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Strategic Capacity Planning in Process Industries under Water Scarcity

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Water scarcity is a serious global problem that will have a big impact on process industries, where water is a key component. Therefore, it would be beneficial for these industries to have water considerations in their capacity planning and use water reuse and regeneration as methods for preventing future water issues and favoring the expansion of the company. This thesis is going to focus on the capacity expansion problem in process industries considering a water scarcity setting. The possibilities of internal water treatment and/or collaboration between plants in a possible industrial symbiosis are going to be explored by means of a multi-objective capacity expansion mixed integer linear program (MILP) model. This will be targeted to optimizing both efficient distribution of water resources and profitability of such exchanges in a collaborative setting. In the end a conclusion regarding the possible solutions to the water scarcity problem and the effect of different parameters on the optimal capacity expansion planning will be presented.

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EIP	Eco-Industrial Park
IPWI	Inter-Plant Water Integration
KPI	Key Performance Indicator
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Nonlinear Programming
MIP	Mixed Integer Programming
NLP	Nonlinear Programming
NPV	Net Present Value
REWARD	REuse of WAteR in the food and bioprocessing inDustry
TUM	Technische Universität München

1 Introduction

Water scarcity is a serious global problem that, since 2012, continuously appears in the annual risk report published by the World Economic Forum as one of the top five largest global risks in terms of potential impact (World Economic Forum, 2018). Furthermore, global water use has increased by a factor of six over the past 100 years and grows steadily at a rate of about 1% per year (UN Water, 2018). The water problem is only worsened by the continued water demand rise caused by increasing world population, improving living standards, changing consumption patterns and expansion of irrigated agriculture among other factors (Ercin and Hoekstra, 2014)

According to a 2008 report by the United Nations Environment Programme (UNEP), freshwater constitutes only 1% of the worldwide water resources and industrial use accounts for about 20% of this percentage, being industry the second largest user of freshwater worldwide, after agriculture with 70%. For this reason, water scarcity also becomes an imminent threat to industries worldwide and particularly to process industries, since many processes are water-intensive and their water demand is increasingly high. Some of the water risks that process industries can face are: freshwater shortages in the supply chain or in its operations, a reputational risk regarding sustainable water use, a risk of governmental interference and regulation and the financial risk of cost increases and revenue reductions due to the effect of growing water scarcity in the availability and price of certain raw materials (Klee and Nielsen, 2014).

High-income countries treat about 70% of the municipal and industrial wastewater they generate. However, over 80% of all wastewater is discharged without treatment from a global point of view (UN Water, 2017). Wastewater is an undervalued resource that is often seen as a burden, but could actually be an affordable and sustainable source of water and energy. In fact, there are strong economic arguments in favor of optimizing freshwater-use efficiency, managing wastewater as a resource and eliminating or reducing pollution at the point of use (UN Water, 2017).

Processes in process industries usually have many polluted effluent streams and therefore water and wastewater management should be highly considered and should take part in their strategy for fighting the water scarcity problem. By making their process more water efficient and reducing their waste, these companies could turn an environmental burden into a resource and therefore avoid serious financial and environmental consequences.

In view of this situation, the philosophy for minimizing freshwater use and wastewater generation becomes more relevant and the investment on water reuse, regeneration and recycle processes becomes more necessary. Water regeneration involves treatment and purification technologies. The combination of these processes with water reuse and recycling in different schemes constitute the water network synthesis problem (Foo, 2009), an important aspect of water management. A better definition for the problem could be the design of the synthesis of water networks which may involve water-using units and/or wastewater treatment operations.

The water network synthesis problem is treated in the literature mainly from an operational point of view, focusing on design and production level. However, there is a lack of literature considering a strategic level that focuses on timing for investing in the water facilities, possibility of capacity expansion in the long term and optimization of the water network from a broader perspective. Process industries in particular are known for having high investment costs. On the other hand, in general strategic capacity planning also requires substantial resources with long payout times (Paraskevopoulos, 1991). For this reason, it is crucial that water management is also present in the strategic capacity planning of the company.

The capacity expansion problem was defined by Luss (1982) as the determination of the sizes of facilities to be added, the associated times at which they should be added and the appropriate location for any expansion. Capacity expansion planning, from the strategic level point of view, is extremely important for every company and integrates decisions regarding all areas in the company. Therefore, it usually happens at the highest management level (Martínez-Costa et al., 2014). Managing the water scarcity problem that is becoming more threatening is also one of the problems to take care of at this level. Consequently, it should be integrated in the capacity expansion strategy of the firm, especially when water is as important element as in the process industries.

Under the previously described water scarcity circumstances, a research community with participants from various academic groups and industries from Germany (TUM) and Denmark appeared and the REWARD project ("REuse of WAteR in the food and bioprocessing inDustry") was established. The REWARD project focuses on process water cases from the food and bioprocessing industries with the aim of reducing water consumption. Some of the partners in this research are closely involved with the Kalundborg industrial park in Denmark, the first one to achieve a full realization of an industrial symbiosis (Chertow, 2000). The members of this eco-industrial park (EIP) share: ground water, surface water, waste water, electricity, and also exchange a variety of residues that become feedstock in other processes. This sets an example for collaborative planning and resource sharing.

The possibility of water sharing and reuse between various plants could be a very attractive option for industrial parks. Furthermore, the application of the water network design problem in the case of EIPs is also very present in the literature. Actually, there is evidence that increasing the symbiotic relationship between plants can highly contribute to a profitable and sustainable industrial development (Boix et al., 2015). With this in mind, it could be very interesting to consider the strategic capacity expansion planning from an EIP point of view, searching the optimality in the multiple alternatives of collaboration or not collaboration with regards to water processes.

To conclude, this thesis is going to focus on the capacity expansion problem in process industries with a water management approach, considering a water scarcity setting. The possibilities of internal water treatment and/or collaboration between plants in a possible industrial symbiosis are going to be explored by means of a multi-objective capacity expansion mixed integer linear program (MILP) model. Said model will be targeted to optimizing both efficient distribution of water resources and profitability of such exchanges in a collaborative setting. In the end, a conclusion regarding the possible solutions to the water scarcity problem and the effect of different parameters on the optimal capacity expansion planning will be provided. Lastly, this master thesis is also framed in the context of the REWARD project.

2 Related Literature

Already since the late 1950s, numerous models with different objectives, applications and assumptions appear in the literature on the topic of capacity expansion planning. Additionally, the water network synthesis problem has also been an active area of research for the last two decades and many models and solutions have been suggested. Regarding the last topic, the focus for this work is going to be on the application of the water network design problem to eco-industrial parks. Elements of these streams of literature constitute the background for this thesis and they are going to be reviewed separately in this chapter.

2.1 Strategic Capacity Expansion Problem

The literature on operations management makes a distinction between tactical and strategic capacity planning. The first one deals with production and inventory management in the medium term, but not with equipment. Instead, strategic planning considers changes in the facilities during the long and medium term. Quantitative methods or mathematical programming models are more likely to be used on the operational and tactical levels, but they are also very helpful for taking decisions on the strategic level. This review is going to focus on strategic capacity planning models.

To clarify some terms, capacity is going to be defined as the volume of products that can be generated in a given period and it is influenced either by the volume of outputs that can be generated or the availability of some resources. As already stated in the introduction, Luss (1982) defined the capacity expansion problem as the determination of the sizes of facilities to be added, the associated times at which they should be added and the appropriate location for any expansion. Facilities could be understood as the smallest production process that produces an output and can be installed or expanded in different periods of time.

Luss (1982) also emphasized the importance of the strategic capacity planning for every company and established a framework and classification for capacity expansion models in the literature such as single-facility or multi-facility (multiple resource or capacity types), and single-site or multi-site.

In 1989, Sahinidis et al. developed a multi-period MILP model for long-range planning in chemical process industries that has been cited many times in later studies. The model has the aim of maximizing the net present value over a given time horizon and determining the following items: selection of new processes, capacity expansion and shut-down policies for all processes, production profiles and sales and purchases of chemicals at each time period. The problem of the computational expense of solving this long range planning problem is also investigated.

Sahinidis et al. (1991) and Liu and Sahinidis (1996) continued the investigation about the different solving strategies and suggested a reformulation of the model. Solution techniques for solving the model involved linear, nonlinear and dynamic programming and integer programming by: branch-and-bound, cutting planes, decomposition and heuristics. The approach by Liu and Sahinidis (1996) using strong cutting plane algorithms is demonstrated to be more robust and faster than conventional approaches for large scale problems with long time horizons.

Sahinidis et al. (1991) also presented a different work with a multi-period MILP investment decision model, which was an extension of their previous model from 1989, showing that it can be adapted to production facilities that are flexible manufacturing systems operating in either continuous or batch operations.

Bok et al. (1998) addressed the problem of long-range capacity expansion planning for chemical processing networks under uncertain demand forecast scenarios. A multi-period mixed integer nonlinear programming optimization model is suggested and its effectiveness is illustrated on a real problem arising from investment planning in the Korean petrochemical industry.

For other fields or applications, many mixed-integer models for capacity expansion have been developed. Some examples are capacity expansion for multi-site batch plants (Lee, 2000), strategic supply chain optimization for pharmaceutical industries (Papageorgiou et al., 2001), environmentally conscious design of supply chain networks (Hugo et al., 2005), multi-site capacity, production, and distribution planning (You, 2011), generation and transmission expansion planning (Pozo et al., 2013), etc.

Martínez-Costa et al. (2014) conducted an extensive literature review of mathematical programming models for strategic capacity planning in manufacturing companies and classified and analyzed many capacity planning models found in the literature. Different settings are addressed in different models and in all of them some decisions must be taken, such as capacity size decisions, possibility of capacity location on different sites, allocation of multiple resources, inventory decisions or workforce planning. Many factors can also be part of the problem statement, such as uncertainty, economies of scale, risks, regulatory factors or taxes, among others. No model is identified as being better than the others, since each of them faces a specific situation. It is observed that mixed integer linear programming (MILP) and linear programming (LP) models are the typical models to deal with planning capacity. However, different objective functions have been proposed, such as total cost minimization, maximization of net present value, minimization of unmet demand or maximization of capacity utilization.

Some of the most recent models on capacity expansion also include the consideration of rational markets and a competitive environment. Garcia-Herreros et al. (2016) developed a bi-level MILP model with an upper-level of NPV maximization and a lower-level representing the response of the market. One year later, Florensa et al. (2017) went a step further and developed a tri-level MILP model with three levels of decision-makers capturing the dynamics of duopolistic markets.

All in all, capacity planning is a very important problem in the industry and it is widely studied in different areas where large capital investments are required and profitability can only be assessed in a long time horizon. However, it can be observed that different problems can be defined for different settings.

2.2 Water Network Synthesis Problem

Water network synthesis is a problem in process systems engineering and can be defined as the design problem of the synthesis and retrofit of water networks for both continuous and batch operations (Khor et al., 2014). One of the most common objectives for solving this problem is minimization of freshwater use and minimization of wastewater generation. This usually involves using water-using units, wastewater operations or both.

In order to clarify some concepts, a water-using unit comprises water sources, such as external freshwater, and water sinks, with some degree of contamination. Wastewater treatment operations are intermediate processes that act as a water regenerator and can be placed before a water source.

There are some commonly used schemes introduced by Wang and Smith (1994) that represent reuse, recycle or regeneration processes and the optimal combination of these schemes is another possible definition of the water network synthesis problem (Foo, 2009).

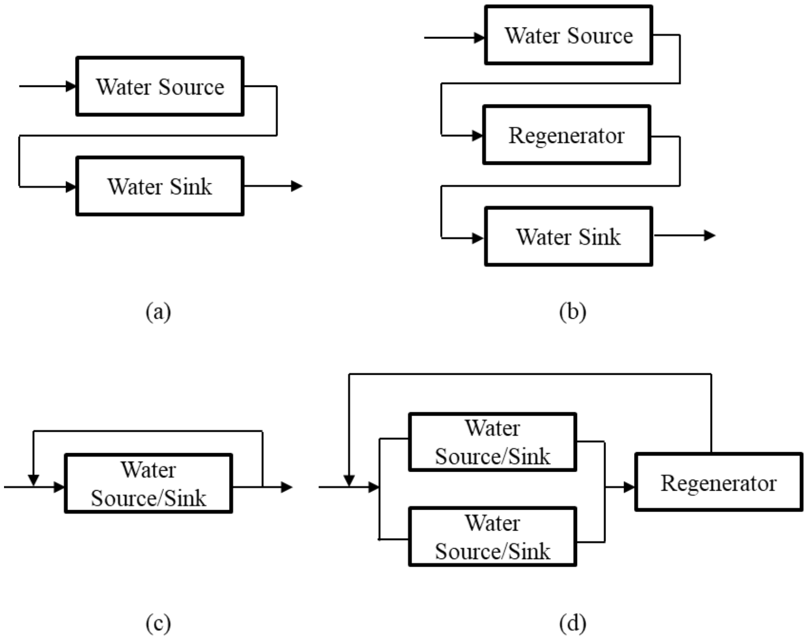


Figure 1: Representation of water recovery schemes: (a) reuse, (b) regeneration-reuse, (c) recycle, and (d) regeneration-recycling

In the context of process integration, water reuse means that the untreated wastewater from the unit that produced it is directly transferred to another unit for its use (figure 1a). Regeneration-reuse considers a partial water treatment (e. g. filter, adsorption, etc.) before reuse in another unit (figure 1b). Water recycle allows reusing water in the same unit where it was generated (figure 1c) and regeneration-recycling considers a partial water treatment before reuse in the same unit. These schemes allow a better understanding of how these options are usually modeled.

In general, there are two main approaches for solving the optimization network design problem and they are: insight-based techniques and model-based optimization methods. The former involves graphical and algebraic methods, such as water pinch analysis techniques, and the latter involves mathematical programming, such as MILP (linear) or MINLP (nonlinear) models.

Some extensive literature reviews on both approaches, water pinch analysis techniques (Foo, 2009) and mathematical programming (Khor et al., 2014), have been done. However, the most important points extracted from these papers are the motivation of the problem and the understanding of the concepts used. For this thesis, it is going to be more relevant to review models solving the water network design problem for eco-industrial parks or capturing water interactions between multiple factories.

2.3 Water Network Design of Eco-Industrial Parks

An eco-industrial park is commonly defined as “an industrial system of planned materials and energy exchanges that seeks to minimize energy and raw material use, minimize waste, and build sustainable economic, ecological and social relationships” (PCSD, 1996). There is evidence that increasing exchange of materials, energy, water or by-products in a symbiotic relationship between plants in the same area, contributes to a more sustainable development (Chertow, 2000). However, it has only been in the past decade that this is a topic of extensive research due to the growing environmental concern (Boix et al., 2015).

In the literature about optimal design of an EIP network, the most common types of cooperation that can be identified are cooperation through the water network, via energy and through exchanges of materials. Water network is the most usual among all of them and many of the rules and methods used to optimizing a single plant water network are also applied to integrating the water network of several plants. Actually, the typical methods for optimizing the water network design of eco-industrial parks are also conceptual graphic design and mathematical programming, the same as in the previous section.

One of the precursors of EIP optimization was Olesen and Polley (1996) and based on the water minimization procedure developed by Wang and Smith (1994), they decided to also address practical considerations such as geographical locations and piping costs. The used methodology was based on the graphical concepts of pinch technology.

In 2000, Chertow reviewed the small amount of industrial symbiosis literature until that moment and examined 12 sample industrial symbiosis projects representing four material exchange types. One of them was the EIP at Kalundborg, Denmark, the first industrial symbiosis to be achieved and an example of how water consumption can be reduced by a collective 25%. Chertow affirmed that there is enormous potential for environmental improvement through industrial symbiosis, reinforced the critical importance of the private sector and also encouraged the further investigation on this topic.

After some years with few publications on this topic, Liao et al. (2007) developed a design methodology for flexible multiple plant water networks combining pinch insight with mathematical programming. This methodology takes into account uncertainty and multi-period issues and has two stages: a targeting stage, which is a MINLP problem for providing the target freshwater usage and cross plant interconnection conditions; and a design stage, which is a MILP problem for obtaining a water network that meets the freshwater target in all periods for individual plants.

Chew et al. (2008) analyzed two different interplant water network schemes using mathematical optimization techniques. The first one is direct integration and represents direct connections between different water networks via cross-plant pipelines. This possibility was formulated through a MILP model with the objective of minimizing total cost and finding the optimal global solution. In the second scheme, which is indirect integration, water from different networks is sent to a centralized utility hub, which collects and redistributes water to the individual plants and could also act as a regeneration unit. In this case the problem is formulated with a MINLP model.

Chew et al. (2009) used a game theory-based approach to analyze the interaction between companies with a direct water integration scheme and reflected on the individual point of view of the participating companies in an EIP. The game theory approach is used as a decision-making tool after having generated a set of schemes. Both cooperative and non-cooperative scenarios are compared. The same authors (Chew et al., 2011) also applied the game theory approach to an indirect water integrated scheme. They also considered the possibility of an intervention by an EIP authority in order to investigate the influence of incentives for participation in the inter-plant water integration (IPWI).

Lovelady and El-Halwagi (2009) suggested a MILNP model with the objective of minimizing the total cost of the EIP and determining optimal design decisions for stream allocation, separation, exchange, and discharge. Some process and environmental constraints are also considered.

Lim and Park (2010) developed a nonlinear model (NLP) with the objective of minimizing industrial water consumption. They did not only synthesize and design an inter-factory and intra-factory water network system for an EIP, but also an environmental and economic feasibility study, using life cycle assessment (LCA) and life cycle costing (LCC), to demonstrate benefits from industrial symbiosis.

