	-374	(a_2)
{C}	0.25	-310	(a_2)
{D}	0.2	-216	(a_2)
{A,B}	0.5	-285	(a_2, a_2)
{A,C}	0.525	-248.25	(a_2, a_2)
{A,D}	0.5	-205	(a_2, a_2)
{B,C}	0.225	-681.5	(a_2, a_2)
{B,D}	0.2	-534	(a_2, a_1)
{C,D}	0.225	-530	(a_2, a_2)
{A,B,C}	0.417	-513.33	(a_3, a_3, a_3)
{A,B,D}	0.4	-554	(a_2, a_2, a_2)
{A,C,D}	0.417	-510.83	(a_2, a_2, a_2)
{B,C,D}	0.217	-837.67	(a_1, a_2, a_2)
{A,B,C,D}	0.363	-812.25	(a_4, a_4, a_4, a_4)

Table 55: "JUF6": Utility values of coalitions, when using JUF method, with $p = 15\%$, $h = 20$, $u_S = u_S^1$ and $w_S = w_S^1$ on data instance "Example 2".

S	w_S	$v^u(S)$	strategy
{A}	0.8	4.17	(a_2)
{B}	0.2	0.25	(a_2)
{C}	0.25	0.33	(a_2)
{D}	0.2	0.25	(a_2)
{A,B}	0.508	1.07	(a_2, a_1)
{A,C}	0.539	1.22	(a_2, a_1)
{A,D}	0.6	1.56	(a_2, a_1)
{B,C}	0.224	0.29	(a_2, a_2)
{B,D}	0.2	0.25	(a_2, a_2)
{C,D}	0.232	0.30	(a_2, a_1)
{A,B,C}	0.426	0.77	(a_2, a_1, a_1)
{A,B,D}	0.445	0.83	(a_2, a_1, a_1)
{A,C,D}	0.469	0.92	(a_2, a_1, a_1)
{B,C,D}	0.219	0.28	(a_2, a_1, a_1)
{A,B,C,D}	0.393	0.68	(a_3, a_3, a_3, a_3)

Table 56: "JUF7": Utility values of coalitions, when using JUF method, with $p = 0$, $h = 0$, $u_S = u_S^2$ and $w_S = w_S^2$ on data instance "Example 2".

B.3 Individualised Utility Function

S	$v^u(S)$	Strategy	Cost Allocation
{A}	54	(a_2)	(240)
{B}	0	(a_1)	(20)
{C}	5	(a_2)	(40)
{A,B}	60	(a_2, a_2)	$(350, 0)$
{A,C}	63	(a_2, a_2)	$(280, 0)$
{B,C}	5	(a_1, a_2)	$(20, 20)$
{A,B,C}	119	(a_3, a_3, a_3)	$(1390, 0, 0)$

Table 57: "IUF1": Utility values of coalitions using IUF method solving the MIP problem in Section 4.1.3 on data instance "Example 1"

S	$v^u(S)$	Strategy	Cost Allocation
{A}	274	(a_3)	(1630)
{B}	0	(a_1)	(0)
{C}	0	(a_1)	(0)
{D}	0	(a_1)	(0)
{A,B}	372	(a_3, a_3)	$(1840, 0)$
{A,C}	412.5	(a_4, a_4)	$(2600, 0)$
{A,D}	312	(a_4, a_4)	$(2440, 0)$
{B,C}	0	(a_1, a_1)	$(0, 0)$
{B,D}	0	(a_1, a_1)	$(0, 0)$
{C,D}	0	(a_1, a_1)	$(0, 0)$
{A,B,C}	542.5	(a_4, a_4, a_4)	$(2800, 0, 0)$
{A,B,D}	442	(a_4, a_4, a_4)	$(2640, 0, 0)$
{A,C,D}	484.5	(a_4, a_4, a_4)	$(2640, 0, 0)$
{B,C,D}	0	(a_1, a_1, a_1)	$(0, 0, 0)$
{A,B,C,D}	614.5	(a_4, a_4, a_4, a_4)	$(2840, 0, 0, 0)$

Table 58: "IUF2": Utility values using IUF method solving the MIP problem in Section 4.1.3 on data instance "Example 2"

