Optimization of industrial water networks. Development of generic design tools and application in a real industrial site

Keivan Nemati-Amirkolaii

Thèse de doctorat

NNT : 2021UPASB036

université PARIS-SACLAY

Optimization of industrial water networks. Development of generic design tools and application in a real industrial site.

Optimisation des réseaux d'eau industriels. Développement d'outils de conception générique et application à un site industriel.

Thèse de doctorat de l'université Paris-Saclay

École doctorale n°581 Agriculture, alimentation, biologie, environnement et santé (ABIES)
Spécialité de doctorat : Génie des procédés
Unité de recherche : Université Paris-Saclay, INRAE, AgroParisTech, UMR SayFood, 91300, Massy, France
Référent : AgroParisTech

Thèse présentée et soutenue à Paris-Saclay, le 31/08/2021, par

Keivan NEMATI-AMIRKOLAII

Composition du Jury

Ludovic MONTASTRUC Professeur, Toulouse INP	Président
Antoine COLLIGNAN Professeur, Institut Agro - Montpellier SupAgro	Rapporteur & Examinateur
Patricia ARLABOSSE Professeure, IMT Mines Albi	Rapporteur & Examinatrice
Assaad ZOUGHAIB Professeur, Mines ParisTech	Examinateur

Direction de la thèse

Marie-Laure LAMELOISE Professeure, AgroParisTech	Directrice de thèse
Hedi ROMDHANA Maître de Conférences, AgroParisTech	Co-Encadrant & Examinateur

To my beloved wife and family,

and all those who have supported me so far.

"Ever tried. Ever failed. No matter.

Try again. Fail again. Fail better."

Samuel Beckett

Table of Contents

Contents

List of Figures

List of Tables

List of Abbreviations

Roman uppercase letters		
BOD	Biochemical Oxygen Demand	
Brix	sugar content	°Bx
C	cold stream/concentration	
COD	Chemical Oxygen Demand	
CP	Heat capacity flowrate	kW/K
C_p	Specific heat	j/kg/K
EC	electrical conductivity	S/m
H2S	Hydrogen Sulfide	
SS	Suspended Solids	
GA	Genetic Algorithm	
GAMS	General Algebraic Modeling System	
H	Hot stream	
ISO 14000	Environmental standard management	
ISO 50001	Energy standard management	
LP	Linear Programing	
MATLAB	numerical computing environment	
MILP	Mix Integer Linear Programing	
MINLP	Mix Integer Non-Linear Programing	
MSA	Mass Separating Agents	
NLP	Non-Linear Programing	
NSGA-II	Non-dominated Sorting Genetic Algorithm II	
PSO	Particle Swarm Optimization	
TOPSIS	Modified Technique for Order of Preference by Similarity to Ideal Solution	
Python	Programming language	
OG	Oils and Grease	
T	Temperature	°C
TDS	Total Dissolved Solids	
TOC	Total Organic Carbon	
TSS	Total Suspend Solid	
AFI	Agro-Food Industry	
WPA	Water Pinch Analysis	
pH	Acidity or Basicity	
ppm	Part Per Million	
BOD5	5 Days Biological Oxygen Demand	
R2A	Reasoner's 2A Agar	
DR	Dry Residues	
NF	Nanofiltration Stage	
RO	Reverse Osmosis	
AOX	Absorbable Organic Halides	
HP	Hardness Properties	
POME	Palm Oil Mill Effluent	
HC	Hydrocarbon	
WIN	Water Use Index	
GEC	Global Equivalent Cost	
EIN	Environmental Performance Index	
TAC	Total Annualized Cost	