Boix et al. (2012) developed a multi-objective optimization strategy for minimizing the freshwater consumption, the regenerated water flow rate and the number of network connections. They formulated a MILP problem and used the ε-constraint method to solve it. To validate their approach, their model is applied to a published example with one contaminant. Afterwards, their MILP strategy is implemented for designing an EIP with three companies. Three scenarios are compared and the best configuration is found. The scenarios are EIP without regeneration unit, EIP where each company has its regeneration unit and EIP where the three companies share the regeneration unit. One year later, Montastruc et al. (2013) extended this work to a flexibility analysis with the goal of giving guidelines to face variations of the economic activity of an EIP. The economic indicators used are the equivalent number of connections (ENC) which reflects the piping and pumping costs in the EIP infrastructure, and the Global Equivalent Cost (GEC) expressed as an equivalent of freshwater flow rate.

Boix et al. (2015) did a literature review of the publications about EIPs and classified them into the different types of symbiotic relationships or cooperation that can be found in the literature. In particular, they focused on the mathematical formulation of the different criteria. It is observed that an EIP can be optimized from different ways and sometimes there are conflicting objectives. The typical objectives are societal, economic, topological and environmental.

Finally, Tiu and Cruz (2017) propose a multi-objective MILP model for optimizing water exchanges in eco-industrial parks considering water quality. This model simultaneously minimizes the economic and the environmental objective functions of an EIP through goal programming. They concluded that economic costs and environmental impacts are dependent on the priorities given to each goal, as well as the treatment quality of the processes.

2.4 Research Gaps

In the review of mathematical programming models for strategic capacity planning in manufacturing, by Martínez-Costa et al. (2014), one of the conclusions was that there are many techniques to model and solve a problem, but before formulating the model, it is more important to define the problem correctly and ensure that all the relevant considerations are taken into account.

This can also be applied to the process industries. For example, it can be observed that there is a gap on the literature regarding water considerations in strategic capacity expansion models. Water is a key component of process industries and it would make sense that it is an important factor in the expansion plans of a company. However, in the reviewed publications, specific constraints or processes modeling this topic are not observed.

From the water network design point of view, no publications have been found that consider a strategic level and address optimal timing for investing in the water facilities, possibility of capacity expansion in the long term and optimization of the water network from a broader perspective. This is also the case with the specific literature on eco-industrial parks. Capacity expansion planning combined with water management from an EIP perspective is a topic yet to be explored.

Lastly, another gap identified by Boix et al. (2015) concerning EIP are the lack of multi-objective optimization studies, since there are few publications that consider several objectives simultaneously and the ideal EIP design problem should address economic, environmental and social objectives. The authors affirm that some improvements have to be made regarding the mathematical formulation of objective functions.

3 Multi-objective, multi-period, multi-factory MILP Model

One of the purposes of this thesis is to present a multi-period, multi-factory MILP model for capacity expansion planning in process industries that also takes water management into consideration. The model represents water exchanges and allows using water reuse and regeneration as methods for preventing future water issues and favoring the expansion of the companies.

A collaborative setting is considered and a trade-off between maximizing the sum of the net present value of all factories and maximizing water reuse over a given time horizon must be achieved by determining the optimal value of these items: capacity expansion and shut-down policy for existing processes; selection of new processes, including water treatment, and their capacity expansion policy; production profiles; sales and purchases of chemicals at each time period; and water consumption and discharge from all sources/to all water sinks. The model is based on the Sahinidis et al. (1989) model for long range planning in the chemical industry, specifically on the later reformulation by Liu and Sahinidis (1996).

3.1 Problem Description

The following model considers one or multiple factories with possibility of water exchanges between them and assumes that a network of processes and chemicals for every factory is given. Each process can have one or more chemicals as an input an also one or more chemicals as an output; which can be intermediate products, meaning inputs for other processes; or end products, which are sold to the market. Processes can be modeled as water intensive, without water or be completely water based. The model has constraints for production and exchanges of chemicals, and constraints for production and exchanges of water. Figure 2 is an example representing one factory.

Usually, water enters a process with a certain quality and exits with a lower one. In this model, water quality is going to be defined with a water classification scheme as shown in figure 3 (Pulluru and Akkerman, 2017). This is an ordinal water quality classification which defines ordered water classes with descending levels of quality based on one or more water quality parameters. The water quality parameters corresponding to each water class should be within a predefined interval and all water streams are designated as a specific water class.

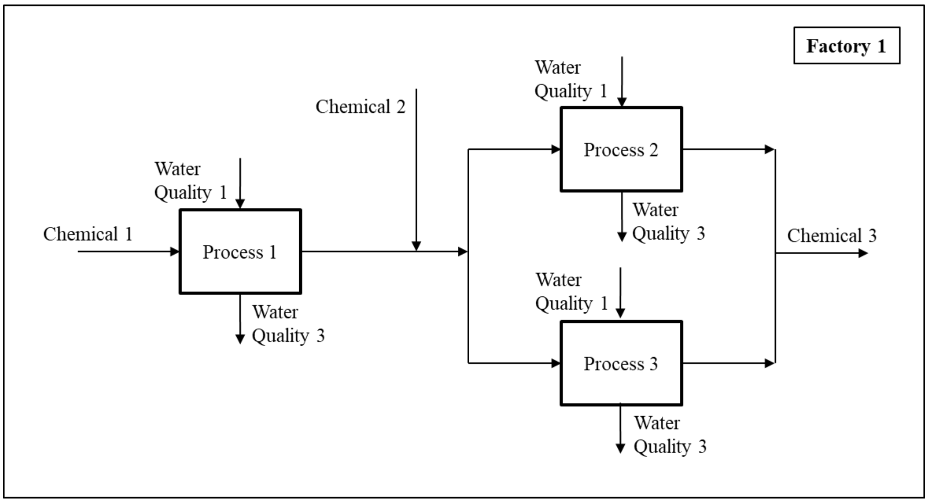


Figure 2: Example representing one factory

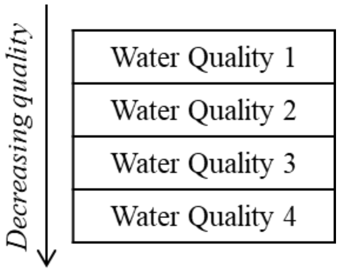


Figure 3: Water quality scheme

For every process a minimum required water quality needs to be set as well as the output water quality. A process can also be modeled as a water regenerator by setting a lower water quality requirement as an input and a higher water quality as an output. In figure 4, an example of a factory with a water treatment process can be observed. It is necessary that the quality class assigned to freshwater extracted from a natural source is lower than the quality class assigned to treated water coming out from the water treatment process, even if they are very similar.

It is also necessary to define a set of water sinks and sources that include not only extern freshwater sources like a lake, but also the factories that are able to sell treated water from their own water treatment plant to other factories. Water, in this case, is treated as a chemical that can be bought and sold in different qualities from one company to another and also can be bought/extracted from and sold/discharged to a natural sink or source, possibly with a certain cost.

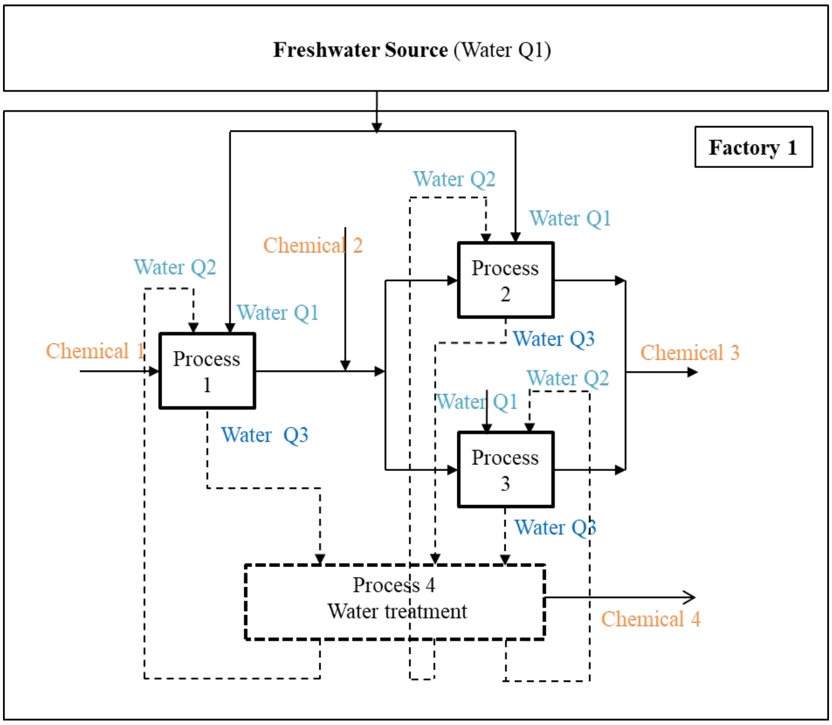


Figure 4: Example representing one factory with water treatment

The model allows the definition of another factory exclusively with water treatment processes and to set the possibility of water exchange of said factory with the other factories, as a central shared facility. In this case, some method for sharing the cost should also be defined. This is shown in figure 5.

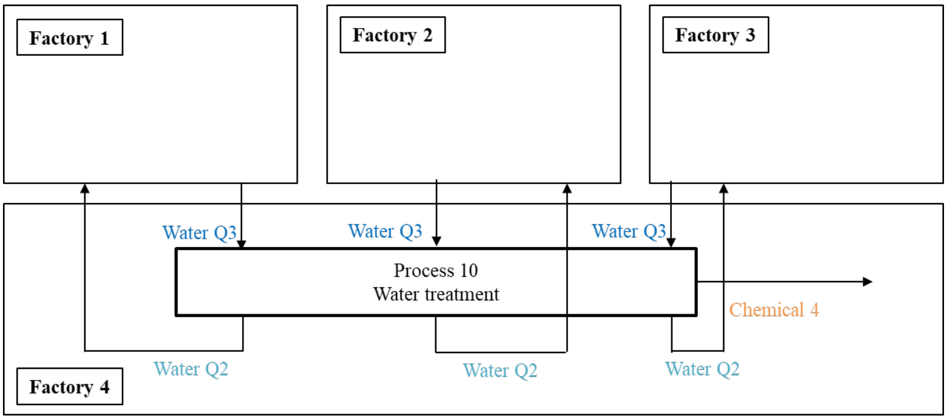


Figure 5: Example representing three factories with central water treatment

Every factory can buy and purchase the chemicals from different markets and the different market alternatives could also be defined with different streams. All processes, existent and possible ones, must be defined even if they are set with an initial capacity of zero. Furthermore, a finite number of time periods is considered and in all of them prices and demands of chemicals, prices and exchange possibilities of water, and investment and operating costs of the processes can vary. Therefore, it is necessary to estimate all prices and costs for all time periods and predefine these parameters.

It is considered that material and water balances in each process can be expressed linearly in terms of the operating level of the process. The same is assumed for the operating cost of each process. The investment costs of the processes and also their expansions are assumed to be linear expressions of the capacities with a fixed and a variable cost.

3.2 Indexes, Parameters and Variables

The following tables describe the indexes (table 1), parameters (table 2) and variables (table 3) contemplated in the model.

Table 1: List of sets & indexes

Index & Set	Description
$f \in F$	Set of factories
$i \in I_f$	Set of processes belonging to factory f
$W_f \subseteq I_f$	Subset of water treatment processes belonging to I_f
$j \in J$	Set of chemicals
$v \in V$	Set of water qualities
$l \in L$	Set of markets
$r \in R$	Set of water sink and sources
$t \in T$	Set of time periods

In table 2, it can be observed that this model requires some assumptions. In order to define all the necessary parameters, trends and forecasts have to be analyzed. Furthermore, assumptions regarding the prices of chemicals and water, the production and investment costs, the availabilities of raw materials, and the demands of the end products have to be made for a long range horizon. Uncertainties are not contemplated in the model.

Table 2: List of parameters

Parameter	Description
Q_{i0}	Existing capacity of process *i* at time *t=0*
QE^L_{it}, QE^U_{it}	Lower/upper bounds for capacity expansions of process *i* in period *t*
a^L_{jlt}, a^U_{jlt}	Lower/upper bound for purchases (availability) of product *j* from market *l* in period *t*
d^L_{jlt}, d^U_{jlt}	Lower/upper bound for sales (demand) of chemical *j* from market *l* in period *t*
$av^{water\_bin}{}_{fvrt}$	Binary parameter indicating possibility (availability) for factory *f* to buy water of quality *v* from source *r* in period *t*
$de^{water\_bin}{}_{fvrt}$	Binary parameter indicating possibility (demand) for factory *f* to sell/discharge water of quality *v* to sink *r* in period *t*
$av^{water\_U}{}_{fvrt}$	Upper bound for purchases (availability) for factory *f* to buy water of quality *v* from source *r* in period *t*
$de^{water\_U}{}_{fvrt}$	Upper bound for sales (discharge) for factory *f* to sell/discharge water of quality *v* to sink *r* in period *t*
μ_{ij}, η_{ij}	Input/output coefficient for material balance for process *i* and chemical *j*
$\mu^{water}{}_i, \eta^{water}{}_i$	Input/output water coefficient for process *i* and chemical *j*
$V^{req}{}_i$	Minimum water quality requirement for process *i*
$V^{eff}{}_i$	Water quality effluent from a process *i*
α_{it}, β_{it}	Variable/fixed term of investment cost for process *i* in period *t*
$\gamma_{fjlt}, \tau_{fjlt}$	Sales/purchase prices of chemical *j* for factory *f* in market *l* in period *t*
$\gamma^{water}{}_{fvrt}, \tau^{water}{}_{fvrt}$	Sales/purchase prices of water of quality *v* for factory *f* from source/to sink *r* in period *t*
δ_{it}	Unit operating cost for process *i* during time period *t*
CI_{ft}	Capital investment limitation of factory *f* in period *t*
$NEXP_i$	Maximum allowable number of expansions for process *i*

Table 3: List of variables

Variable	Description
Q_{it}	Total capacity of the plant of process *i* which is available

	in period t
QE_{it}	Capacity expansion of the plant of process i which is installed in period t
W_{it}	Operating level of process i during time period t
y_{it}	Binary variable which is 1 whenever there is an expansion for process i at the beginning of time period t, 0 otherwise
$I_{ijt,}O_{ijt}$	Amount of chemical j consumed/produced by process i during period t
MWI_{ivt}, MWO_{ivt}	Amount of water of quality v consumed/produced by process i during period t
P_{fjlt}, S_{fjlt}	Amount of product j purchased from/sold to market l by factory f at the beginning of period t
MWP_{fvrt}, MWS_{fvrt}	Amount of water of quality v bought from/discharged to source/sink r by factory f at the beginning of period t

Apart from the parameters and variables described in tables 2 and 3, the option of modeling a natural freshwater source like a lake is also presented. Even though this must be adapted for different settings, in the case of one lake as the only freshwater source it would be necessary to define the initial water level of the lake as parameter $MWLL_0$ and the water level of the lake in every period t as a new variable $MWLL_t$.

3.3 Constraints

To describe the problem it is necessary to define constraints regarding: capacity planning of processes, material balances, chemical availabilities and demands, possibility of water exchanges and water quality requirements.

First of all, equation (1) sets an upper and lower bound QE^L_{it}, QE^U_{it} for the capacity expansion QE_{it} in each process i and each period t. The variable y_{it} indicates occurrence of the expansion, so the bounds are only applied if y_{it}=1 and the expansion takes place. If variable y_{it} takes a value of zero then capacity expansion QE_{it} is also forced to zero.

$$y_{it}\, QE^L_{it} \le QE_{it} \le y_{it} QE^U_{it} \quad \forall i \in I_f, f \in F, t \in T \tag{1}$$

Equation (2) defines the total capacity Q_{it} that is available in each time period t, which is the expanded capacity in period t added to the capacity in the previous time period $t-1$. For this, it is necessary to define the initial capacity Q_{i0} of all processes in time $t=0$.

$$Q_{it} = Q_{i,t-1} + QE_{it} \quad \forall i \in I_f, f \in F, t \in T \tag{2}$$

Equation (3) ensures that the operating level W_{it} of a process does not exceed its capacity Q_{it}. Operating level W_{it} means, in this case, amounts of chemicals and water being consumed or produced/discharged in process i and period t.

$$W_{it} \leq Q_{it} \quad \forall i \in I_f, f \in F, t \in T \tag{3}$$

Equations (4) and (5) are material balances for the chemicals. The flow of every input I_{ijt} and output O_{ijt} of chemical j in process i and period t is defined as proportional to the operating level W_{it} of that process. Therefore, it is necessary to set the parameters μ_{ij} and η_{ij}, which are the proportions of each chemical in the total input and output of each process.

$$I_{ijt} = \mu_{ij}\, W_{it} \quad \forall i \in I_f, f \in F, j \in J, t \in T \tag{4}$$

$$O_{ijt} = \eta_{ij}\, W_{it} \quad \forall i \in I_f, f \in F, j \in J, t \in T \tag{5}$$

Equation (6) is a material balance of all chemicals in each factory. The amount of chemicals that a factory purchases from various markets plus the amounts produced within the network is equal to the amount of chemicals that a factory sells to various markets plus the amounts consumed within the network. That means that chemicals entering one process can be purchased from an external market, be an output from another process of the factory or both, and chemicals produced in a process can be sold to an external market, be used as an input in another process of the factory or both.

$$\sum_{l \in L} P_{fjlt} + \sum_{i \in I_f} O_{ijt} = \sum_{l \in L} S_{fjlt} + \sum_{i \in I_f} I_{ijt} \quad \forall f \in F, j \in J, t \in T \tag{6}$$

Equations (7) and (8) set an upper and lower bound for the availabilities a^L_{jlt}, a^U_{jlt} and for the demands d^L_{jlt}, d^U_{jlt} of the chemicals in every market l and every period

t. Therefore, purchases P_{fjlt} and sales S_{fjlt} of chemicals must be within these ranges.

$$a^{L}_{jlt} \leq \sum_{f \in F} P_{fjlt} \leq a^{U}_{jlt} \quad \forall j \in J, l \in L, t \in T \tag{7}$$

$$d^{L}_{jlt} \leq \sum_{f \in F} S_{fjlt} \leq d^{U}_{jlt} \quad \forall j \in J, l \in L, t \in T \tag{8}$$