B.4 Repeated cost allocation

S	$v^u(S)$	Strategy	Cost Allocation
{A}	54	(a_2)	(240)
{B}	0	(a_1)	(0)
{C}	5	(a_2)	(40)
{A,B}	54	(a_2, a_1)	$(240, 0)$
{A,C}	59	(a_2, a_2)	$(240, 40)$
{B,C}	5	(a_1, a_2)	$(0, 40)$
{A,B,C}	59	(a_2, a_1, a_2)	$(240, 0, 40)$

Table 59: "RCA1": v(S) values and cost allocation using RCA algorithm on configurations "RCA1"

S	$v^u(S)$	Strategy	Cost Allocation
{A}	54	(a_2)	(240)
{B}	0	(a_1)	(0)
{C}	5	(a_2)	(40)
{A,B}	54	(a_2, a_1)	$(240, 0)$
{A,C}	59	(a_2, a_2)	$(240, 40)$
{B,C}	5	(a_1, a_2)	$(0, 40)$
{A,B,C}	75	(a_3, a_3, a_3)	$(950, 250, 190)$

Table 60: "RCA2": v(S) values and cost allocation using RCA algorithm on configurations "RCA2"

S	strategy	$v^u(S)$	cost allocation	$argmin(NS_G)$	$min(NS_G)$	$avg(NS_G)$
{A}	a_2	37	240	-	-	-
{B}	a_2	11	250	-	-	-
{C}	a_2	31	200	-	-	-
{D}	a_1	0	0	-	-	-
{E}	a_2	1	60	-	-	-
{F}	a_2	11	30	-	-	-
{A,B}	(a_2, a_2)	48	(240,250)	-	-	-
{A,C}	(a_2, a_2)	68	(240,200)	-	-	-
{A,D}	(a_2, a_1)	37	(240,0)	-	-	-
{A,E}	(a_2, a_2)	38	(240,60)	-	-	-
{A,F}	(a_2, a_2)	48	(240,30)	-	-	-
{B,C}	(a_2, a_2)	41	(250,200)	-	-	-
{B,D}	(a_2, a_1)	11	(250,0)	-	-	-
{B,E}	(a_2, a_2)	12	(250,60)	-	-	-
{B,F}	(a_2, a_2)	22	(250,30)	-	-	-
{C,D}	(a_2, a_1)	31	(200,0)	-	-	-
{C,E}	(a_2, a_2)	31	(200,60)	-	-	-
{C,F}	(a_2, a_2)	42	(200,30)	-	-	-
{D,E}	(a_1, a_2)	1	(0,60)	-	-	-
{D,F}	(a_1, a_2)	11	(0,30)	-	-	-
{E,F}	(a_2, a_2)	12	(60,30)	-	-	-
{A,B,C}	(a_2, a_2, a_2)	79	(240,250,200)	-	-	-
{A,B,D}	(a_2, a_2, a_1)	48	(240,250,0)	-	-	-
{A,B,E}	(a_2, a_2, a_2)	49	(240,250,60)	-	-	-
{A,B,F}	(a_2, a_2, a_2)	59	(240,250,30)	-	-	-
{A,C,D}	(a_2, a_2, a_1)	68	(240,200,0)	-	-	-
{A,C,E}	(a_2, a_2, a_2)	68	(240,200,60)	-	-	-
{A,C,F}	(a_2, a_2, a_2)	79	(240,200,30)	-	-	-
{A,D,E}	(a_2, a_1, a_2)	38	(240,0,60)	-	-	-
{A,D,F}	(a_2, a_1, a_2)	48	(240,0,30)	-	-	-
{A,E,F}	(a_2, a_2, a_2)	49	(240,60,30)	-	-	-
{B,C,D}	(a_2, a_2, a_1)	42	(250,200,0)	-	-	-
{B,C,E}	(a_2, a_2, a_2)	42	(250,200,60)	-	-	-
{B,C,F}	(a_2, a_2, a_2)	53	(250,200,30)	-	-	-
{B,D,E}	(a_2, a_1, a_2)	12	(250,0,60)	-	-	-
{B,D,F}	(a_2, a_1, a_2)	22	(250,0,30)	-	-	-
{B,E,F}	(a_2, a_2, a_2)	23	(250,60,30)	-	-	-
{C,D,E}	(a_2, a_1, a_2)	31	(200,0,60)	-	-	-