ATEX	ATmospheres EXplosible	
AFI	Agro Food Industry	
WWTP	Wastewater Treatment Plant	
WAN	Water Allocation Network	
HEN	Heat Exchanger Network	
MEN	Mass Exchanger Network	
MSA	Mass Separating Agents	
LCA	Life Cycle Assessment	
FU	Functional Unit	
WEUI	Water And Energy Use Indicator	
IPPC	Integrated Pollution Prevention and Control	
HACCP	Hazard Analysis Critical Control Point	
CRF	Capital Recovery Factor	
PCP	Parallel Coordinate Plots	
Emergy	Embodied Solar Energy	
U	Unit	
Roman lowercase letters		
$\dot{m}$	Mass Flowrate of Water	m^3/h
F_i	Freshwater supply from a water source to process (i)	m^3/h
R_{ij}	Water-reuse from the process (i) to process (j)	m^3/h
W_i	Wastewater release from the process (i)	m^3/h
m_i	Mass Flowrate of Water for process i	m^3/h
$m_{i,in}$	Inlet Mass Flowrate of Water for process i	m^3/h
$m_{i,out}$	Outlet Mass Flowrate of Water for process i	m^3/h
Q_{ki}	Mass load of the contaminant (k) from side to side of the process (i)	kg/h
C_{in}	Inlet Concentration	ppm
C_{out}	Outlet Concentration	ppm
$C_{ki,in}$	Inlet Concentrations of contaminant (k) at the boundaries of the process (i)	ppm
$C_{ki,out}$	Outlet Concentrations of contaminant (k) at the boundaries of the process (i)	ppm
$C_{ki,in}^{max}$	Maximum Possible Inlet Concentration	ppm
$C_{ki,out}^{min}$	Maximum Possible Outlet Concentration	ppm
C_{eq}	Equipment Cost	$k€$
C_{op}	Operating Cost	$k€$
IR	The Interest Rate	
L_f	Lifetime Expressed	$year$
C_m	Membrane Unit Cost	$k€/m^2$
C_p	Pump Unit Cost	$k€/kWh$
E_p	Pump Power	kWh
C_e	Cost of Electricity	$€/kWh$
C_{rc}	Membrane Replacement And Cleaning Cost	$k€/m^2/year$
t_y	Annual Operating Time	h/year
F_r	Flowrate of Reused Water	m^3/h
d	Fiber Diameter	m
L	Fiber Length	m
u	Water Velocity Through the Fiber	m/s
A	Water Permeability	$m/s/bar$
ρ	Water Density Expressed	kg/m^3
S	Membrane Area	
Greek letters		
ΔH	Latent Heat	kJ/kg

ΔP_m	Membrane Pressure	bar
ΔT	Temperature Difference	°C
Subscripts		
in	Input	
out	Output	
min	Minimum	
max	Maximum	
i , j	Processes	
k	Contaminants	
s	Supply	
t	Target	
w	Water	

General introduction

Freshwater is the high-priority source for human beings to survive. It's necessary to use it reasonably and try to save the rest of the freshwater sources as much as possible. The explosion of the population and economic development leads to consuming more water recourses. Based on the works of (Alcamo et al., 2003) and (Flörke et al., 2013) approximately, freshwater consummation becomes six-time more than in 1900. The world's total freshwater demand (agriculture, industry, and municipal uses) had a smooth trend before 1950. From 1950 up to 2000, the trend had increased sharply. After the year 2000, it seems that the growth rate is slowing down, but water scarcity remains a serious problem. There is a proportional percentage between agriculture, industry, and municipal sectors (World Dev. Rep. 2008, 2007). Globally around 70% of freshwater goes to the agricultural sector, the industrial sector uses around 19% of total freshwater withdrawals in the world and the rest goes to municipal uses (Ritchie and Roser, 2017).

Sustainable water management is a priority for all industries, especially the food sector, as a vital sector of human food security. The use of efficient water purification equipment is highly recommended by the European IPPC directive (96/61/CE). Nevertheless, the annual cost of this equipment can be around 2.5-3.5 million euros (Jiri Klemes et al., 2010). Therefore, it is essential to find possibilities to minimize water demand and contaminant load before integrating purification equipment using a set of methods such as mass integration tools. The mass integration techniques are a global and systematic approach to minimize water consumption and discharges, especially for the most energy-intensive and water-consuming factories. As one of the mass integration techniques, the water pinch method consists of identifying reuse streams throughout the water network. Economically, it is interesting to reduce the required investments to increase the plant's production rhythm by saving water and by reducing the effluent to be treated. Such analysis can be applied to most processes in the food industries. The initial graphical development of the water pinch method is more suitable for small and simple cases. In reality, most industries involve complex water networks with several pollutants. In this case, it is difficult to deal with the problem with traditional graphics approaches. To manage this problem, numerical tools inspired by the logic of the pinch method are proposed to deal with real cases. In addition, the development of multi-criteria optimization methods for water systems where many pollutants are involved seems necessary.