Equations (9) and (10) are the equivalent equations to (4) and (5) but with water instead of chemicals. The parameters $\mu^{water}{}_{i}$ and $\eta^{water}{}_{i}$ are the water proportion in the total input and output of material of each process i. As explained in the section 3.1., a water classification scheme is used in this model and it is necessary to set some ranges of contamination and classify all water flows into different quality classes. The parameter $V^{req}{}_{i}$ defines the minimum water quality class required for the process i and the sum of all water flows MWI_{ivt} with quality class inferior (better quality) to this minimum, that constitute the water input to the process. Quality classes higher than $V^{req}{}_{i}$ (worse quality) cannot enter the process. There is an exception with the water treatment processes, defined by the set W_f, where input quality class must be exactly $V^{req}{}_{i}$. Water flow MWO_{ivt} is the water output to process i and must have the quality defined by the parameter $V^{eff}{}_{i}$. All water inputs and outputs with other qualities are set to zero in equations (11), (12) and (13).

$$\sum_{v \in V \mid v \leq V^{req}{}_{i}} MWI_{ivt} = \mu^{water}{}_{i} \, W_{it} \quad \forall i \in I_f, f \in F, t \in T \tag{9}$$

$$\sum_{v \in V \mid v = V^{eff}{}_{i}} MWO_{ivt} = \eta^{water}{}_{i} \, W_{it} \quad \forall i \in I_f, f \in F, t \in T \tag{10}$$

$$MWI_{ivt} = 0 \quad \forall i \in I_f, f \in F, v \in V, t \in T | v > V^{req}{}_{i} \tag{11}$$

$$MWI_{ivt} = 0 \quad \forall i \in W_f, f \in F, v \in V, t \in T | v < V^{req}{}_{i} \tag{12}$$

$$MWO_{ivt} = 0 \quad \forall i \in I_f, f \in F, v \in V, t \in T | v \neq V^{eff}{}_{i} \tag{13}$$

Equation (13) is the equivalent to equation (6), a material balance for each water quality in each factory. The set R defines the possible water sinks and sources, which can be for example natural resources and other factories with a water treatment plant.

$$\sum_{r \in R} MWP_{fvrt} + \sum_{i \in I_f} MWO_{ivt} = \sum_{r \in R} MWS_{fvrt} + \sum_{i \in I_f} MWI_{ivt} \quad \forall f \in F, v \in V, t \in T \tag{14}$$

Equation (13) means that for every quality *v* and every period *t* the amount of water that a factory purchases from various sources (lake, other factory with a treatment plant,..) plus the amount of water produced within the network is equal to the amount of water that a factory discharges to different sinks (lake, other factory with a treatment plant,..) plus the amounts consumed within the network.

This equation requires having some considerations that make it different from equation (6). In equation (6), purchases and sales of chemicals are made to external markets that are not modeled with equations. However, in the case of water purchases and sales there are two possibilities. Water can either be bought from or discharged to an extern source or sink, or be bought from or discharged to another factory that also belongs to the set of factories F. In this case, all parameters such as price or availability must be written twice in both directions. For example, if two factories are in set F and also in set R, the price of factory one for buying treated water from factory two must be the same as the price of factory two for selling treated water to factory one.

Another consideration is also necessary. If factory one wants to discharge water with a low quality to factory two, which has a water treatment plant and is able to treat it, then factory one must pay a price to factory two. However, in the model this is seen as if factory one is selling low quality water and factory two is purchasing it. Therefore, this price must be defined two times as a negative number, factory one has a negative price for selling low quality water to factory two and factory two has the same negative price for buying low quality water from factory one.

Equation (14) is another necessary balance in order to make a correlation between factories acting as sinks and sources in the same eco-industrial park. The amount of water that factory one purchases from factory two must be the same amount of water that factory two sells to factory one. This equation is only valid for the elements in set F (factories) that also belong to set R (water sources and sinks).

$$MWP_{fvrt} = MWS_{rvft} \quad \forall f \in F, v \in V, r \in R, t \in T \tag{15}$$

Equations (15) and (16) define the possibility of the water exchange between factory *f* and sink or source *r* for water of quality *v* in period *t*. The parameters $av^{water\_bin}{}_{fvrt}$ and $de^{water\_bin}{}_{fvrt}$ are binary, and must be 1 if it is possible for factory *f* to purchase from or sell to source or sink *r* and 0 otherwise.

$$MWP_{fvrt} \leq MWP_{fvrt}\, av^{water\_bin}{}_{fvrt} \quad \forall f \in F, v \in V, r \in R, t \in T \tag{16}$$

$$MWS_{fvrt} \leq MWS_{fvrt}\, de^{water\_bin}{}_{fvrt} \quad \forall f \in F, v \in V, r \in R, t \in T \tag{17}$$

The parameters $av^{water\_U}{}_{fvrt}$ and $de^{water\_U}{}_{fvrt}$ set an upper bound for these water purchases and discharges, and they could be for example a government regulation. Equations (18) and (19) define these limits.

$$MWP_{fvrt} \leq av^{water\_U}{}_{fvrt} \quad \forall f \in F, v \in V, r \in R, t \in T \tag{18}$$

$$MWS_{fvrt} \leq de^{water\_U}{}_{fvrt} \quad \forall f \in F, v \in V, r \in R, t \in T \tag{19}$$

Equations (20) and (21) express that the sum of water purchases of a factory *f* from all sources cannot exceed the amount of water entering their processes. Similarly, the sum of water discharges of a factory *f* to all sinks cannot exceed the amount of water coming out of their processes. This is to eliminate the possibility of factories trading with water and purchasing and discharging water that they do not use in their processes.

$$\sum_{r \in R} MWP_{fvrt} = \sum_{i \in I_f} MWI_{ivt} \quad \forall f \in F, v \in V, t \in T \tag{20}$$

$$\sum_{r \in R} MWS_{fvrt} = \sum_{i \in I_f} MWO_{ivt} \quad \forall f \in F, v \in V, t \in T \tag{21}$$

Equation (22) expresses a limit on the number of expansions for each process *i* and equation (23) expresses a limit of the capital available for investment for each factory *f* and time period *t*.

$$\sum_{t \in T} y_{it} \leq NEXP_i \quad \forall i \in I_f, f \in F \tag{22}$$

$$\sum_{i \in I_f} (\alpha_{it}\, QE_{it} + \beta_{it} y_{it}) \leq CI_{ft} \quad \forall f \in F, t \in T \tag{23}$$

In the case of considering a natural water source like a lake, this element could be modeled with equation (24). The water level of the lake *MWLL* in a certain period *t+1* is equal to the water level in the previous period *t* minus all water purchases or consumptions from the lake in period *t* plus all water discharges to the lake in period *t*. Two extra parameters $MWwithoth_t$ and $MWdischoth_t$ are added in order to represent other withdrawals and other discharges such as rain water.

$$\begin{aligned} MWLL_{t+1} = MWLL_t - \sum_{f\in F}\sum_{v\in V}\sum_{r\in R|r=lake} MWP_{fvrt} \\ + \sum_{f\in F}\sum_{v\in V}\sum_{r\in R|r=lake} MWS_{fvrt} - MWwithoth_t \\ + MWdischoth_t \quad \forall t \in T \end{aligned} \tag{24}$$

In this case, it is also necessary to add constraint (25). The amount of water withdrawn from the lake must be lower than the water level of the lake.

$$\sum_{f\in F} MWP_{fvrt} \leq \; MWLL_t \quad \forall v \in V, r \in R, t \in T | r = lake \tag{25}$$

It is also assumed that the lake has water of high quality, for example quality 1, and therefore it must be set that the only type of water that factories can consume from the lake is quality 1. It is also considered that the lake is big enough that even if factories discharge water of lower quality to the lake, it does not affect its quality and it remains water of quality 1.

3.4 Objective Function

Several key performance indicators (KPIs) could be chosen in order to define the objective function of this model. Of course, economic objectives are very important for companies, since they need to make their businesses profitable. However, sustainability objectives are also very relevant in order to maintain their business over time and avoid future environmental regulations or the possibility of depleting their own resources. For this reason, the objective function of the model is going to be a trade-off between maximizing the total net present value of all factories and maximizing the total water reuse. It is necessary to predefine a weight representing the importance of each objective, hence, a trade-off analysis comparing different weighs might be useful in order to take a decision of which weights to use. Weighted goal programming is the multi-objective method that is going to be used. Tiu and Cruz already tested its effectiveness in their model from 2017.

In order to use the weighted goal programming method it is necessary to solve the model three times. The first two times the model must be solved for both objectives individually and the last time it must be solved with the goal programming objective. The reason for this is that NPV and water reuse values have different scales and therefore they must be normalized in order to have the same impact in the multi-objective equation. In order to normalize these values, it is necessary to define the range by which NPV and water reuse may vary and these limits, obtained in the first two runs of the model, are going to be an input in the multi-objective equation.

The first objective is maximizing the net present value of all factories, which is defined by equation (26). Equation (27) shows the NPV calculation for each factory.

$$max\ Obj_1 = \sum_{f \in F} NPV_f \tag{26}$$

$$\begin{aligned} NPV_f = \frac{1}{(1+r)^t} [- \sum_{i \in I_f} \sum_{t \in T} (\alpha_{it}\, QE_{it} + \beta_{it} y_{it}) \\ - \sum_{i \in I_f} \sum_{t \in T} \delta_{it} W_{it} + \sum_{j \in J} \sum_{l \in L} \sum_{t \in T} (\gamma_{fjlt}\, S_{fjlt} - \tau_{fjlt}\, P_{fjlt}) \\ + \sum_{v \in V} \sum_{r \in R} \sum_{t \in T} ({\gamma^{water}}_{fvrt}\, MWS_{fvrt} - {\tau^{water}}_{fvrt}\, MWP_{fvrt})] \quad \forall f \in F \end{aligned} \tag{27}$$

The first term of this equation belongs to the NPV formula and expresses that all cash flows must be discounted with a certain discount rate r. The next four terms define the cash flows of one factory. The first one is a negative cash flow and represents the investment costs for the capacity expansions. The parameters α_{it} and β_{it} are the variable and fixed terms for the investment cost. The second one is also a negative cash flow and represents the operating costs. The parameter δ_{it} is the unit operating cost. The third term represents the chemical sales minus the chemical purchases and the parameters γ_{fjlt} and τ_{fjlt} are, respectively, the sales and purchases prices for the chemicals. Finally, the last term represents the water discharges minus the water purchases and γ^{water}_{fjlt} and τ^{water}_{fjlt} are, respectively, the discharges and purchases prices or costs for water. After solving the model with this objective, the optimal NPV value must be saved as the parameter NPV_{max} and the corresponding total water reuse value must be saved as $Reusewater_{min}$.

The second objective is maximizing the water reuse value of all factories, which is defined by equation (28). Equation (29) shows the water reuse calculation for each factory. This calculation is the sum of all water inputs, with the water quality class corresponding to the treated water, to the processes of each factory. After solving the model with this objective, the optimal water reuse value must be saved as $Reusewater_{max}$ and the corresponding total NPV value must be saved as NPV_{min}.

$$max\ Obj_2 = \sum_{f \in F} Reusewater_f \tag{28}$$

$$Reusewater_f = \sum_{i \in I_f} \sum_{v \in V | v = Qtreatment} \sum_{t \in T} MWI_{ivt}\ \forall f \in F \tag{29}$$

Finally the model is solved for maximizing the weighed goal programming objective shown in equation (30). In this equation the objectives are normalized with the parameters previously obtained, which are $NPV_{max,}$ $NPV_{min,}$ $Reusewater_{min}$ and $Reusewater_{max}$, and it is also necessary to define the weights $weight_1$ and $weight_2$ representing the importance of each goal. The sum of both weights must be 100%.

$$\begin{aligned} max\ Obj_{goal} = weight_1 & \frac{Obj_1 - NPV_{min}}{NPV_{max} - NPV_{min}} \\ + \ weight_2 & \frac{Obj_2 - Reusewater_{min}}{Reusewater_{max} - Reusewater_{min}} \end{aligned} \tag{30}$$

From a mathematical perspective, the maximal value of Obj_{goal} is 100. This is impossible to happen unless the maximum total NPV and the maximum total water reuse are achieved at the same time. Otherwise, the objective maximize Obj_{goal} is trying to approximate the total NPV and the total water reuse to their maximum values, favoring one objective over the other according to their weights.

4 Numerical Experiments

A base setting has been designed and different parameter variations have been implemented in order to test the model and explore some scenarios. In this chapter, a sensitivity analysis, a trade-off analysis with the economical vs. the sustainable objective and a profit distribution analysis are presented and discussed.

All experiments have been implemented with the programming language Python 3.6. through the environment Spyder and using the Gurobi Optimizer as a solver. It has been allowed a gap of 5% between the found solution and the optimal solution and it has been set a time limit of 100 seconds in each iteration. All experiments have been performed on a computer with 8GB RAM, dual core Intel® Core™ i7-7500U processor and 2.7 GHz speed.

4.1 Base Setting and Data

The base setting that has been designed is constituted by three identical chemical industries in an industrial park, which use a relatively high amount of water in their processes. This setting is shown in figure 6. Each of the factories has an identical scheme with three processes and consume freshwater from a nearby lake, which has a cost. Each factory buys some chemicals from a market and sells a chemical to the same market, so only one market is considered.

Since the freshwater from the lake is a limited resource and all factories want to expand in the next ten years, they decide to investigate the possibility of adding a water treatment plant either individually with no water sharing possibility or collectively, with the possibility of treating the polluted water of the neighbor factory for a certain price. In that case, all factories and the lake would be water sinks and sources and could purchase and sell water from one to another.

The three factories want to maximize their net present value, but they are also concerned about minimizing the freshwater consumption / maximizing water reuse on their processes due to possible government regulations in the future. Therefore, they also have to decide which importance to give to each objective. In order to decide whether to invest or how to invest in a water treatment process, the presented MILP model for capacity expansion planning can be applied.

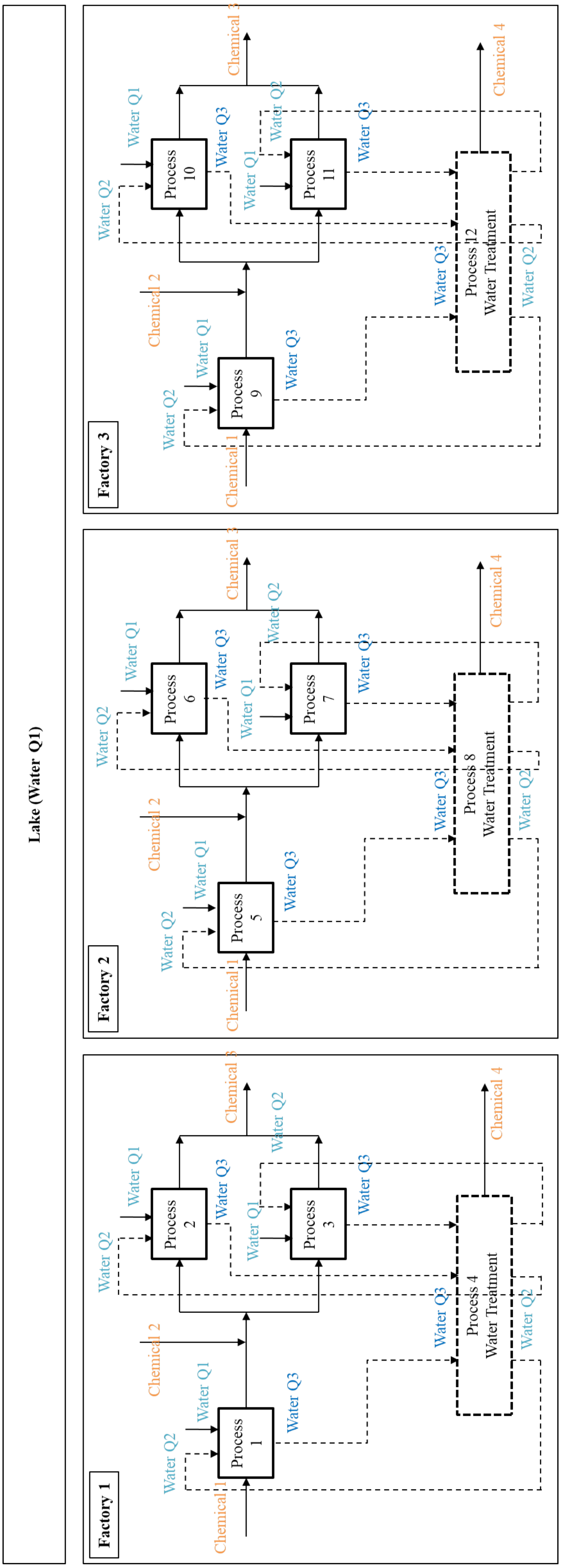


Figure 6: Three factories with possibility of water treatment plant and one lake

For the base setting the following sets are considered: a period of time of ten years (T), three factories (F), four processes in each factory (I_f), one possible water treatment process in each factory (W_f), one market for chemical purchases and sales (L), four different chemicals (J), three water quality classes (V) and finally four water sink and sources (R), which are the three factories and the lake. Since all three factories are identical, the data for processes 1, 2, 3 and 4 is going to be the same for the equivalent processes of the other factories. The data from tables 4, 5 and 7 is based on the data used by Sahinidis et al. (1991) for testing their model.

It is determined that the initial capacity (Q_{i0}) of process 1 is 7.5 kton/year, processes 2 and 3 have an initial capacity of 20 kton/year, and process 4, which is the water treatment plant, has zero initial capacity because it has not been installed yet. The upper bound for all capacity expansions is QE^{U}_{it} = 200 kton/year and the lower bound is QE^{L}_{it} = 0 kton/year.