{C,D,F}	(a_2, a_1, a_2)	42	(200,0,30)	-	-	-
{C,E,F}	(a_2, a_2, a_2)	43	(200,60,30)	-	-	-
{D,E,F}	(a_1, a_2, a_2)	12	(0,60,30)	-	-	-
{A,B,C,D}	(a_2, a_2, a_2, a_1)	79	(240,250,200,0)	-	-	-
{A,B,C,E}	(a_4, a_4, a_4, a_4)	305	(864,850,846,180)	A/B/C/E	225	451
{A,B,C,F}	(a_2, a_2, a_2, a_2)	90	(240,250,200,30)	-	-	-
{A,B,D,E}	(a_2, a_2, a_1, a_2)	49	(240,250,0,60)	-	-	-
{A,B,D,F}	(a_2, a_2, a_1, a_2)	59	(240,250,0,30)	-	-	-
{A,B,E,F}	(a_2, a_2, a_2, a_2)	60	(240,250,60,30)	-	-	-
{A,C,D,E}	(a_2, a_2, a_1, a_2)	68	(240,200,0,60)	-	-	-
{A,C,D,F}	(a_2, a_2, a_1, a_2)	79	(240,200,0,30)	-	-	-
{A,C,E,F}	(a_2, a_2, a_2, a_2)	80	(240,200,60,30)	-	-	-
{A,D,E,F}	(a_2, a_1, a_2, a_2)	49	(240,0,60,30)	-	-	-
{B,C,D,E}	(a_2, a_2, a_1, a_2)	42	(250,200,0,60)	-	-	-
{B,C,D,F}	(a_2, a_2, a_1, a_2)	53	(250,200,0,30)	-	-	-
{B,C,E,F}	(a_2, a_2, a_2, a_2)	54	(250,200,60,30)	-	-	-
{B,D,E,F}	(a_2, a_1, a_2, a_2)	23	(250,0,60,30)	-	-	-
{C,D,E,F}	(a_2, a_1, a_2, a_2)	43	(200,0,60,30)	-	-	-
{A,B,C,D,E}	$(a_4, a_4, a_4, a_4, a_4)$	371	(864,850,850,36,180)	D	246	291
{A,B,C,D,F}	$(a_4, a_4, a_4, a_4, a_2)$	328	(864,850,839,157,60)	A/B/C	238	238
{A,B,C,E,F}	$(a_4, a_4, a_4, a_4, a_4)$	340	(864,850,816,180,60)	F	25	204
{A,B,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	60	(240,250,0,60,30)	-	-	-
{A,C,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	80	(240,200,0,60,30)	-	-	-
{B,C,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	54	(250,200,0,60,30)	-	-	-
{A,B,C,D,E,F}	$(a_4, a_4, a_4, a_4, a_4, a_4)$	398	(840,850,779,101,180,60)	F	16	177

Table 61: “RCA4”: v(S) values, cost allocation and negotiation space using RCA algorithm on configuration “RCA4”

B.5 Predetermined Rules and Regulations

S	$v^u(S)$	Strategy	(Cost, Environmental benefits) Allocation
{A}	135	(a_2)	$((240, 250))$
{B}	0	(a_1)	$((0, 0))$
{C}	10	(a_2)	$((40, 50))$
{A,B}	135	(a_2, a_1)	$((240, 250), (0, 0)$
{A,C}	145	(a_2, a_2)	$((240, 250), (40, 50))$
{B,C}	10	(a_1, a_2)	$((0, 0), (40, 50))$
{A,B,C}	145	(a_2, a_1, a_2)	$((240, 250), B : (0, 0), (40, 50))$

Table 62: "PRR1": v(S) values and cost and environmental benefits allocation using PRR algorithm on configuration "PRR1"