A new generic method for water/wastewater minimization and water network design has been developed. It's suitable for food processes and able to handle either single or multi-contaminant systems. Considering several pollutants in the water network requires the use of mathematical tools such as multi-objective optimization. This work ultimately initiates a generic methodology and demonstrates its feasibility and benefits by applying it to the real case study of the food industry. The resolution of the mathematical model is implemented in *Python®* software. As part of this thesis, we have developed two optimization tools: *(1)* manual optimization using manual tradeoffs between all possible reuse streams and *(2)* automatic optimization using multi-objective optimization algorithms like evolutionary algorithms. Both of these methods are based on water pinch logic but implemented in numerical tools. Each of these approaches follows different instructions that lead to different ways of use. The developments within this thesis work are and will be the subject of publications in international journals. All of these works are presented in detail in this thesis manuscript, in the order that is explained in the following paragraphs.

This thesis work is part of a research program entitled ***"Minimizing water consumption in food industries by developing an integrated approach combining Water Footprint and Pinch analyses"****. This project is supported by the* ***French Research Agency (ANR)*** *and coordinated* ***by AgroParisTech*** *and includes a research institute* ***(IRSTEA)****, an engineering software company* ***(ProSim)*** *and five engineering centers* ***(ACTALIA, ITERG, CTCPA, IFV and CRITT)****.*

In this thesis, there are three main chapters in the following order. Firstly, *State of the art* contains a general bibliographic analysis on mass integration techniques and pinch method variation (minimization of different sources: energy, raw materials, fluids including water). Deep bibliographic analysis was performed on the water pinch method. Some numerical examples about water pinch implementation and other pinch variations are also presented in this chapter.

The second chapter deals with the development of two original optimization methods. In this chapter, manual and numerical optimization tools based on water pinch analysis are proposed. Classical pinch methodology can help to target minimum required freshwater, and the re-design the mono-contaminant water networks. For this reason, we have combined the classic approach with advanced numerical methods. This chapter includes two subsections. Each sub-section is the subject of a scientific publication. A user-friendly tool that helps to find the reuse possibilities in the processing industry has been proposed in the first sub-section. This tool aims to minimize the total freshwater of the network in both single and multi-contaminant systems. This method provides the optimized design of the network by using the tradeoff between the maximum possible contaminants concentrations, the maximum water reuse, and the minimum mass transfer of pollutants within each process. All the steps of this optimization are managed manually by the user and numerically assisted by the tool. A multi-contaminant case study from the literature was used to demonstrate the use of the tool. In the second section of the second chapter, an optimization tool based on NSGA-II was developed to optimize industrial water networks. The designed approach targets the minimum freshwater for different mono or multi-contaminants systems using the maximum possibility of reuse. Two case studies, both mono, and multi contaminant selected and tested to show the efficiency of the proposed tool.

The third and last chapter concerns the *industrial application of the two methods explained in chapter 2*. This part focused on the industrial application of the optimization tools by adding some new contributions like cost analysis. The real case study was applied to a French edible oil company. This chapter includes two subsections. Each sub-section will be the subject of a scientific publication. Both methodologies (i.e., manual tradeoffs, and NSGA-II based optimization algorithms) have been applied with the same dataset. Furthermore, an additional discussion about other expected and unexpected decision-making parameters has been proposed. Finally, the results are presented and discussed in detail for each method.

A short introduction is provided at the beginning of each chapter. In addition, a French summary related to each published or submitted and the under-submission article has been presented. At the end of the current thesis, insights and summaries of results are presented to be useful for practitioners. Further research and outlooks are provided as well.

Chapter 1: State of art - Mass integration tools and Pinch methods

As discussed in the previous section; It's vital to reduce the amount of industrial freshwater consummation and effluents in a cost-efficient and optimum way. By considering that, the necessity of using mass integration tools as an efficient method in different types of industries is undeniable. To go in deep and know more about the different applications of mass integration tools in different types of industries (especially the food sector) a survey review has been proposed. This part of the thesis belongs to a comprehensive state of the art about different variations of pinch method and mass integration tools. Besides, the main focus is on water pinch analysis and its applications in food industries. Benefits, challenges, R&D needs, and future research potential of the water pinch method have been discussed in different sections of this chapter. This chapter is built based on the article entitled*" Pinch Methods for Efficient Use of Water in Food Industry: A Survey Review"*. This article was already *accepted (2019)* in the journal of "*Sustainability*" as the first outcome of this thesis. In this chapter; firstly, a short French summary of the current article has been developed. This summary contains two-part: the main contents and results, and, the order of topics within the article. Secondly, the original text of the published article is embedded within the chapter.