Table 4 shows all upper bounds for chemical availabilities and demands a^{U}_{jlt}, d^{U}_{jlt} and also the chemical purchases and sales prices $\tau_{fjlt}, \gamma_{fjlt}$. All upper bounds for chemical availabilities and demands that do not appear in the table have a value of zero. The only exception is the demand of chemical 4, which is residual waste from the water treatment plant that cannot be sold and must have a high demand upper bound for not limiting the use of the water treatment plant. All lower bounds for chemical availabilities and demands a^{L}_{jlt}, d^{L}_{jlt} are set to zero and all chemical prices that do not appear in table 4 as well. Water availabilities and discharge restrictions $av^{water\_U}_{fvrt}$, $de^{water\_U}_{fvrt}$ for the base case are defined with a very high value.

Table 4: Upper bounds for chemical availabilities and demands and chemical prices

Item	**t=1**	**t=2**	**t=3**	**t=4**	**t=5**	**t=6**	**t=7**	**t=8**	**t=9**	**t=10**
Avail. chem. 1 a^{U}_{jlt} (kton/year)	90	120	135	136	140	140	140	145	145	145
Avail. chem. 2 a^{U}_{jlt} (kton/year)	300	375	450	451	452	453	454	455	456	457
Dem. chem. 3 d^{U}_{jlt} (kton/year)	195	225	270	280	290	300	310	320	330	340
Buy price ch. 1 τ_{fjlt} (10^3\$/kton)	73.2	52.4	40	39	39	39	35	35	35	30

Buy price ch. 2 τ_{fjlt} (10^3\$/kton)	135.2	115.2	96	96	90	90	90	86	86	86
Sell price ch. 3 γ_{fjlt} (10^3\$/kton)	450	400	360	360	330	330	300	300	300	250

Table 5 shows the proportions of water and chemicals in the total input and output of each process μ_{ij}, η_{ij}, μ^{water}_{i}, η^{water}_{i}. A minimum water quality class requirement for processes 1, 2 and 3 of $V^{req}_i = 2$ and for process 4 of $V^{req}_i = 3$ is defined. The water quality class of the effluent is $V^{eff}_i = 3$ for the processes 1, 2 and 3 and $V^{eff}_i = 2$ for process 4.

Table 5: Mass balances for chemicals and water

Item	Input coeff. in process				Output coeff. in process			
	1	2	3	4	1	2	3	4
Chemical 1 μ_{ij}, η_{ij}	0.3	0	0	0	0	0	0	0
Chemical 2 μ_{ij}, η_{ij}	0	0.4	0.4	0	0.3	0	0	0
Chemical 3 μ_{ij}, η_{ij}	0	0	0	0	0	0.4	0.4	0
Chemical 4 μ_{ij}, η_{ij}	0	0	0	0	0	0	0	0.3
Water $\mu^{water}_{i}, \eta^{water}_{i}$	0.7	0.6	0.6	1	0.7	0.7	0.6	0.7

Table 6 presents the different water purchase and discharge prices/costs τ^{water}_{fjlt}, γ^{water}_{fjlt} and table 7 shows all variable and fixed investment costs α_{it}, β_{it} and all operating costs δ_{it}. All water prices that do not appear in table 6 are zero.

Table 6: Water prices

Prices (10^3 \$/kton)	t=1-10
Buy freshwater v=1 from lake τ^{water}_{fjlt}	1.5
Buy treated water v=2, from another factory τ^{water}_{fjlt}	1.4
Buy dirty water v=3 from another factory τ^{water}_{fjlt}	-3
Sell treated water v=2 to another factory γ^{water}_{fjlt}	1.4
Sell dirty water v=3 to another factory γ^{water}_{fjlt}	-3
Discharge dirty water v=3 to the lake γ^{water}_{fjlt}	-3

Table 7: Variable and fixed investment coefficients and operating cost coefficients

Item	t=1	t=2	t=3	t=4	t=5	t=6	t=7	t=8	t=9	t=10
Var. C. Proc. 1 α_{it}	15.8	13.6	12.8	12.6	12.3	12.0	11.9	11.6	11.3	11

$(10^{3}\$/(\text{kton}\cdot\text{year}))$										
Var. C. Proc. 2 α_{it} $(10^{3}\$/(\text{kton}\cdot\text{year}))$	44	31.2	25.2	25.2	25.2	25.2	25.2	25.2	25.2	25.2
Var. C. Proc. 3 α_{it} $(10^{3}\$/(\text{kton}\cdot\text{year}))$	46.4	32.4	25.6	25.2	25.2	25.2	25.2	25.2	25.2	25.2
Var. C. Proc. 4 α_{it} $(10^{3}\$/(\text{kton}\cdot\text{year}))$	1.32	1.32	1.32	1.32	1.32	1.32	1.32	1.32	1.32	1.32
Fix. C. Proc. 1 β_{it} $(10^{5}\$)$	11.2	9.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5
Fix. C. Proc. 2 β_{it} $(10^{5}\$)$	10.2	8.2	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3
Fix. C. Proc. 3 β_{it} $(10^{5}\$)$	11.4	9.7	8.9	8.9	8.9	8.9	8.9	8.9	8.9	8.9
Fix. C. Proc. 4 β_{it} $(10^{5}\$)$	5	5	5	5	5	5	5	5	5	5
Op. C. Proc. 1 δ_{it} $(10^{3}\$/\text{kton})$	6	5	4	4	4	4	4	4	4	4
Op. C. Proc. 2 δ_{it} $(10^{3}\$/\text{kton})$	8	7	6	6	6	6	6	6	6	6
Op. C. Proc. 3 δ_{it} $(10^{3}\$/\text{kton})$	9	8	7	7	7	7	7	7	7	7
Op. C. Proc. 4 δ_{it} $(10^{3}\$/\text{kton})$	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28

A maximum number of 5 expansions for each process $NEXP_i$ is set, and a maximum capital available for investment CI_{ft} of 1500000$ is set for each factory. Additionally, the initial level of the lake is set to $MWLL_0 = 10^7$ kton. For the NPV calculation it has been used a discount rate of 10%.

In order to test the model and modify some parameters, the scenarios shown in table 8 have been designed. Table 9 shows the material balances in the case of less water intensive processes, which corresponds to sub-sub-scenario 2.

Table 8: Experiment Scenarios

Scenario	Description
Scenario 1	Water exchanges are not allowed between factories
Scenario 2	Water exchanges are allowed between factories
Sub-scenario 1	All companies have the same investment capital of 1500000$

Sub-scenario 2	All companies have a different investment capital: 2500000$, 1500000$ and 500000$.
Sub-sub-scenario 1	Processes are water intensive (table 5)
Sub-sub-scenario 2	Processes are less water intensive (table 9)

Table 9: Mass balances for chemicals and water – Sub-sub-scenario 2

Item	Input coeff. in process				Output coeff. in process			
	1	2	3	4	1	2	3	4
Chemical 1 μ_{ij}, η_{ij}	0.7	0	0	0	0	0	0	0
Chemical 2 μ_{ij}, η_{ij}	0	0.6	0.6	0	0.7	0	0	0
Chemical 3 μ_{ij}, η_{ij}	0	0	0	0	0	0.6	0.6	0
Chemical 4 μ_{ij}, η_{ij}	0	0	0	0	0	0	0	0.3
Water $\mu^{water}_{i}, \eta^{water}_{i}$	0.3	0.4	0.4	1	0.3	0.4	0.4	0.7

4.2 Sensitivity and Trade-off Analysis: Economic Objective vs. Sustainable Objective

The effects of the variation of several parameters are presented in this section, mainly focusing on the changes in NPV, freshwater consumption and water reuse percentage. Furthermore, it is analyzed how the variation of some parameters affect the optimal solution in a different way depending on the weights of maximizing the NPV and maximizing water reuse in the objective function. Some comments about the presented experiments must be made. The 5% MIP gap allows that quite different solutions can be found for each small variation of a parameter. However, this considerably reduces the computational effort and trends can be observed anyway. Sub-scenario 2 is ignored in this section because the differences in investment capital did not bring clear conclusions related to the variation of other parameters.

The first parameter that has been analyzed is the discharge cost of water with quality class 3 to the lake. This price is initially set to 3 $/ton. Figures 7 and 8 show a sensitivity analysis with this parameter and a trade-off analysis with the two objectives. Each curve in the graph corresponds to an increase or decrease of the value of this parameter and each point in the curve corresponds to different weights in the objective function. The left end of every curve correspond to the objective of maximizing the NPV with a weight of 100% and the right end of every curve correspond to the objective of maximizing water reuse with a weight of

100%. In every curve of figures 7 and 8, there are 11 points corresponding to a 10% increase or decrease in the weights of the two objectives. For example, the second point in each curve starting from the left represents the optimal solution with the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%.

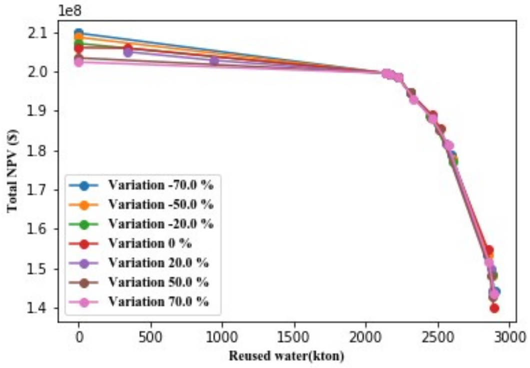


Figure 7: Sensitivity and trade-off analysis: water v=3 discharge to lake price variation. Scenario 1-1-1

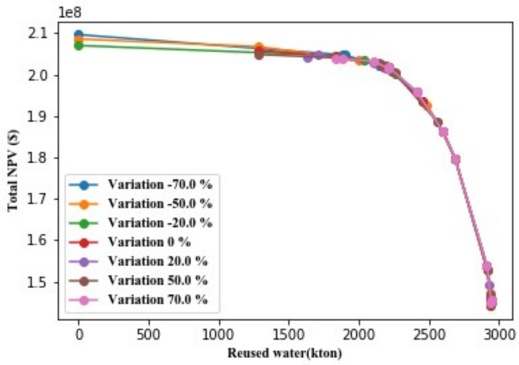


Figure 8: Sensitivity and trade-off analysis: water v=3 discharge to lake price variation. Scenario 2-1-1

Figure 7 is obtained with scenario 1, sub-scenario 1 and sub-sub-scenario 1, and scenario 1 means that water exchanges are not allowed between factories, so they can only withdraw and discharge water individually to the lake and they have to decide individually whether to install or not a water treatment process for their own use. Figure 8 is obtained with scenario 2 and the same sub-scenarios, and in this case it is also possible that only one or two factories install a water treatment process and the others make use of this process by paying a certain fee. This means that in scenario 2 it is always more likely that installing a water treatment process at least in one of the factories is profitable.

From figures 7 and 8 it can be observed that small variations of the discharge price of water with quality class 3 to the lake have little effect on the optimal solution. In the case of only maximizing the NPV (weight 100%) and scenario 1, all optimal solutions have zero water reuse independently of the price variation, which means not installing a water treatment plant in any factory. The lower the discharge price the higher the NPV is and vice versa, but without water reuse. However in the same case in scenario 2, if the discharge price of water with quality class 3 to the lake is equal or superior to 3 $/ton (variation of 0%), then it is profitable to at least install one water treatment process in one of the factories, even if the objective is only maximizing the total NPV. If water is being treated, less water with quality class 3 is being discharged to the lake and therefore, the discharge price of water with quality class 3 to the lake has little impact on the optimal solution.

The same happens if maximizing water reuse is also included in the objective function, even if it is with a small weight. If the water treatment processes are installed, much less water with quality class 3 is being discharged and the discharge price of water with quality class 3 makes an insignificant difference in the objective function. For this reason all curves look aligned if water reuse is prioritized. However, the difference between taking into account the sustainable objective with a weight of 0% and a weight of 10% is the decrease of the total NPV in a range between 1 and 4%, but in the last case 40-60% of the water can be reused.

Another test can be performed and it is to keep increasing the discharge price of water with quality class 3 until a variation of +900% (30 $/ton) and see how the model behaves.

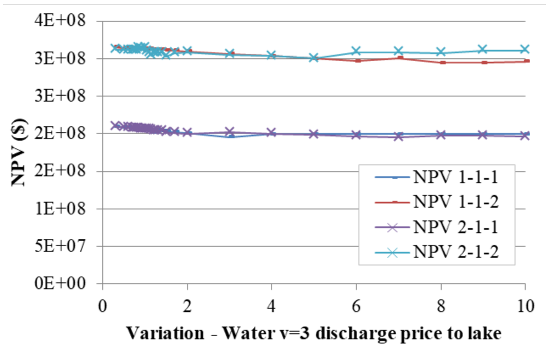


Figure 9: Sensitivity analysis: water v=3 discharge to lake price variation. NPV. Objective: 100% NPV - 0% Reuse Water

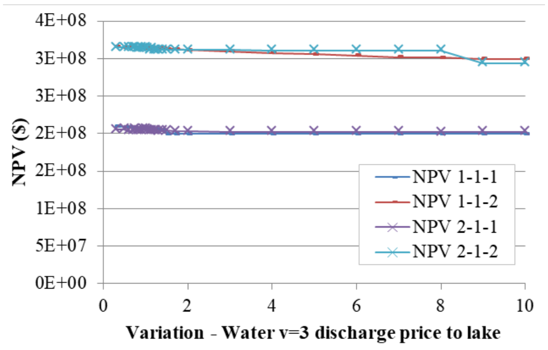


Figure 10: Sensitivity analysis: water v=3 discharge to lake price variation. NPV. Objective: 90% NPV - 10% Reuse Water

In figures 9-14, the variation of the parameter is given with a multiplicative factor instead of a percentage and factor 1 equals to a variation of 0%. These figures also show the difference between sub-sub-scenario 1 and sub-sub-scenario 2, which is a higher percentage of water in the processes or a lower percentage of water in the processes, respectively.

Figure 9 and figure 10 compare the NPV variation if the objective is maximizing the NPV with a weight of 100% or with a weight of 90%. As previously said, for small variations of the discharge price, NPV is a bit higher with the objective of maximizing the NPV with a weight of 100% than with a weight of 90%. However if the discharge price increases a lot, practically the same NPV is achieved independently of using a weight of 100% or 90% in the objective, or independently of allowing the possibility of water exchanges between the factories or not. It always comes to a point where either it is more profitable to invest in a water treatment plant or practically the same NPV is achieved if the decision is to install the water treatment process or not. This is because the investment cost of the plant is compensated by the cost of discharging water with quality class 3 to the lake. Regarding the difference in NPV between sub-sub-scenario 1 and sub-sub-scenario 2, this only has to do with how the material balances are defined. If processes have less water, they are producing and selling more chemicals and therefore the NPV is higher. This is not a meaningful conclusion and must be ignored. Only the behavior with regards to the water consumption and reuse is meaningful in case of sub-sub-scenario 2.

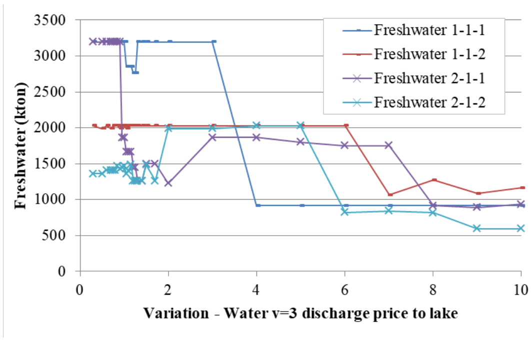


Figure 11: Sensitivity analysis: water v=3 discharge to lake price variation. Freshwater. Objective: 100% NPV - 0% Reuse Water

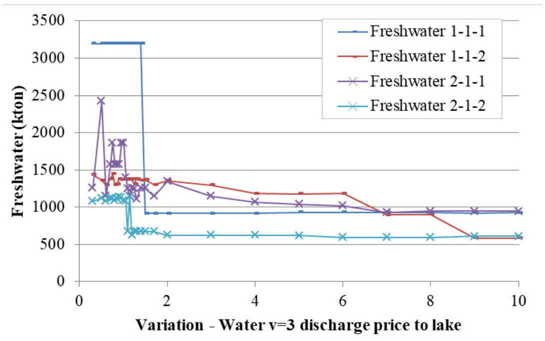


Figure 12: Sensitivity analysis: water v=3 discharge to lake price variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

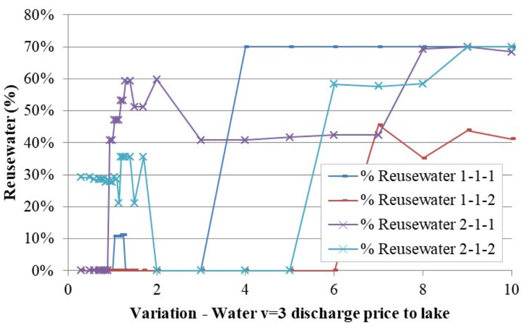


Figure 13: Sensitivity analysis: water v=3 discharge to lake price variation. Water reuse. Objective: 100% NPV - 0% Reuse Water

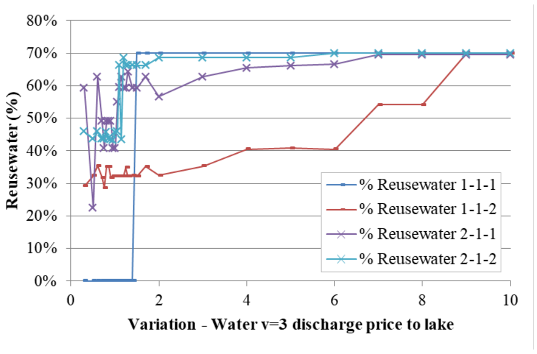


Figure 14: Sensitivity analysis: water v=3 discharge to lake price variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

Figures 11-14 show the different freshwater consumption values and reused water percentages in case of maximizing the NPV with a weight of 100% or with a weight of 90% and also show the different combinations of scenarios and sub-sub-scenarios. In the case of maximizing the NPV with a weight of 100%, the obtained discharge price of water with quality class 3 to the lake that makes the installation of a water treatment plant be profitable is: 3 $/ton (multiplicative factor 1) for scenario 2-1-1, 9 $/ton (multiplicative factor 3) for scenario 1-1-1, 15 $/ton (multiplicative factor 5) for scenario 2-1-2, and 18 $/ton (multiplicative factor 6) for scenario 1-1-2. However in case of maximizing the NPV with a weight of 90% and maximizing reuse water with a weight of 10%, the obtained discharge price of water with class quality 3 to the lake that makes the installation of a water treatment plant be profitable is 0$/ton for scenarios 2-1-1, 1-1-2 and 2-1-2; and 5.4$/ton (multiplicative factor 1.8) for scenario 1-1-1. This means that in this problem there are multiple optimal solutions and just including the objective of reusing water with a 10% weight in the objective function, practically the same NPV is achieved but with much higher water reuse percentages. This also means that the discharge price of water with quality class 3 to the lake is much more significant for scenario 1-1-1. This is an expected result because if all factories work individually, it is less likely that they invest in a water treatment plant. However, if only one of them installs a water treatment plant, then all the others could make use of it. This is the case for scenario 2-1-1; here to have water reuse in the system is more likely to be profitable independently on the water discharge price to the lake. Of course in scenarios 1-1-2 and 2-1-2, water plays a less important role, and variations on parameters related to water have a lower effect.