S	strategy	$v^u(S)$	cost allocation	$argmin(NS_G)$	$min(NS_G)$	$avg(NS_G)$
{A}	a_2	85	240	-	-	-
{B}	a_2	25	250	-	-	-
{C}	a_2	80	200	-	-	-
{D}	a_1	0	0	-	-	-
{E}	a_2	2	60	-	-	-
{F}	a_2	31	30	-	-	-
{A,B}	(a_2, a_2)	110	(240,250)	-	-	-
{A,C}	(a_2, a_2)	165	(240,200)	-	-	-
{A,D}	(a_2, a_1)	85	(240,0)	-	-	-
{A,E}	(a_2, a_2)	87	(240,60)	-	-	-
{A,F}	(a_2, a_2)	116	(240,30)	-	-	-
{B,C}	(a_2, a_2)	105	(250,200)	-	-	-
{B,D}	(a_2, a_1)	25	(250,0)	-	-	-
{B,E}	(a_2, a_2)	27	(250,60)	-	-	-
{B,F}	(a_2, a_2)	56	(250,30)	-	-	-
{C,D}	(a_2, a_1)	80	(200,0)	-	-	-
{C,E}	(a_2, a_2)	82	(200,60)	-	-	-
{C,F}	(a_2, a_2)	111	(200,30)	-	-	-
{D,E}	(a_1, a_2)	2	(0,60)	-	-	-
{D,F}	(a_1, a_2)	31	(0,30)	-	-	-
{E,F}	(a_2, a_2)	33	(60,30)	-	-	-
{A,B,C}	(a_4, a_4, a_4)	581,2281	(937,900,863)	A/B/C	391	391
{A,B,D}	(a_2, a_2, a_1)	110	(240,250,0)	-	-	-
{A,B,E}	(a_2, a_2, a_2)	112	(240,250,60)	-	-	-
{A,B,F}	(a_2, a_2, a_2)	141	(240,250,30)	-	-	-
{A,C,D}	(a_2, a_2, a_1)	165	(240,200,0)	-	-	-
{A,C,E}	(a_2, a_2, a_2)	167	(240,200,60)	-	-	-
{A,C,F}	(a_2, a_2, a_2)	196	(240,200,30)	-	-	-
{A,D,E}	(a_2, a_1, a_2)	87	(240,0,60)	-	-	-
{A,D,F}	(a_2, a_1, a_2)	116	(240,0,30)	-	-	-
{A,E,F}	(a_2, a_2, a_2)	118	(240,60,30)	-	-	-
{B,C,D}	(a_2, a_2, a_1)	105	(250,200,0)	-	-	-
{B,C,E}	(a_2, a_2, a_2)	107	(250,200,60)	-	-	-
{B,C,F}	(a_2, a_2, a_2)	136	(250,200,30)	-	-	-
{B,D,E}	(a_2, a_1, a_2)	27	(250,0,60)	-	-	-
{B,D,F}	(a_2, a_1, a_2)	56	(250,0,30)	-	-	-
{B,E,F}	(a_2, a_2, a_2)	58	(250,60,30)	-	-	-
{C,D,E}	(a_2, a_1, a_2)	82	(200,0,60)	-	-	-
{C,D,F}	(a_2, a_1, a_2)	111	(200,0,30)	-	-	-
{C,E,F}	(a_2, a_2, a_2)	113	(200,60,30)	-	-	-
{D,E,F}	(a_1, a_2, a_2)	33	(0,60,30)	-	-	-
{A,B,C,D}	(a_4, a_4, a_4, a_1)	581,2281	(937,900,863,0)	A/B/C	391	391
{A,B,C,E}	(a_4, a_4, a_4, a_4)	741,1667	(900,865,830,145)	E	158	451
{A,B,C,F}	(a_4, a_4, a_4, a_4)	612,2281	(937,900,863,30)	A/B/C	391	391
{A,B,D,E}	(a_2, a_2, a_1, a_2)	112	(240,250,0,60)	-	-	-
{A,B,D,F}	(a_2, a_2, a_1, a_2)	141	(240,250,0,30)	-	-	-
{A,B,E,F}	(a_2, a_2, a_2, a_2)	143	(240,250,60,30)	-	-	-
{A,C,D,E}	(a_2, a_2, a_1, a_2)	167	(240,200,0,60)	-	-	-
{A,C,D,F}	(a_2, a_2, a_1, a_2)	196	(240,200,0,30)	-	-	-
{A,C,E,F}	(a_2, a_2, a_2, a_2)	198	(240,200,60,30)	-	-	-
{A,D,E,F}	(a_2, a_1, a_2, a_2)	118	(240,0,60,30)	-	-	-
{B,C,D,E}	(a_2, a_2, a_1, a_2)	107	(250,200,0,60)	-	-	-
{B,C,D,F}	(a_2, a_2, a_1, a_2)	136	(250,200,0,30)	-	-	-
{B,C,E,F}	(a_2, a_2, a_2, a_2)	138	(250,200,60,30)	-	-	-
{B,D,E,F}	(a_2, a_1, a_2, a_2)	58	(250,0,60,30)	-	-	-
{C,D,E,F}	(a_2, a_1, a_2, a_2)	113	(200,0,60,30)	-	-	-
{A,B,C,D,E}	$(a_4, a_4, a_4, a_1, a_4)$	741,1667	(900,865,830,0,145)	E	158	451
{A,B,C,D,F}	$(a_4, a_4, a_4, a_1, a_2)$	612,2281	(937,900,863,0,30)	A/B/C	391	391
{A,B,C,E,F}	$(a_4, a_4, a_4, a_4, a_2)$	772,1667	(900,865,830,145,30)	E	158	451
{A,B,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	143	(240,250,0,60,30)	-	-	-
{A,C,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	198	(240,200,0,60,30)	-	-	-
{B,C,D,E,F}	$(a_2, a_2, a_1, a_2, a_2)$	138	(250,200,0,60,30)	-	-	-
{A,B,C,D,E,F}	$(a_4, a_4, a_4, a_1, a_4, a_2)$	772,1667	(900,865,830,0,145,30)	E	158	451