1.1 Méthodes de pincement pour une utilisation efficace de l'eau dans l'industrie alimentaire : Analyse bibliographique

Mots-clés : Intégration des procédés ; Analyse Pincement ; Industrie alimentaire ; Eau

La mise en œuvre de pratiques d'une gestion durable, de recyclage et la réutilisation de l'eau, sont essentielles pour minimiser les coûts de production et l'impact environnemental de l'industrie alimentaire. La consommation d'eau et la production d'eaux usées dans l'industrie alimentaire pourraient être réduites en remplaçant les technologies existantes par de nouvelles. Cependant, la mise en place d'équipements innovants nécessitera beaucoup d'investissements, de temps de recherche et de développement. En outre, compte tenu du faible prix de l'eau, l'investissement dans des équipements de purification est difficilement justifiable d'un point de vue financier. L'optimisation des réseaux d'eau par l'analyse Pincement est une opportunité d'augmenter l'efficacité de l'utilisation de l'eau dans l'industrie alimentaire avec des coûts d'investissement réduits. L'analyse du pincement appliquée à l'eau permet une réduction de la consommation d'eau allant de 20 à 40% avec un coût réduit. Son développement et sa disponibilité pour l'industrie alimentaire devraient encourager les équipementiers et industriels à adopter cette approche et réaliser des économies d'eau. L'idée clé pour minimiser l'eau avec l'analyse Pincement est d'identifier les flux d'eau qui peuvent être réutilisés dans une opération pour laquelle la qualité de l'eau est acceptable. Les besoins minimaux en eau peuvent être ciblés à l'aide d'outils graphiques ou de méthodes de conception automatisées. Les méthodes graphiques fournissent un aperçu conceptuel (théorique) du problème et mettent en évidence les conceptions appropriées. Cependant, lorsque d'autres composants sont ajoutés au problème et que le besoin d'optimisation des coûts se fait sentir, ces problèmes deviennent trop compliqués pour ces procédures graphiques. L'extraction des données est l'étape la plus critique pour réaliser une analyse optimale. La plupart des méthodes discutées dans la littérature sont basées sur des systèmes d'eau à un seul contaminant. La prise en compte d'un seul contaminant de l'eau et du nombre limité de sources d'eau dans un cadre simple permet de présenter le fonctionnement de l'analyse du pincement de l'eau, alors que de nombreux contaminants devraient être pris en compte. Dans l'industrie alimentaire, il est presque impossible d'inclure tous les composants qui influencent la chimie de l'eau, l'aspect microbiologique et la qualité du produit alimentaire. Dans certains secteurs de l'industrie alimentaire, il est courant de sélectionner des indicateurs de contamination représentatifs. L'application de la méthode graphique pour les systèmes d'eau multi-contaminants n'est pas facile à utiliser. Pour cela, le développement d'outils numériques semble une étape cruciale pour le développement de l'analyse du pincement et son application dans l'industrie alimentaire. La programmation mathématique semble mieux adaptée pour résoudre des problèmes complexes.

Le travail actuel a passé en revue la littérature complète sur les différentes variantes de l'analyse par pincement. La méthode du pincement de l'eau a fait l'objet d'une discussion approfondie et certaines données pertinentes concernant le processus d'utilisation de l'eau et les indicateurs de polluants ont été examinées en mettant l'accent sur le secteur de l'industrie alimentaire. Dans les sections suivantes, différentes méthodes de pincement comme l'analyse du pincement énergétique, la réduction des émissions de CO2, l'analyse du pincement de l'hydrogène ont été expliquées en détail à l'aide d'exemples pratiques afin de donner une vision claire de leur déploiement. Dans les sections suivantes, des explications sur de nouvelles variantes du pincement comme l'analyse du pincement de l'oxygène, le pincement de l'énergie, le budget-temps-revenu ont été données. L'accent ayant été mis sur les analyses du pincement de l'eau, une section complète sur cette méthode est fournie. Dans cette section, différents articles dans ce domaine de recherche ont été examinés et des exemples pratiques du pincement de l'eau ont également été expliqués. Enfin, l'utilisation de l'analyse du pincement de l'eau dans l'industrie alimentaire est présentée. Certaines difficultés sont dues à la diversité des utilisations de l'eau dans l'industrie alimentaire, aux contraintes liées à la qualité de l'eau utilisée et aux diverses substances rejetées. Les différents aspects comme la question économique ont été considérées.