The same experiments are made with the freshwater (quality class 1) purchase price from the lake. This price is initially set to 1 $/ton (variation 0%, multiplicative factor 1). Figures 15-18 are obtained and they show very similar results to the last experiments. In this case, small variations in the freshwater price have even a smaller effect because the initial price is very low compared to all other costs. The biggest effect can be observed comparing scenario 1-1-1 with scenario 2-1-1. Figures 15 and 16 show that for the objective of only maximizing the NPV, even if the purchase price is decreased by 20% (0.8 $/ton), having at least one water treatment plant between the three factories is profitable (scenario 2). However, if they have to install the water treatment process individually, the purchase price which makes this profitable is slightly higher (scenario 1). Figure 17 shows that if the NPV maximization objective is 90%, then the freshwater price must be 2 \$/ton (multiplicative factor 2) in order for the individual installation of a water treatment plant to be profitable.

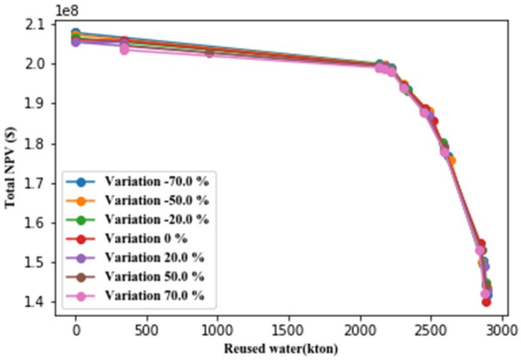


Figure 15: Sensitivity and trade-off analysis: water v=1 purchase from lake price variation. Scenario 1-1-1

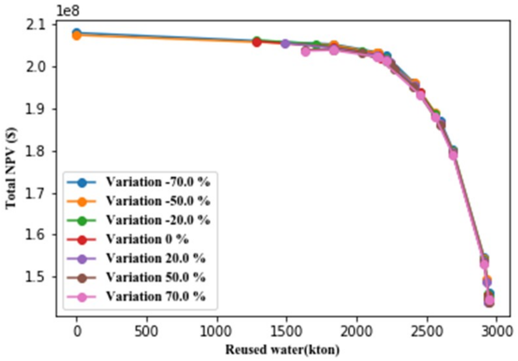


Figure 16: Sensitivity and trade-off analysis: water v=1 purchase from lake price variation. Scenario 2-1-1

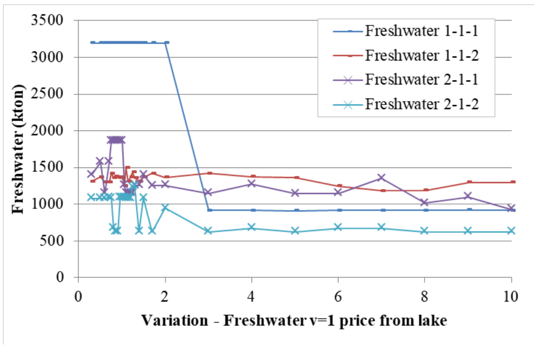


Figure 17: Sensitivity analysis: water v=1 purchase from lake price variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

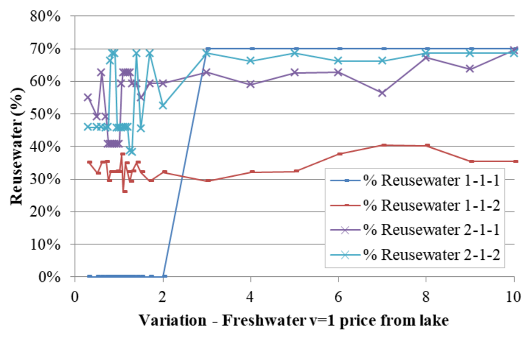


Figure 18: Sensitivity analysis: water v=1 purchase from lake price variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

The next set of experiments has been done by adding two different freshwater restrictions with different decreasing slopes during the years. This is achieved with the parameter $av^{water\_U}_{fvrt}$. Availability restriction 1 has a lower slope than availability restriction 2. The values are shown in figure 19.

These availabilities are made more or less restrictive by varying their values with a certain percentage and the results are shown in figures 20-22 for the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%. Figure 20 shows the expected NPV results. The NPV is maximum when there are no availability restrictions and it is the same if water exchanges are allowed between the factories (scenario 1) or not (scenario 2). However, there is a difference between the two restrictions. In restriction 2 the availability decreases at a higher pace every year than in restriction 1, therefore the NPV with restriction 2 is always lower than with restriction 1, which is also lower than with no restriction. Independently of which restriction is applied, the NPV is always a bit higher if water exchanges are allowed between the factories than if they are not allowed. In all cases, the lower the freshwater availability, the lower the NPV is because less freshwater is available for production.

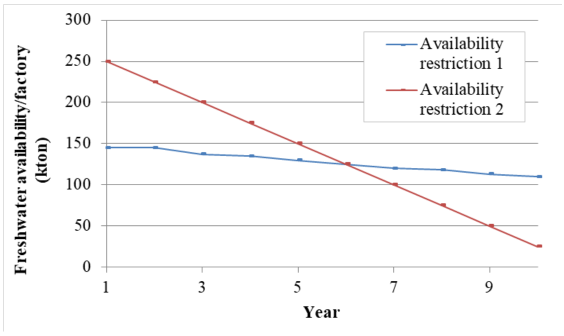


Figure 19: Freshwater v=1 availability restriction per factory from the lake

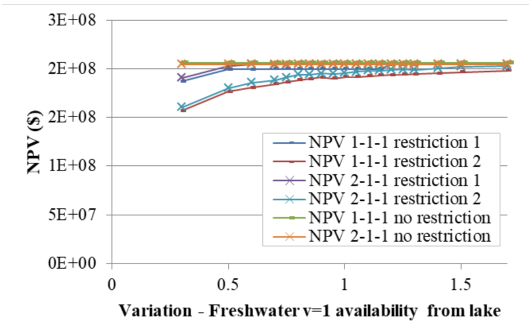


Figure 20: Sensitivity analysis: freshwater v=1 availability from lake variation. NPV. Objective: 90% NPV - 10% Reuse Water

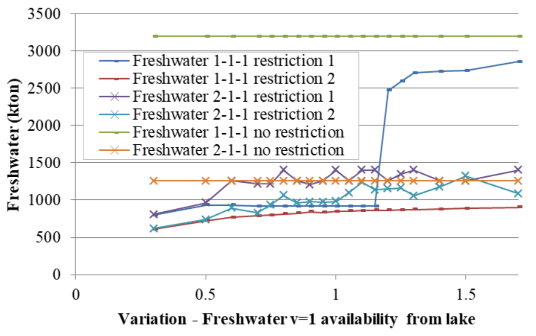


Figure 21: Sensitivity analysis: freshwater v=1 availability from lake variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

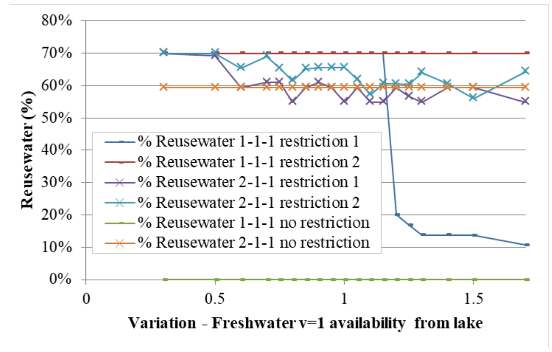


Figure 22: Sensitivity analysis: freshwater v=1 availability from lake variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

Figures 21 and 22 show that, independently from the restriction, it is always more profitable and more sustainable to collaborate for reusing water. Collaborating (scenario 2) also mitigates the effects of the availability restrictions. However, if the factories do not collaborate, they are more affected by the restrictions. Restriction 2 is stricter and for this reason, even if increasing or decreasing the values by 70% (multiplicative factors 0.3 and 1.7), with scenario 1 it is always more profitable to install a water treatment process in each factory. However, with restriction 1, which is less strict, it can be observed in the figure that if the availability values are increased 20% (multiplicative factor 1.2) then it stops being that profitable to invest on water treatment processes in scenario 1.

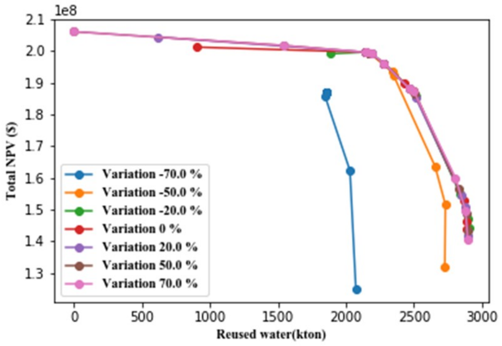


Figure 23: Sensitivity and trade-off analysis: freshwater v=1 availability from lake variation. Restriction 1, scenario 1-1-1

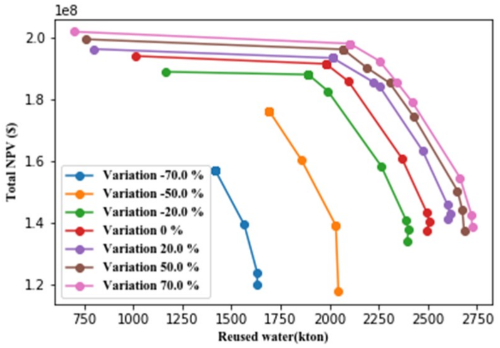


Figure 24: Sensitivity and trade-off analysis: freshwater v=1 availability from lake variation. Restriction 2, scenario 1-1-1

Figures 23 and 24 show a comparison between the two restrictions. It can be observed that if the availability values in restriction 2 increase, this has a higher effect on the NPV than if the availability values in restriction 1 increase. In both cases, it can be observed that for higher availability values, the trade-off curve between the objectives is very broad. This means that the maximum NPV is obtained with a much lower water reuse percentage than the maximum water reuse percentage. And the more weight the water reuse objective has, the less NPV is obtained. However, in the case of very low availabilities like a decrease of the values in 70%, the trade-off curve becomes almost vertical. This means that the maximum NPV is obtained with a very close water reuse percentage to the maximum water reuse possible.

The same experiment is now tested by adding two different discharge restrictions on water with quality class 3, with different decreasing slopes during the years. This is done with the parameter $de^{water\_U}_{fvrt}$. Discharge restriction 1 has a lower slope than discharge restriction 2 and the values are shown in figure 25.

Once more, these availabilities are made more or less restrictive by varying their values with a certain percentage. The results shown in figures 26, 29 and 30 are for the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%. In figure 26, only very small variations in the

NPV in scenario 1 are observed with both restrictions, but in general the NPV remains almost constant. The explanation is that if water treatment processes are profitable, independently of the restriction, water discharge is minimized and discharge restrictions lose their negative effect since only the minimum amount of water is being discharged. This is also shown in figures 27 and 28, where hardly any changes in NPV can be observed.

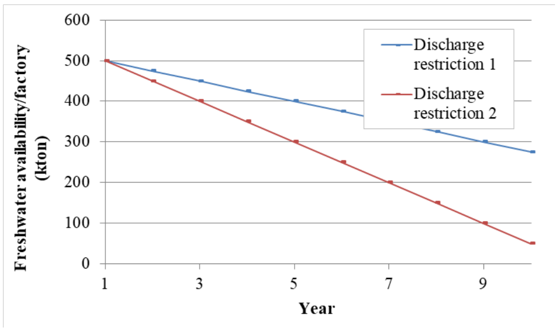


Figure 25: Water v=3 discharge restriction per factory to the lake

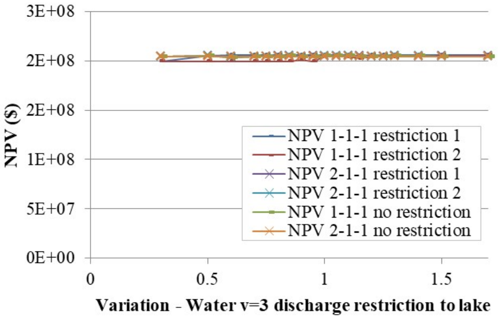


Figure 26: Sensitivity analysis: water v=3 discharge restriction to lake variation. NPV. Objective: 90% NPV - 10% Reuse Water

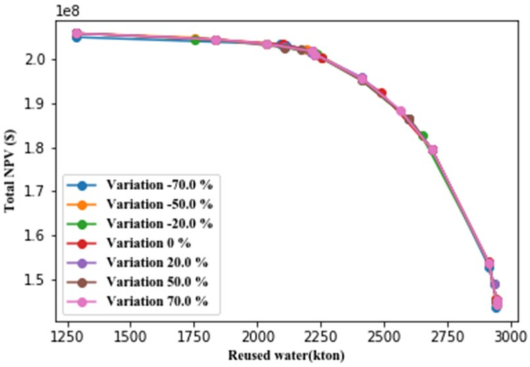


Figure 27: Sensitivity and trade-off analysis: water v=3 discharge restriction to lake variation. Restriction 1, scenario 2-1-1

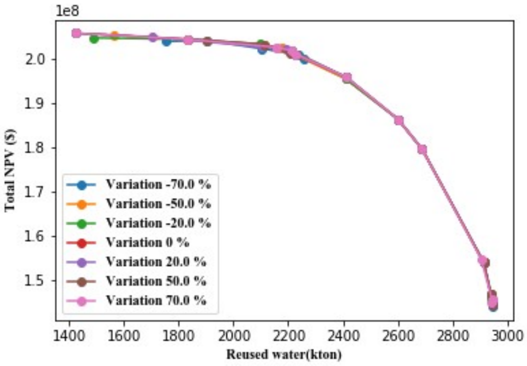


Figure 28: Sensitivity and trade-off analysis: water v=3 discharge restriction to lake variation. Restriction 2, scenario 2-1-1

Figures 29 and 30 show freshwater consumption and water reuse percentage and this has only an effect in scenario 1, where water exchanges are not allowed. If restrictions are strong, it is always profitable to install a water treatment plant, but the more relaxed they are, the less likely it is that installing a water treatment plant for each factory individually is profitable. The high slopes in the dark blue and red lines represent the variation in the discharge restriction for which installing a water treatment plant stops or starts being profitable.

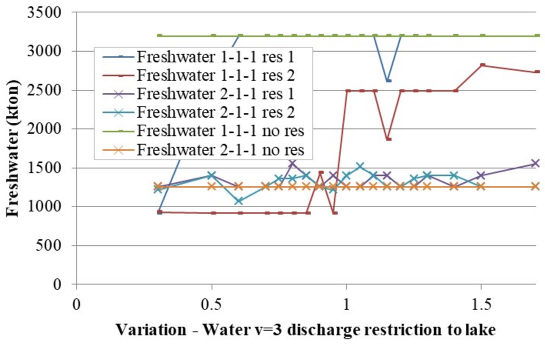


Figure 29: Sensitivity analysis: water v=3 discharge restriction to lake variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

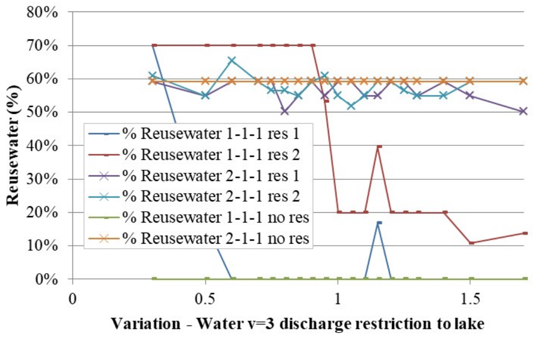


Figure 30: Sensitivity analysis: water v=3 discharge restriction to lake variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

The next parameter that has been tested is the demand upper bound of chemical 3, which is a way of increasing or decreasing the need for production. Chemical 3 is the only chemical that is sold to the market and brings profit to the companies. Figures 31 and 32 compare scenario 1 and scenario 2 for different variations of the parameter and different variations in the weights of the objectives. It is observed that a high upper bound demand of chemical 3 does not affect the model. However, if demand is very low, less production is needed and the companies have less profit. The lower the demand of chemical 3, the narrower the trade-off curves, and the closer the optimal water reuse value is, with maximum NPV, to the maximum water reuse value. The reason for this is that if demand is very low, optimizing the production in order to make it more efficient becomes more important for increasing the NPV. In this case, this translates into avoiding the costs of discharging water of quality class 3 to the lake and favoring water reuse and the installation of water treatment processes.