Table 63: "PRR6": $v^u(S)$ values, cost allocation and negotiation space using PRR algorithm on configuration "PRR6".

	r_1^e	r_2^e	r_3^e	r_4^e
r_1^c	-	-	-	-
r_2^c	$(a_1, a_1, a_0, a_0, a_1, a_0)$	-	$(a_1, a_1, a_0, a_0, a_1, a_0)$	$(a_1, a_1, a_0, a_0, a_1, a_0)$
r_3^c	-	-	-	-
r_4^c	$(a_1, a_1, a_0, a_0, a_1, a_0)$	-	$(a_3, a_3, a_3, a_3, a_1, a_3)$	$(a_1, a_1, a_0, a_0, a_1, a_0)$
r_5^c	$(a_1, a_1, a_0, a_0, a_1, a_0)$	-	$(a_1, a_1, a_0, a_0, a_1, a_0)$	$(a_1, a_1, a_0, a_0, a_1, a_0)$
r_6^c	$(a_1, a_1, a_0, a_0, a_1, a_0)$	-	$(a_1, a_1, a_0, a_0, a_1, a_0)$	$(a_1, a_1, a_0, a_0, a_1, a_0)$
r_7^c	$(a_1, a_1, a_0, a_0, a_1, a_0)$	-	$(a_1, a_1, a_0, a_0, a_1, a_0)$	$(a_1, a_1, a_0, a_0, a_1, a_0)$
r_8^c	-	-	-	-

Table 64: Chosen strategy by the grand coalition for different rules and regulation on data instance "Chemelot 3".

	r_1^e	r_2^e	r_3^e	r_4^e
r_1^c	-	-	-	-
r_2^c	min = -, mean = -	-	min = -, mean = -	min = -, mean = -
r_3^c	-	-	-	-
r_4^c	min = -, mean = -	-	min = 50, mean = 138	min = -, mean = -
r_5^c	min = -, mean = -	-	min = -, mean = -	min = -, mean = -
r_6^c	min = -, mean = -	-	min = -, mean = -	min = -, mean = -
r_7^c	min = -, mean = -	-	min = -, mean = -	min = -, mean = -
r_8^c	-	-	-	-

Table 65: Summary of negotiation space of companies, investing in group decarbonisation options, in the grand coalition for different rules and regulation on data instance "Chemelot 3" corresponding to the chosen strategies in Table 64.