The First Article General Text

1.2 Pinch methods for efficient use of water in food industry: A survey review

1.2.1 Abstract

The implementation of sustainable water management practices, through the recycling and reuse of water, is essential in terms of minimizing production costs and the environmental impact of the food industry. This problem goes beyond the classical audit and housekeeping practices through developing a systemic water-using reduction strategy. The implementation of such an approach needs R&D development, especially for the food industry, where there is a lack of knowledge on (a) process integration and (b) data on the pollutant indicators or (c) volumes of water used and discharged at specific steps of the food processing line. Since energy pinch analysis emerged, different variations of pinch methods have been developed. As a variation of pinch, Water pinch analysis is a global and systematic approach to minimize water consumption and discharges, especially for the most energy-intensive and water-consuming factories. Based on the nature of the food industry, the real systems are

complex, multi-source multi-contaminant systems, the problem should be well-formulated, including mathematical constraints (inequalities thresholds). Current work has reviewed comprehensive literature about different variations of pinch analysis. To continue, the water pinch method is deeply discussed and some relevant data concerning the water using process and pollutant indicators have been reviewed with emphasis on the food industry sector.

Keywords: process integration; pinch analysis; food industry; water

1.2.2 Introduction

Setting energy targets is the first fundamental concept of pinch analysis (B Linnhoff, J Flower, 1978). This approach is based on the optimization of resources and tries to allocate limited sources to the demands in the best way. Based on this definition, the method has been developed for different applications, especially for minimizing water consumption. Further developments have resulted in methods for minimizing water use (Wang and Smith, 1994) and various industrial utilities like hydrogen, oxygen, etc.

Water pinch is a global and systematic approach to minimize freshwater and wastewater, especially for the most energy-intensive and water-consuming factories. Wang and Smith (1994) showed that mass pinch analysis appears as a particular case of mass integration, especially to minimize the consumption of water or any other fluid. Later, El-Halwagi, F. Gabriel, and Harell (2003) and Prakash and Shenoy (2005) illustrated a systematic approach to optimize water networks of the industrial site by applying analogy with thermal pinch analysis. This approach provides results just as spectacular as energy analysis to optimize water consumption. Almató et al. (1997) identified potential water savings of 63–72% in a fruit juice production industry. The work of Thevendiraraj et al. (2003) and Tokos and Novak Pintarič (2009) identified potential water savings of 30% respectively in a brewery workshop and a citrus juice production workshop. Recently, the parallel application of water pinch and mathematical optimization was considered as well, which find a water savings of 30% in a corn refinery (Bavar et al., 2018).

In the food industry, energy efficiency has become more than ever a priority to improve the environmental and economic performance of industrial sites. The environmental and economic regulations impose a variety of measures in the food industry. Water resources must be saved as much as possible, especially for certain regions where water is becoming increasingly scarce because of climatic hazards due to human activities and the denaturation of freshwater sources. On the other hand, the new regulations require more constraints to reduce and/or optimize the discharges loaded with organics like carbon, nitrogen, phosphorus, acid, etc. The new European rules aim for zero discharges into polluted water (2455/2001/EC and 2000/60/EC). Faced with these increasingly serious issues, the food industry has to go beyond simple measures (best practices) and employ more efficient methods. The integration of high-performance equipment for water purification is strongly recommended by the European IPPC Directive (96/61/EC). However, the annual cost of these techniques can amount to 2.5–3.5 million euros (Jiri Klemes et al., 2010). It is therefore essential to identify the possibilities of minimizing the consumption of water and the polluting load before integrating the purification equipment by using mass integration tools.

Despite the development of Pinch Mass Analysis in many studies, this technique still occupies a small place in the industry, particularly in the food sector. As mentioned before, different variations of pinch have been developed after emerging off the energy pinch concept. In this work, all different variations of the pinch method have been reviewed with the main focus on water pinch analysis. In the following sections, at first different pinch methods like energy pinch analysis, CO_2 emission targeting, hydrogen pinch analysis have been explained in detail by using practical examples to make a clear vision of their functions and in the next sections, some explanation about new variations of a pinch like oxygen pinch analysis, emergy pinch, budget-time-income have been explained. As an important part of this study, the main focus was on water pinch analyses, so a comprehensive section about this method was presented. In this section, different articles in this area of research have been reviewed and practical examples of water pinch explained as well. In the end, the utilization of water pinch analysis in the food industry was presented. Some difficulties are due to the diversity of uses of water in the food industry, the constraints related to the quality of the water used, and the various substances released. The different aspects of view like economic issue have been considered.

1.2.3 Key concept of Pinch analysis

The challenges of developing the pinch method for the optimization of primary resources (e.g., energy, water, raw material), are significant and involve intensive efforts in many application areas. The purpose of this subsection is to summarize the main research and the significant results in the area of pinch analysis.