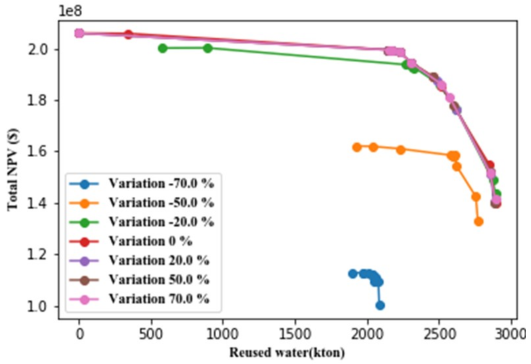


Figure 31: Sensitivity and trade-off analysis: chemical 3 demand variation. Scenario 1-1-1

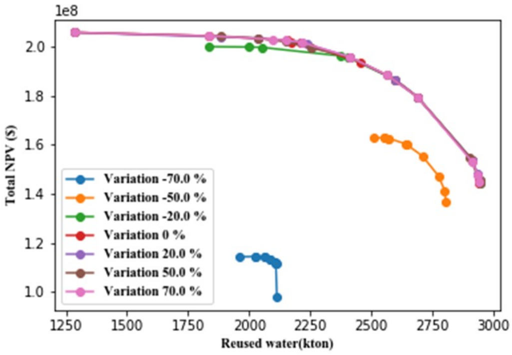


Figure 32: Sensitivity and trade-off analysis: chemical 3 demand variation. Scenario 2-1-1

Figures 33-35 show the NPV, freshwater consumption and water reuse percentage for different variations of the parameter and with the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%. It is observed again in figure 33 that if the demand of chemical 3 increases, the NPV remains constant or increases slightly, but if this parameter decreases, the NPV also decreases considerably for the reasons explained previously.

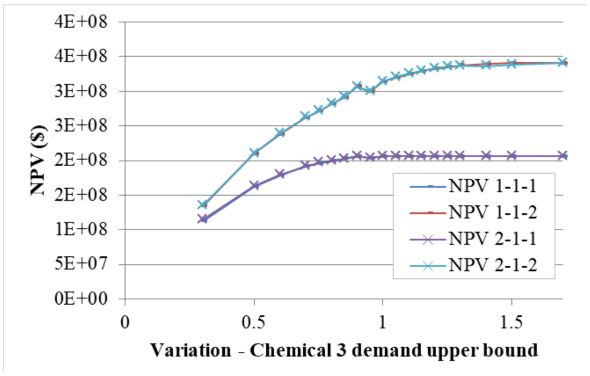


Figure 33: Sensitivity analysis: chemical 3 demand variation. NPV.
Objective: 90% NPV - 10% Reuse Water

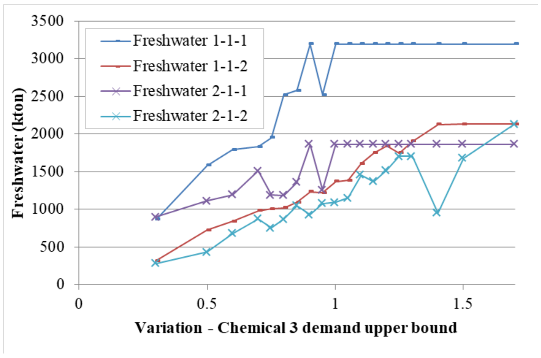


Figure 34: Sensitivity analysis: chemical 3 demand variation. Freshwater.
Objective: 90% NPV - 10% Reuse Water

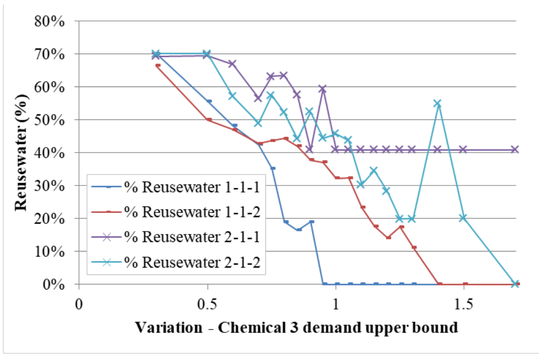


Figure 35: Sensitivity analysis: chemical 3 demand variation. Water reuse.
Objective: 90% NPV - 10% Reuse Water

Figures 34 and 35 show that for sub-sub-scenario 1, which are processes which require more water, the variations on this parameter start affecting the model when the demand of chemical 3 is lower than the values presented in the base data (variation 0%, multiplicative factor 1). At this point, the use of water treatment processes starts being more important for lower demand values. However, if processes require less water (sub-sub-scenario 2), that means that they are producing more chemicals due to the way that material balances are defined. Therefore, they are more affected by the chemical demand and water reuse and the installation of water treatment processes are optimal also for higher demand upper bounds. The explanation is the same. If the main product of the production has a low demand and the NPV is lower than expected, then it is more beneficial to make the processes more efficient.

The next experiment is the variation of sale price of chemical 3. Since the demand is not changed, the higher the sale price of the main product, the more profit the company is making. Figures 36 and 37 show scenarios 1 and scenario 2 for different variations of the parameter and different variations in the weights of the objectives. This time the curves are very broad. This is because the higher the profit that the company makes, the less important water and sustainability are from an economic perspective. When the objective weights are changed and water reuse appears in the objective function, water reuse increases, but this is imposed by the weight of the sustainable objective. These figures show that if the objective is 100% maximizing the total NPV, for a high sale price the optimal solution is not to install a water treatment plant. However if the sale price is low, installing a water treatment plant might be profitable, especially if companies are collaborating. Nevertheless, for very low prices (variation -70%) the best decision is not to have any production at all.

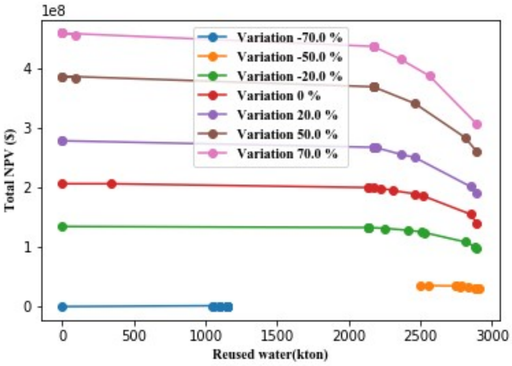


Figure 36: Sensitivity and trade-off analysis: chemical 3 sale price variation. Scenario 1-1-1

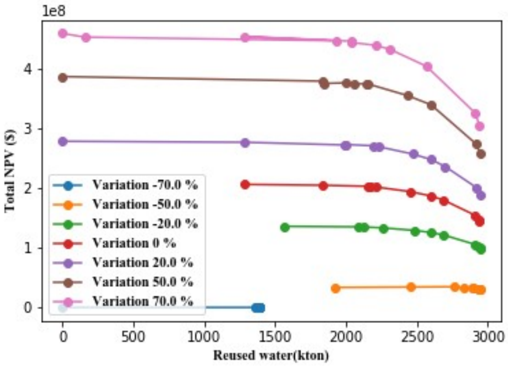


Figure 37: Sensitivity and trade-off analysis: chemical 3 sale price variation. Scenario 2-1-1

Figures 38-40 show the NPV, freshwater consumption and water reuse percentage for different variations of the sale price and with the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%. Figure 38 show the expected direct relation of the NPV with the sale price of chemical 3. The higher the sale price the higher the NPV and vice versa. In figures

39 and 40 it can be observed that in sub-sub-scenario 2, where processes require less water, the variation of the sale price of chemical 3 has a low effect on the water decisions and it is always profitable to invest in a water treatment plant due to the 10% weight of water reuse in the objective function. However, for sub-sub-scenario 1, where processes require more water, the effect of this parameter is stronger. For this sub-sub-scenario if the sale price of chemical 3 is high, water costs have little importance on the NPV because companies are making a lot of profit selling this chemical, and investing in a water treatment plant is less beneficial than expanding their production processes.

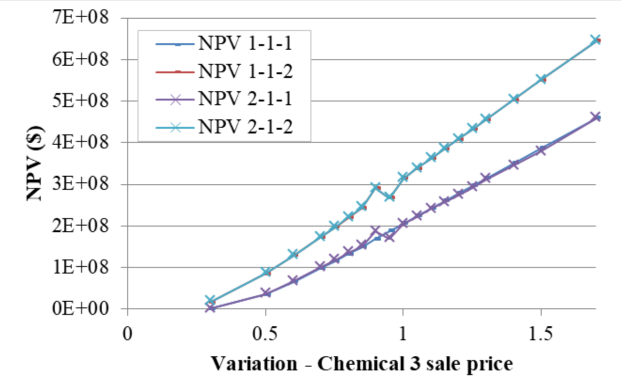


Figure 38: Sensitivity analysis: chemical 3 sale price variation. NPV. Objective: 90% NPV - 10% Reuse Water

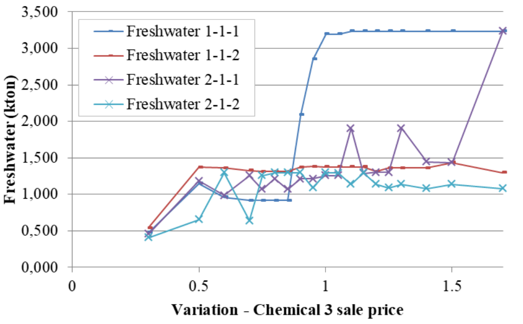


Figure 39: Sensitivity analysis: chemical 3 sale price variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

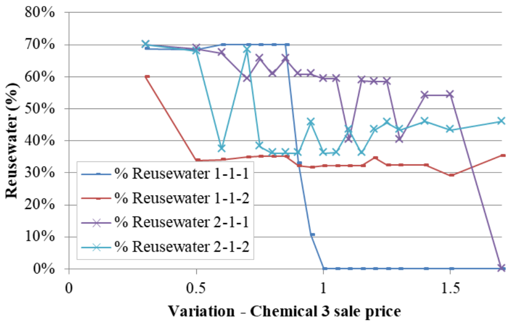


Figure 40: Sensitivity analysis: chemical 3 sale price variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

Especially in scenario 1, where factories do not collaborate, it is not profitable to invest on a water treatment process if the sale price of chemical 3 is higher than the base case (multiplicative factor 1). It is profitable in scenario 1 to invest in the water treatment process, if the sale price is lower than the sale price in the base case. However in scenario 2, where water exchanges are allowed, these effects are more mitigated and it is profitable to share at least a water treatment process between the three factories even for high sale prices of chemical 3. It is only for a very high sale price (variation +70%, multiplicative factor 1.7) that not even one water treatment plant is profitable in scenario 2.

Variations in initial capacity are also tested and figures 41-44 are obtained. Figures 41 and 42 show broad curves and there is a big difference in the optimal water reuse value between the case of only maximizing the NPV in the objective function and the case of only maximizing water reuse. Water reuse if the objective function is only maximizing the NPV is much lower than if the objective is only maximizing water reuse. In general, the higher the initial capacity the higher the NPV and vice versa. For both scenario 1 and 2, for small initial capacities and the objective of only maximizing the NPV, the investment on a water treatment plant is not profitable, because it is more beneficial to expand the production processes. However if the initial capacities are high, it would be more profitable to invest in water treatment processes, especially if the factories are collaborating (scenario 2).

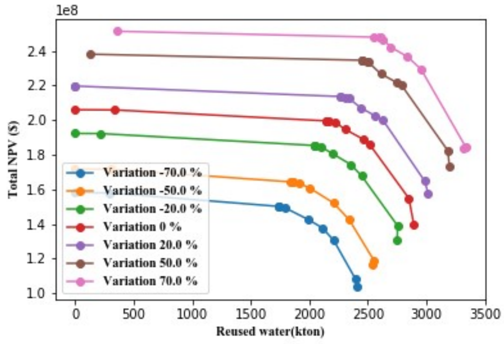


Figure 41: Sensitivity and trade-off analysis: initial capacity variation. Scenario 1-1-1

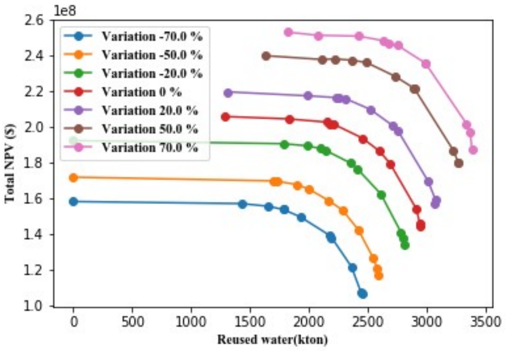


Figure 42: Sensitivity and trade-off analysis: initial capacity variation. Scenario 2-1-1

Figures 43 and 44 show that only if the initial capacities are increased over 40% (multiplicative factor 1.4) from the base case it is profitable in scenario 1 and sub-sub-scenario 1 to invest on a water treatment plant. However in scenario 2, it is always profitable to have at least one water treatment process. This reiterates the benefits of the collaborative setting. These figures correspond to the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%. In the appendix, the NPV figure which is just an increasing line is shown (figure 63).

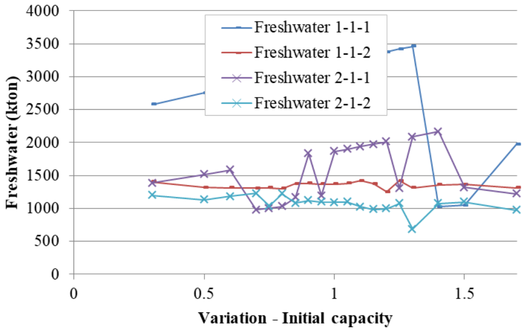


Figure 43: Sensitivity analysis: initial capacity variation. Freshwater.
Objective: 90% NPV - 10% Reuse Water

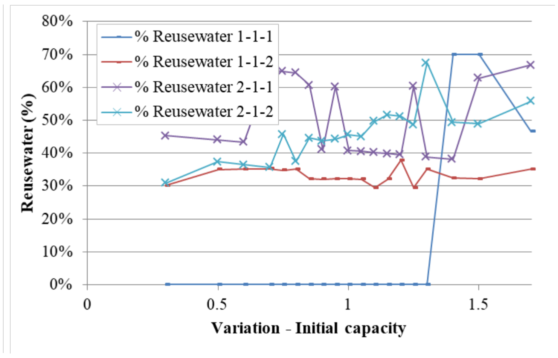


Figure 44: Sensitivity analysis: initial capacity variation. Water reuse.
Objective: 90% NPV - 10% Reuse Water

The capacity expansion upper bound has also been varied and figures 45-48 have been obtained. Figures 45 and 46 show that no water reuse is needed in case of maximizing the NPV with a weight of 100%, independently of the capacity expansion upper bound. However if maximizing water reuse has a weight in the objective function, the higher the capacity expansion upper bound the higher the NPV.

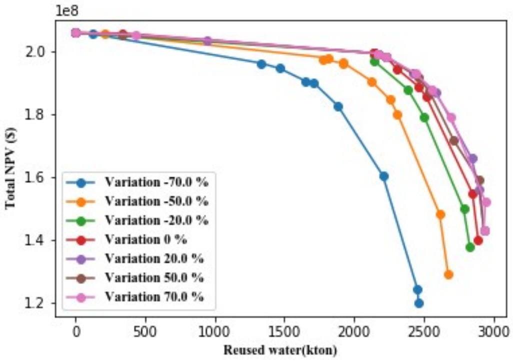


Figure 45: Sensitivity and trade-off analysis: capacity expansion upper bound variation.
Scenario 1-1-1

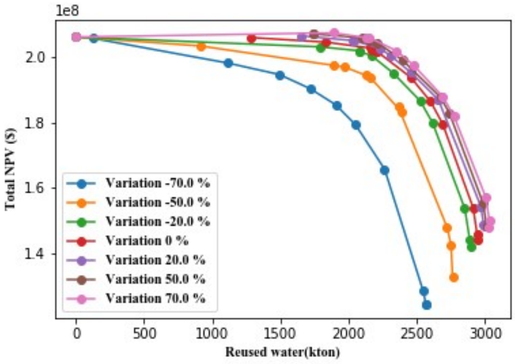
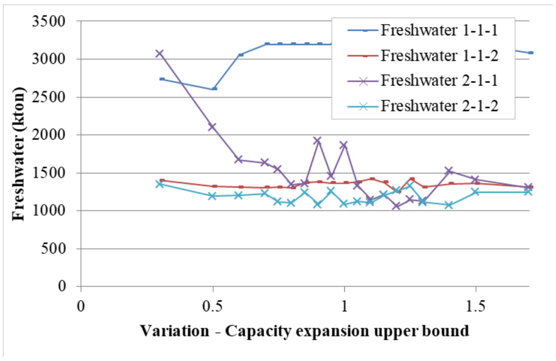


Figure 46: Sensitivity and trade-off analysis: capacity expansion upper bound variation.
Scenario 2-1-1

Figures 47 and 48 correspond to the objective of maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10% and they show again that in the case of non-collaborating factories it is not profitable to invest in a water treatment plant, but it is profitable in case of collaborating. NPV is in this case just a constant line that is shown in the appendix (figure 64). This is due to the fact that for small weights in the water reuse objective, the variations of the capacity expansion upper bound have little effect.



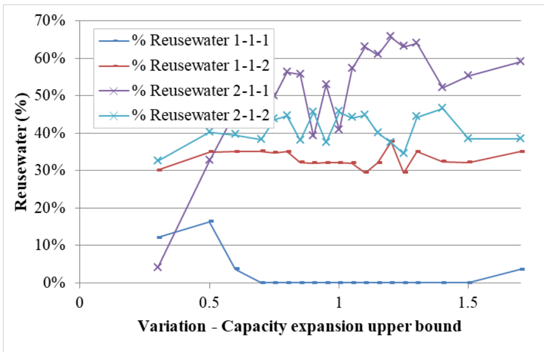
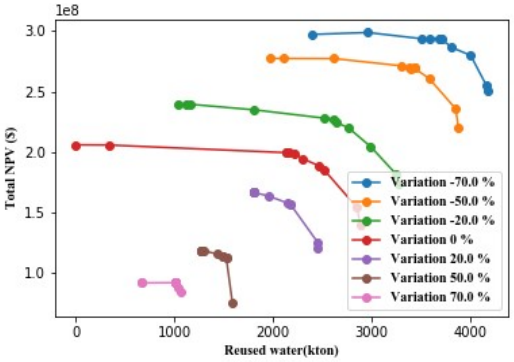


Figure 47: Sensitivity analysis: capacity expansion upper bound variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

Figure 48: Sensitivity analysis: capacity expansion upper bound variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

The fixed investment cost has also been varied and figures 49 and 50 have been obtained. Similar results are shown in the appendix (figures 65 and 66) for the variations in the variable investment cost.