Regarding literature, pinch analysis was initially developed for heat integration (Linnhoff and Flower, 1978). By analogy with the thermal pinch, further applications are developed in various fields, especially, mass integration (Wang and Smith, 1994), design and management of hydrogen networks (Alves, 1999), minimization of oxygen consumption of the microorganisms used for waste degradation (Zhelev and Ntlhakana, 1999), emergy analysis (Odum, 1983) (Zhelev and Ridolfi, 2006), CO_2 emission targeting (Linnhoff and Dhole, 1993) (Tan and Foo, 2007), and supply chain management (Zhelev, 2005). Development in energy integration, territorial energy plan, and hydrogen network management are addressed in detail. Further development for emergy, oxygen pinch, and chain management are shortly mentioned. In the end, as the main review, the mass integration (water pinch) addressed in detail and discussed different aspects of this approach in different kinds of food industries like brewing, sugar, and citrus.

1.2.3.1 Energy Pinch analysis

Energy pinch analysis was developed to optimize heat exchanger networks HENs. (Linnhoff and Hindmarsh, 1983) developed the basic principle of minimization of energy utilities by optimizing the coupling between hot and cold streams. El-Halwagi and Manousiouthakis (1990) were succeeded to identify a useful analogy between the synthesis of two networks of HENs and mass exchanger network (MENs) that are heat exchanger and mass exchanger networks, respectively. The authors explored a novel algorithm-based procedure to synthesize the MENs automatically. It was formulated based on mixed-integer linear programming (MILP). In turn, MILP generated MENs that characterized the minimum number of heat exchangers, exposed to the least amount of mass separating agents (MSA) costs. The lean stream utilized in a unit operation such as a distillation column or liquid extraction is entitled MSA. Targeting the minimum number of units does not fundamentally cause the least cost. This statement results from the graphical technique reported by Hallale and Fraser (1998). Based on the minimum number of trays, this technique was then examined as a new route for capital cost targeting for MENs. To obtain the closely approached targets, a new design method was also developed (Hallale and Fraser, 1998) (Hallale and Fraser, 2000). In recent years, different methods have been developed to improve HEN efficiency. One of the widely discussed subjects is HEN network retrofitting. Different methods like retrofitting without considering additional heat transfer area (Akpomiemie and Smith, 2015), area ratio approach (Akpomiemie and Smith, 2016), cost-effective strategy (Akpomiemie and Smith, 2018), intensified heat transfer (Wang et al., 2012), and retrofitting with fix structure (Jiang et al., 2014) have been applied to improve these networks function. A new graphical method is also developed by Gadalla (2015) to handle both energy integration and network retrofitting. To handle both continuous and discrete variables simultaneously in HEN retrofitting and also increase the efficiency of calculation IDE (integrated differential evolution) method was developed (Zhang and Rangaiah, 2013).

Using the targets inferred from pinch analysis, the proper designs in the view of thermal efficiency were achievable. The retrofitting of the network structure is required by the relocation of an existing heat exchanger to a new duty or the addition of a new exchanger or change of the stream. Composite curves were constructed from hot and cold stream data at which the targeting was acquired. Consequently, the graphical representation of the mass and heat balance of the system is presented through plotting temperature versus enthalpy of the process streams. While the minimum hot and cold utility targets are acquired, the pinch point is discovered when the two composite curves are fitted together. To illustrate the energy pinch procedure, hypothetical data was gathered in **Table 1** with a set of hot and cold streams. Each stream is characterized in term of supply temperature T_s, target temperature T_t and heat capacity flowrate CP assumed to be constant **(Equation 1)**:

$$\mathrm{CP(kW/K)} = \dot{\mathrm{m}}\mathrm{(kg/s)} \times \begin{cases} \mathrm{C_p(kJ/kg/K)} & \text{for stream requiring heating or cooling} \\ \frac{\Delta \mathrm{H(kJ/kg)}}{1\ \mathrm{K}} & \text{for phase} - \text{changing stream} \end{cases} \quad (1)$$

Table 1. Data set for energy pinch analysis

	Hot Streams				Cold Streams		
	$T_s\ (°C)$	$T_t\ (°C)$	$CP\ (kW/°C)$		$T_s\ (°C)$	$T_t\ (°C)$	$CP\ (kW/°C)$
H_1	200	100	20	C_1	80	120	80
H_2	150	60	40	C_2	50	220	15

With, ṁ is the mass flow rate, C_p is the specific heat and ΔH is the latent heat of phase change (i.e., condensing or boiling). To visualize the heat exchange of each stream, a temperature-enthalpy diagram can be used. The individual representations of hot and cold streams are shown in **Figures 1** and **2**, respectively. Since the arbitrary choice of the enthalpy reference, a given stream can be plotted anywhere in the enthalpy axis. The streams are initially drawn by selecting enthalpy references at 60 °C and 50 °C, respectively for hot and cold streams. To provide useful information about the energy coupling between the hot and cold streams, a single composite of all hot streams and a single composite of all cold streams can be plotted in the temperature-enthalpy diagram, and handled in just the same way as two streams. To draw the composite curve, the streams existing over any given temperature range are grouped by adding their heat capacity flowrates. The composite curves are shown in **Figure 3**. The cold composite is shown shifted on the $x-$ axis relative to the hot composite. The overlap between the composite curves represents the maximum amount of energy recovery within the process (4850 kW). A minimum temperature difference ΔT_{min} (in this case, 10 °C) is respected. Further shifting implies larger energy recovery and then a larger heat exchanger. The overshoot at the bottom of the hot composite and for which no cold streams are available represents the minimum cooling utility (750 kW external cooling). The overshoot at the top of the cold composite and for which no hot streams are available represents the minimum heating utility (900 kW external heating). The selection of the minimum temperature difference is of great practical importance. Generally, the higher values of ΔT_{min} give higher hot and cold utility requirements and inversely. Therefore, targeting procedure is essential to identify the most economical ways of maximizing heat recovery and of minimizing the demand for external utilities