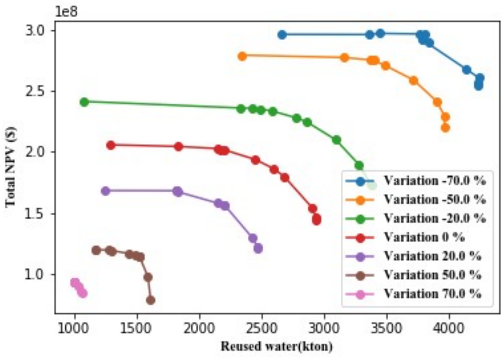


Figure 49: Fixed investment cost variation. Scenario 1-1-1

Figure 50: Fixed investment cost variation. Scenario 2-1-1

Since the fixed investment costs are higher in the production processes than in the water treatment process, the variations in this parameter affect the production processes the most. The results in both scenarios are very similar. If the investment costs are very high (variation 70%), the curves are very narrow because the benefit that can be obtained is very limited independently of the objective function weights. Nevertheless, even in that case it is preferred to invest in a water treatment plant because the investment in expanding the current production processes would be more expensive, due to the way in which the base data set is defined. On the other hand, if investment costs are much lower, NPV would be much higher and then it is profitable to invest in expanding all kind of processes, including the water treatment plant. It is only for variation 0% and scenario 1 that to invest in a water treatment plant is not profitable in case of only maximizing the NPV.

The last experiment is the variation of the operating cost and figures 51-52 are obtained. As expected, the lower the operating cost of the processes the higher the NPV and vice versa. In these graphs, once again, the difference between scenario 1 and scenario 2, for the objective of only maximizing the NPV, is illustrated. From these, the conclusion that it is only profitable to invest in the water treatment plant in scenario 2, where the factories are collaborating and can exchange water, can be made. In case of scenario 1, the operating cost only has an effect on the NPV and practically no effect on the water reuse decisions. However, in scenario 2, it is observed that for lower operating costs more water is being reused and this could be due to an earlier installation of the water treatment plant or due to the installation of multiple water treatment processes.

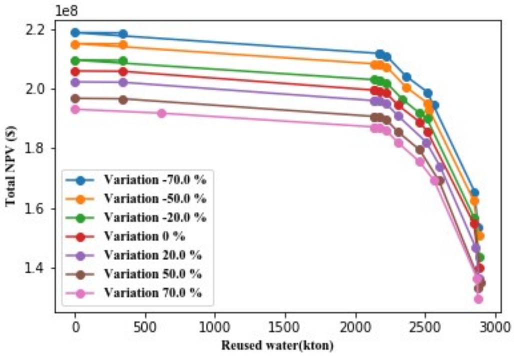


Figure 51: Sensitivity and trade-off analysis: operating cost variation. Scenario 1-1-1

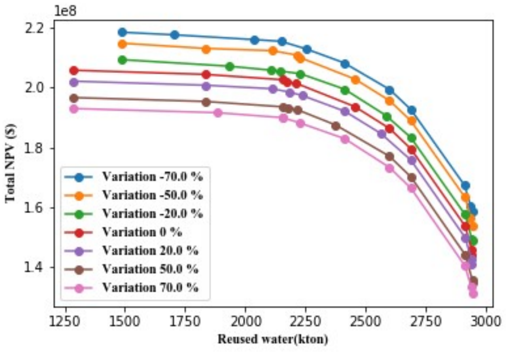


Figure 52: Sensitivity and trade-off analysis: operating cost variation. Scenario 2-1-1

Variations in the chemical availabilities and chemical purchase prices have also been done but have been moved to the appendix (figures 67-76) due to the lack of relevant conclusions.

4.3 Profit Distribution Analysis

The analysis of how the total NPV is distributed between the three companies and also the effect of having different investment capitals in the factories is carried out in this section. Figures 53 and 54 show the capital investment distributions in sub-scenario 1 and sub-scenario 2, which has not been contemplated in the last section.

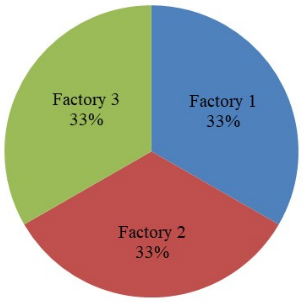


Figure 53: Capital investment distribution. Sub-scenario 1

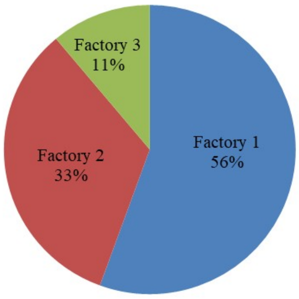


Figure 54: Capital investment distribution. Sub-scenario 2

Figure 55 shows the NPV distribution in scenarios 1 and 2, which mean factories without and with the possibility of water exchanges respectively; in sub-scenarios 1 and 2, which mean equal investment capitals and different investment capitals respectively; and in sub-sub-scenario 1, which mean processes that require a high amount of water.

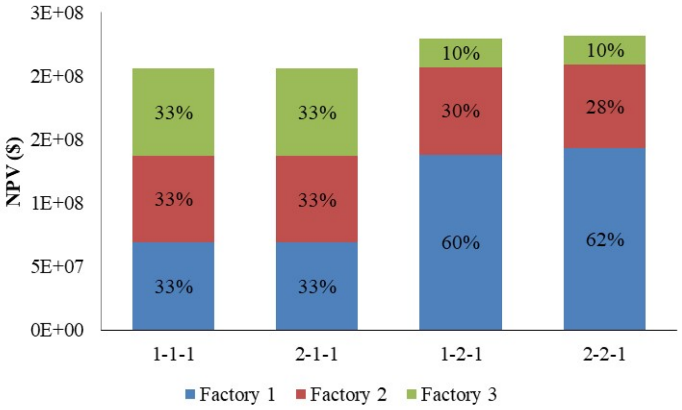


Figure 55: NPV distribution for each factory in different scenarios
Objective: 90% NPV - 10% Reuse Water

Figure 55 represents the optimal NPV with the base data without any variations. The first and the third column correspond to scenario 1, and must be compared respectively to the second and the fourth column to see how the individual NPV changes when collaboration between factories is allowed, and the total NPV is what is being optimized. In this particular case, it is observed that when the factories have the same investment capital, they also generate their individual NPV in the same proportion. However with different investment capitals, it might happen that for achieving a total maximum NPV, the individual NPV of one factory is lower than its individual maximum. This is the case of factory 2 that decreases its NPV a 2% of the total in scenario 2-2-1.

All the experiments shown in the section 4.2. have also been repeated for sub-scenario 2 and one example is presented in this section, focusing on the NPV distribution and the effect of different investment capitals. Figures 55-60 are created with variations on the freshwater availability restriction 1, which has been presented in figure 19. The objective function has been defined again for maximizing the NPV with a weight of 90% and maximizing water reuse with a weight of 10%.

Figure 55 proves that a higher NPV can be obtained if companies collaborate and share water reuse facilities, especially in case of a strict freshwater availability restriction from a lake.

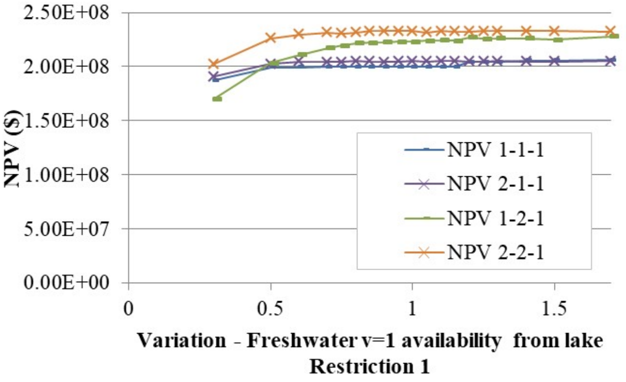


Figure 56: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. NPV. Objective: 90% NPV - 10% Reuse Water

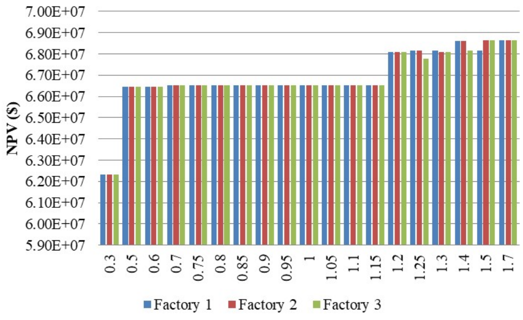


Figure 57: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. NPV/each factory. Scenario 1-1-1 Objective: 90% NPV - 10% Reuse Water

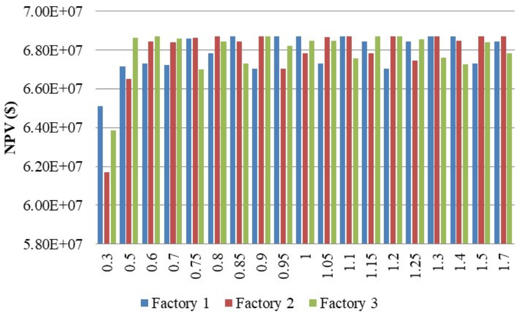


Figure 58: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. NPV/each factory. Scenario 2-1-1 Objective: 90% NPV - 10% Reuse Water

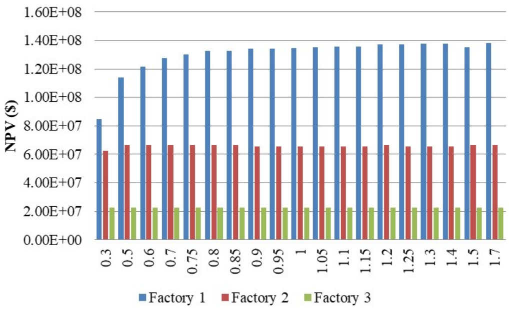


Figure 59: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. NPV/each factory. Scenario 1-2-1 Objective: 90% NPV - 10% Reuse Water

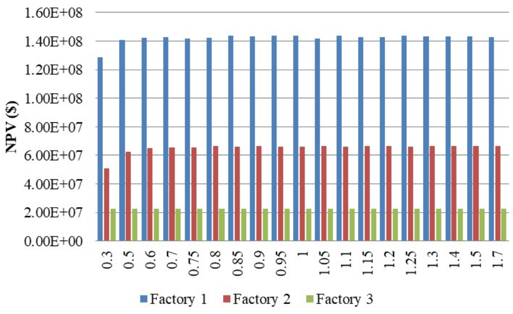


Figure 60: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. NPV/each factory. Scenario 2-2-1 Objective: 90% NPV - 10% Reuse Water

Furthermore, figure 55 shows that the fact of collaborating seems to have a bigger increase in the total NPV if the capital investments are unequal in the factories (sub-scenario 2), than if they are equal (sub-scenario 1). Actually this effect is not related with the fact of being unequal, but with the fact of having one factory with a very high investment capital being able to make a lot of expansions for their own profit and for the benefit of the system, even if another factory is making no expansions. In general, a higher NPV is achieved in sub-scenario 2 because if one company has a very high investment capital, this translates into a higher relative profit than with less investment capital, independently of the other factories.

Figures 56-60 show the NPV of each factory for each variation of the freshwater availability restriction. Figure 56 is compared to figure 57 and it is observed that contrarily to the figure 55, all individual NPVs are different for each variation, even when all factories have invested the same capital. This is because no weights have been defined for the NPV of each individual factory and the model maximizes the total NPV, which can lead to multiple optimal solutions with a random factory being favored each time. Even when the same NPV is achieved in scenario 1 and in scenario 2, for example for an increase of 70% in the freshwater restriction (multiplicative factor 1.7), it can be observed that if factories don't have water exchanges they all achieve the same NPV and if they collaborate the individual NPVs are different.

Figures 59 and 60 can also be compared and if one company has a higher capital investment, a relatively higher NPV is achieved than the others in the optimal solution. As already mentioned, this might be because it is less expensive or more profitable to expand the already existing processes than investing in new ones, and for that reason if one company has more capital to invest than the others, the model will favor the investments and the benefits of this factory. If this is the case, it is possible that the benefits for one or two factories are not aligned with the benefits of the system as a whole. However, it could also be that the model is giving one of the multiple optimal solutions and the same total NPV can be achieved without any factory having less individual NPV in the water exchange setting than in the no water exchange setting.

Figures 61 and 62 present the freshwater consumption and water reuse behavior for the four combinations of scenarios and sub-scenarios. The fact of having a factory with a high capital investment helps to mitigate the effects of the water availability restriction. Independently of the collaboration between factories or not, the company with the very high investment capital can afford a water treatment plant, which is beneficial both them and the system.

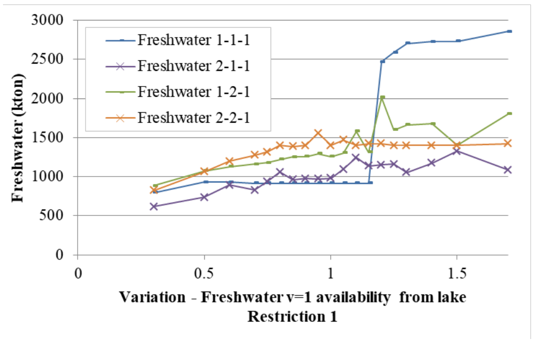


Figure 61: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. Freshwater.

Objective: 90% NPV - 10% Reuse Water

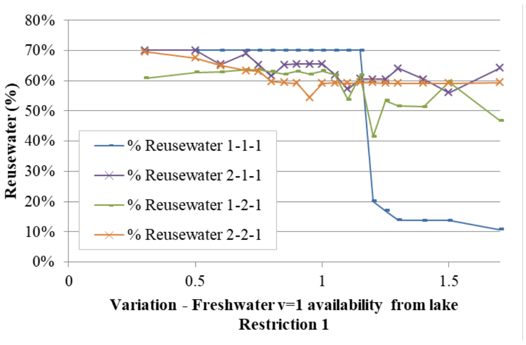


Figure 62: Sensitivity analysis: freshwater v=1 availability from lake variation. Restriction 1. Water reuse.

Objective: 90% NPV - 10% Reuse Water

These figures reiterate the fact that, independently from the restriction, it is always more profitable and more sustainable to collaborate for reusing water. In general, collaborating (scenario 2) mitigates the effects of the availability restrictions. If factories do not collaborate they are more affected by the restrictions and, in this case if the availability values are increased 20% (multiplicative factor 1.2) in scenario 1-1-1, it stops being profitable to invest on water treatment processes. However, the fact of having a strong player in the system, or a company that is willing to invest a lot in their expansion, can also mitigate these effects because they can take care of the sustainable objective almost on their own.

4.4 Results and Discussion

The results presented in this chapter focus on how the variation of some parameters and the variation of the weights in the objective function have an effect on the optimal NPV, freshwater consumption and water reuse. Some conclusions are repeated throughout all the experiments. One of the most important ones is the fact that allowing the possibility of collaboration and water sharing between factories is always beneficial for the system in terms of total NPV and water reuse in a sustainability mindset. Circumstances of stronger regulations or lower water availability must be given in order to be profitable to install a water treatment plant in each individual factory. However, it is more likely that sharing a water treatment facility between all factories in a close location is profitable. As expected, it is observed that factories with processes with less water requirements are less affected by parameter changes in the decision of investing in water treatment or not. In any case, they follow the same trends as factories with water-intensive processes.

The discharge price of water with quality class 3 to the lake has been analyzed and if no water is being reused, the higher the discharge price the lower the NPV is and vice versa. However if the decision is to invest in a water treatment plant, less water with quality class 3 is being discharged to the lake and therefore, the discharge price of water with quality class 3 to the lake has very little impact on the optimal NPV and water reuse. If the discharge price increases, it always comes to a point where it is more profitable to invest in a water treatment plant. After that point, the optimal solution is hardly unchanged by increments of the discharge price. NPV can remain practically the same if the investment cost of the water treatment plant only compensates for avoiding the cost of discharging water with quality class 3 to the lake. On the other hand, the weights on the objective function can strongly change the values of optimal NPV and water reuse.

Very similar results are obtained by analyzing the effect of the variations in the freshwater (quality class 1) purchase price from the lake. Small variations in the freshwater price have a small effect because the price of water is very low compared to all the other costs. However if the price increases, a price is always found for which investing on a water treatment plant is profitable and the freshwater consumption is reduced. The weights on the objective function are again very decisive for finding the optimal NPV and water reuse.

When some restrictions to the freshwater consumption from the lake are added, a higher effect on the optimal NPV and water reuse is observed. Also depending on weather the restriction is very strict or not, the weights on the objective function have a larger or a minor effect. If water availability is high enough, the need for a water treatment plant is lower. Then, depending on the weight for the importance of water reuse in the objective function, the optimal values can change a lot. In other words, the higher the importance of maximizing the NPV the lower the preference for installing water treatment processes and vice versa. However if not much water is available, independently of the weight of water reuse in the objective function, the optimal solution that maximizes NPV also includes high water reuse percentages. As expected, if the freshwater consumption is strongly restricted, the installation of water treatment processes is very profitable.

The effects of adding a restriction on the discharge of water of quality class 3 to the lake is very similar to the effects of increasing the cost of discharging this water class to the lake. If there is a very strict regulation, the installation of water treatment plants is optimal. Then, if the installation of a water treatment plant is profitable, this restriction doesn’t have an effect on the optimal NPV value anymore, because less water is being discharged. However the weight on the water reuse objective will be affected if the optimal solution is installing more or less water treatment processes, or sooner or later in time.

Variations on the demand upper bound of chemical 3 have also been tested. Chemical 3 represents the product that the company is selling in order to make profit. If the demand upper bound is high, the model is not affected by this parameter and the weight of NPV and water reuse will determine the optimal solution. However if the demand of this chemical is low, optimizing the production in order to make it more efficient becomes more important for increasing the NPV and this translates into avoiding the costs of discharging water of quality class 3 to the lake and favoring water reuse and the installation of water treatment processes.

If the price of chemical 3 is changed instead of the demand, the results are different. Since the demand is not changed, the higher the sale price of the main product, the more profit the company makes. Then, the higher the profit that the company makes, the less important water and sustainability are from an economic perspective and the weight of water reuse in the objective function will determine if the water treatment plant installation is encouraged or not. However, if the price is low, installing a water treatment plant might be profitable in order to reduce the water discharge costs, especially if companies are collaborating.

Variations in initial capacity have also been tested and in general the higher the initial capacity the higher the NPV and vice versa. For small initial capacities the investment on a water treatment plant is not profitable, because it is more beneficial to expand the production processes. However if the initial capacities are high, it would be more profitable to invest in water treatment processes, especially if the factories are collaborating. The weights on the objective function will have a big impact on the optimal solution.

Experiments with capacity expansion upper bound show that no water reuse is needed in case of maximizing the NPV with a weight of 100%, independently of the capacity expansion upper bound. Otherwise, the higher the capacity expansion upper bound, the higher the NPV, and the higher the weight of maximizing water reuse in the objective function, the lower the NPV. Depending on the importance given to water reuse, having higher or lower capacity upper bounds favors the expansion of water treatment processes more or less respectively.

The conclusions regarding the variation in the fixed investment cost are specific to this data set, where the cost of the production processes is higher than the cost of the water treatment processes. If the investment costs are very high it is preferred to invest in a water treatment plant, because the investment in expanding the current production processes would be more expensive and increasing water reuse can avoid some discharge costs. If the investment costs are very high it is also optimal to invest in a water treatment plant, because then it is profitable to expand all kinds of processes.

The last parameter variation is the operating cost. As expected, the lower the operating cost of the processes the higher the NPV is, and vice versa. In this experiment, the weight of water reuse in the objective function is the main parameter that can force the implementation of water treatment processes.

Regarding the profit distribution analysis, the total NPV achieved when the investment capital of the factories are different is higher than the total NPV achieved when their investment capital is the same. The explanation is that one factory with a very high investment capital is able to make a lot more expansions and a lot more profit than with a lower investment capital. This is also beneficial for the system in case of a water sharing scenario, even if other factories are making no expansions.

This model only contemplates a collaborative setting that aims to maximize the total NPV value. However, the individual benefit of all factories is neglected in case of a water sharing scenario. Since no weights have been defined for the NPV of each individual factory, multiple optimal solutions can exist, and as a result a random factory is selected each time for the installation of a water treatment plant. It would be interesting to adapt this model to a competitive setting, but this model is still useful in a cooperation setting where the objective is the benefit of the system as a whole.

The experiments presented in this chapter focus on the two objectives in the objective function: NPV and water reuse. However, with this model the optimal values of the following variables are also obtained: the total capacity of the process i in the year t (Q_{it}), the capacity expansion of the plant of process i which is installed in the year t (QE_{it}), the operating level of process i during the year t (W_{it}), the amount of chemical j consumed or produced by process i during the year t (I_{ijt} and O_{ijt}), the amount of water of quality v consumed and produced by process i during the year t (MWI_{ivt} and MWO_{ivt}), the amount of product j purchased from and sold to market l by factory f during the year t (P_{fjlt} and S_{fjlt}) and the amount of water of quality v bought from and discharged to the source or sink r by factory f during the year t (MWP_{fvrt} and MWS_{fvrt}). With the variable QE_{it} the optimal year to install the water treatment plant is also obtained. The optimal values of all these variables constitute the strategic capacity expansion planning.

5 Conclusion

Global water use grows steadily at a rate of about 1% per year (UN Water, 2018) and this will be a big problem for the industry, since it is the second largest user of water with a consumption of 20% of the freshwater worldwide (UNEP, 2008). For this reason, water scarcity becomes an imminent threat, particularly to process industries as many processes are water-intensive and their water demand is increasingly high. However, if these companies made an investment in making their processes more water efficient and reducing their waste, they could turn an environmental burden into a resource and therefore avoid serious financial and environmental consequences.

With this background, the need for including water management strategies in the strategic capacity planning of process industries, including the goal of minimizing freshwater use and wastewater generation, has become a necessity. There is evidence that increasing the symbiotic relationship between plants can highly contribute to a profitable and sustainable industrial development. Consequently, a multi-factory and multi-period capacity expansion mixed integer linear program (MILP) model that contemplates the possibilities of internal water treatment and water sharing between plants, has been presented. This model also has a multi-objective function, allowing a trade-off between maximizing the sum of the net present value of all factories and maximizing water reuse, in a collaborative setting and over a given time horizon.

The developed MILP model is based on the Sahinidis et al. (1989) model for long range planning in the chemical industry and can be used to determine the optimal value of the following variables: capacity expansion and shut-down policy for existing processes; selection of new processes, including water treatment, and their capacity expansion policy; production profiles; sales and purchases of chemicals at each time period; and water consumption and discharge from all sources/to all water sinks.

This model is tested in a theoretic case with three identical companies which have the possibility of installing a water treatment process in every factory during the next ten years and want to plan their capacity expansion with a collaborative mindset. The effect of the variation of several water-related and production-related parameters in the optimal expansion decision has been investigated as well as the effect of the importance of the goals in the multi-objective function. One of the main conclusions obtained is that water sharing between players is a good opportunity to mitigate the impact of water scarcity. Collaboration between factories is always beneficial for the system in terms of total NPV and water reuse. Furthermore, it is likely that sharing a water treatment facility between all factories in a close location is more profitable than installing a water treatment plant in each individual factory.

The experiments show that, in difficult conditions of low freshwater availability, strict freshwater consumption/water discharge restrictions, or high freshwater purchase/discharge costs, the installation of a water treatment plant is very profitable, independently of the weights of maximizing the NPV and water reuse on the objective function. On the other hand, the higher the water reuse the lower the total NPV. Therefore, if there are no sustainability penalties or regulations, the investment in water treatment processes may not be profitable. However, especially in a water sharing setting and if conditions are not very extreme, just to have a 10% weight in the water reuse objective might only mean a decrease on the total NPV of 1-4% but an increment in the total water reuse of 40-60%. In the long run this is very beneficial not only for the system but also for the environment.

The profit distributions in the presented experiments have been analyzed and this model only considers a collaborative setting where only the general benefit is prioritized. Nevertheless, the model is very valid to observe the effect of some parameters on the optimal capacity expansion planning. The next step to continue with this investigation could be to adapt the model to a competitive setting, where maximizing the individual NPV of the players is also considered and the individual interests are contemplated. This could lead to some game theory experiments and the search for the Nash equilibrium.

To conclude, the importance of confronting the water scarcity crisis must be remarked. Furthermore, the multiple benefits of collaboration and water sharing between factories, for approaching this problem, have been confirmed and explained. All in all, this project encourages the integration of water consideration to the industries’ strategic planning through the use of enhanced MILP production models, such as a capacity expansion model.

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Appendices

The following graphs could also have been presented in section 4.2.:

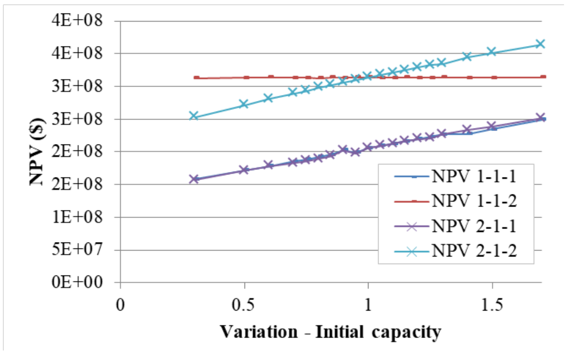


Figure 63: Sensitivity analysis: initial capacity variation. NPV. Objective: 90% NPV - 10% Reuse Water

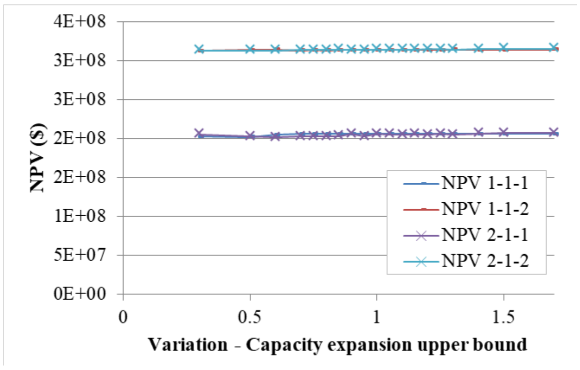


Figure 64: Sensitivity analysis: initial capacity variation. NPV. Objective: 90% NPV - 10% Reuse Water

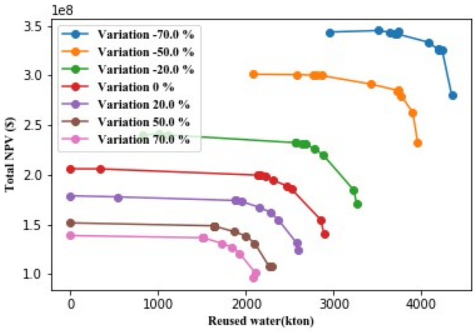


Figure 65: Variable investment cost variation. Scenario 1-1-1

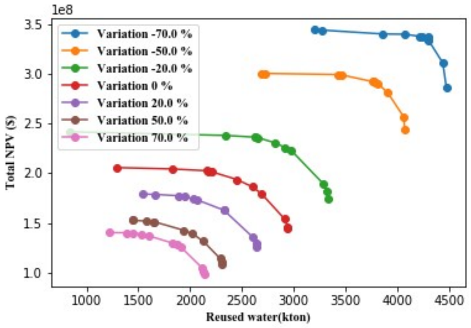
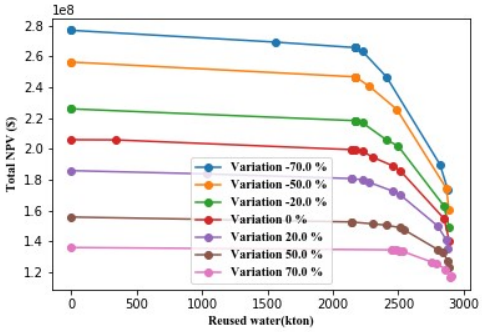


Figure 66: Variable investment cost variation. Scenario 2-1-1

The following parameters have also been varied:

- Variation on the chemical purchase prices:



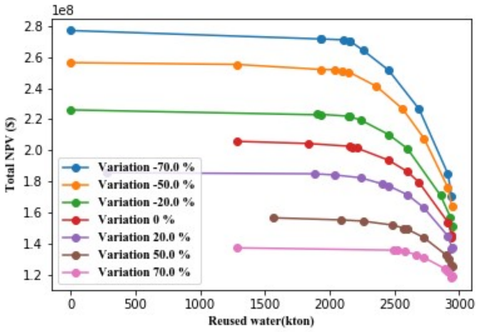


Figure 67: Sensitivity and trade-off analysis: chemicals 1 and 2 purchase price variation. Scenario 1-1-1

Figure 68: Sensitivity and trade-off analysis: chemicals 1 and 2 purchase price variation. Scenario 2-1-1

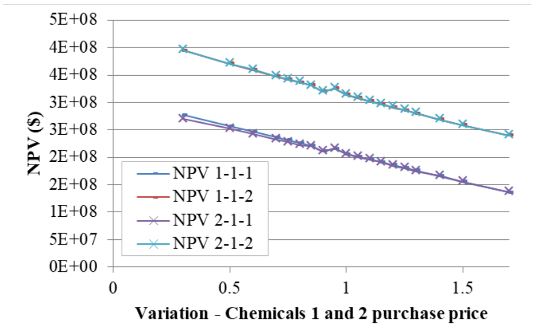
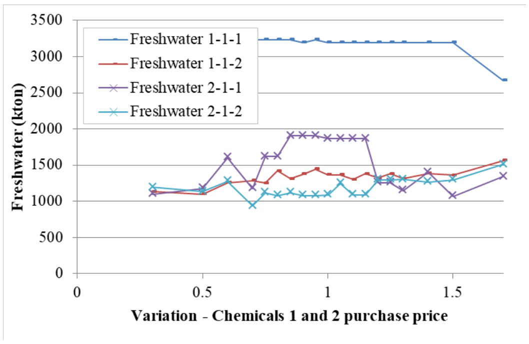


Figure 69: Sensitivity analysis: chemicals 1 and 2 purchase price variation. NPV. Objective: 90% NPV - 10% Reuse Water



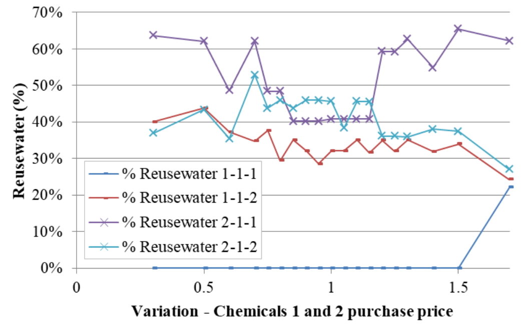
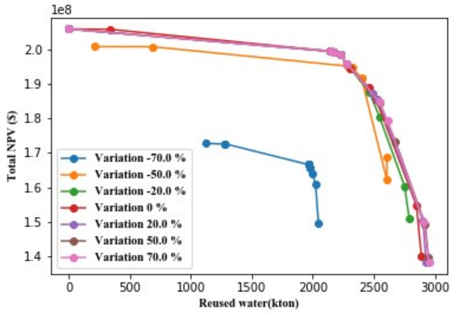


Figure 70: Sensitivity analysis: chemicals 1 and 2 purchase price variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

Figure 71: Sensitivity analysis: chemicals 1 and 2 purchase price variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

- Variation on the chemical availabilities:



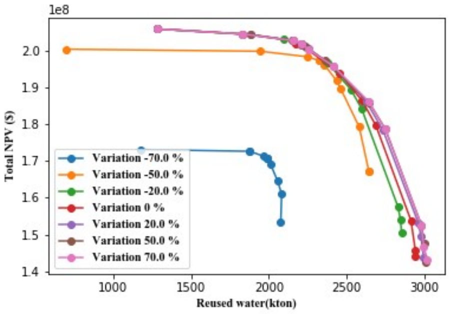


Figure 72: Sensitivity and trade-off analysis: chemicals 1 and 2 availabilities variation. Scenario 1-1-1

Figure 73: Sensitivity and trade-off analysis: chemicals 1 and 2 availabilities variation. Scenario 2-1-1

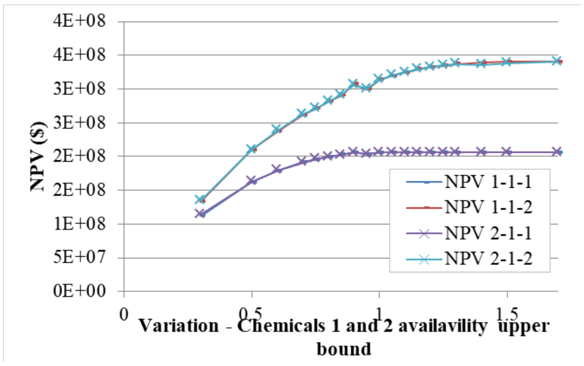
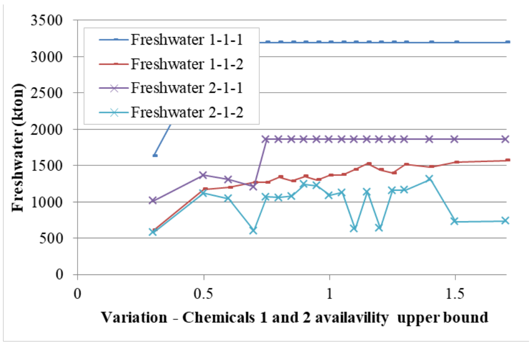


Figure 74: Sensitivity analysis: chemicals 1 and 2 availabilities variation. NPV. Objective: 90% NPV - 10% Reuse Water



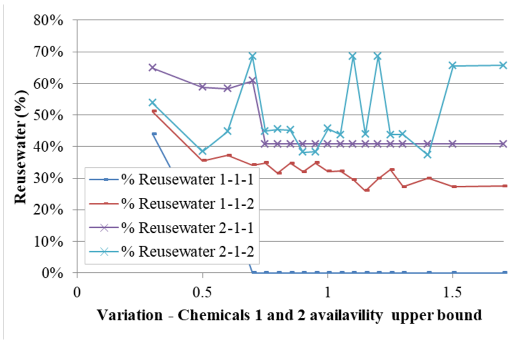


Figure 75: Sensitivity analysis: chemicals 1 and 2 availabilities variation. Freshwater. Objective: 90% NPV - 10% Reuse Water

Figure 76: Sensitivity analysis: chemicals 1 and 2 availabilities variation. Water reuse. Objective: 90% NPV - 10% Reuse Water

Ehrenwörtliche Erklärung

Ich erkläre hiermit ehrenwörtlich, dass ich die vorliegende Arbeit selbständig angefertigt habe. Die aus fremden Quellen direkt und indirekt übernommenen Gedanken sind als solche kenntlich gemacht.

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Die Arbeit wurde weder einer anderen Prüfungsbehörde vorgelegt noch veröffentlicht.

München, den 11.07.2018

Paloma Aparicio Escuder