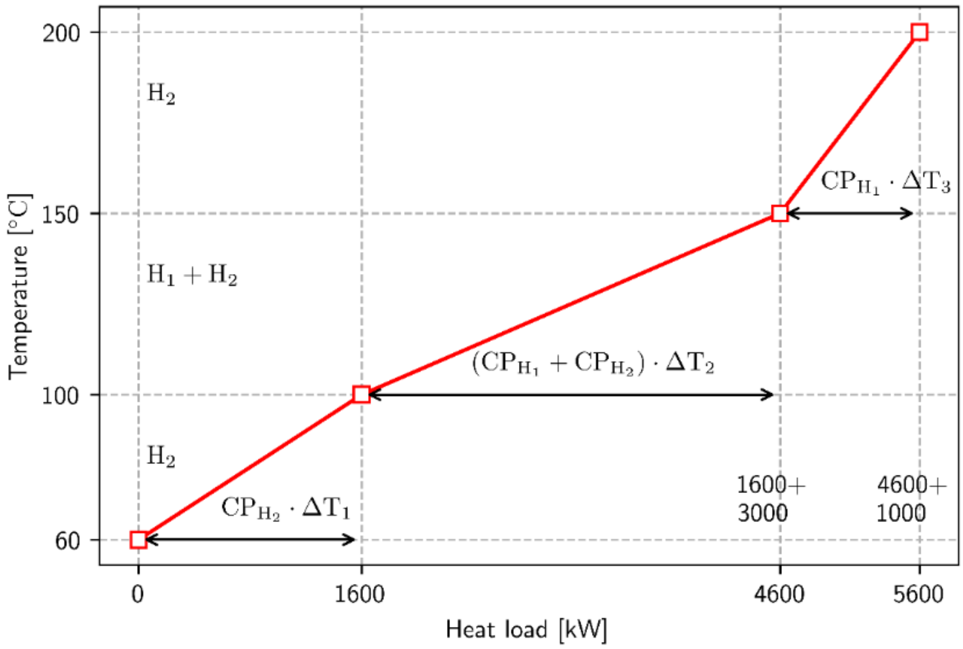

Figure 1. Hot composite curve

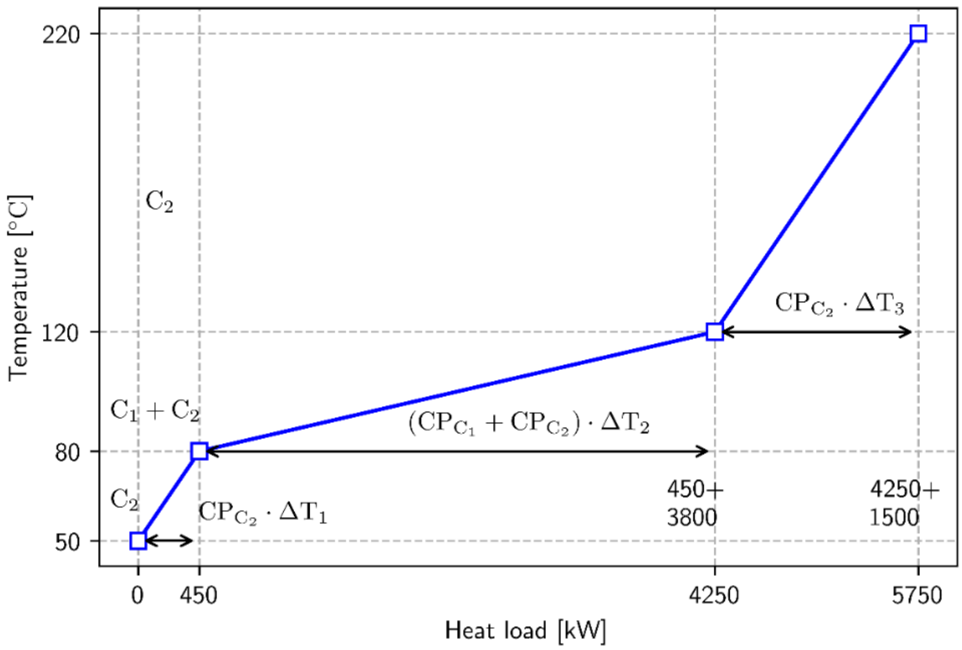

Figure 2. Cold composite curve

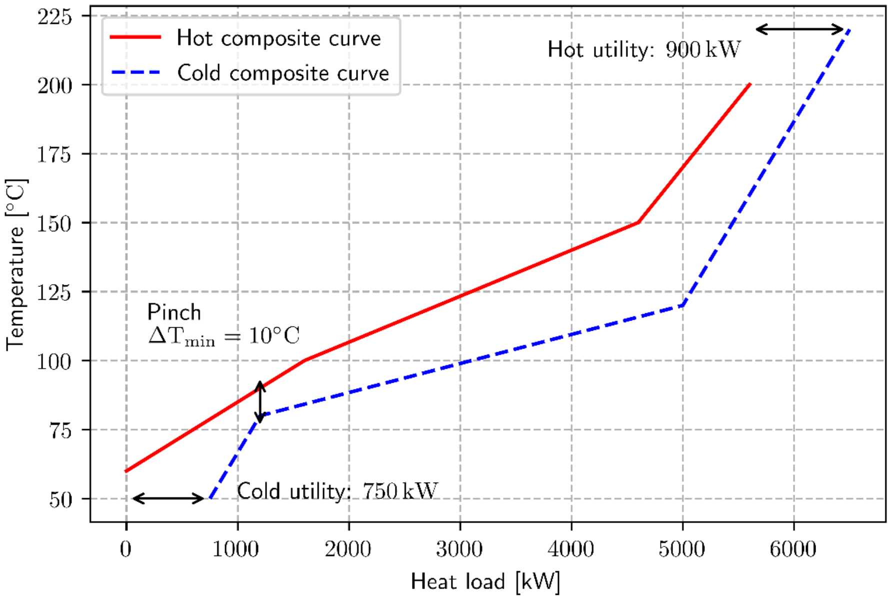

Figure 3. Balanced composite curves and energy recovery target

1.2.3.2 Territorial energy plan (CO_2 emission targeting)

An economic sector is the subject of inevitable energy demand (e.g., territorial regions). To meet national or regional greenhouse emissions limits, energy planning is required. For this purpose, the pinch analysis can be used for determining how the energy resources should be assigned among the energy demands. After the proposition of the first concept by Tan and Foo (2007), a different variation of this method like the mix of graphical and automated targeting approach (Lee et al., 2009), unified pinch with considering different periods and regions (Diamante et al., 2014), a hybrid algebraic graphical method for carbon capture and storage (CCS) (Ooi et al., 2013), Waste Management Pinch Analysis (WAMPA) (Ho et al., 2015) have been developed. In addition, its application in different industries like the Irish electricity generation sector (Crilly and Zhelev, 2008) and the New Zealand electricity sector (Atkins et al., 2010) have been tested. In recent years, the Carbon emissions pinch method mixed with new concepts like Life cycle assessment and carbon footprint which can be useful to analyze the economic and environmental aspect of the system simultaneously (Tan et al., 2018). To illustrate the pinch procedure, hypothetical data was reported from Tan and Foo's (2007) study. **Table 2** shows a set of expected demands for energy in three geographical regions. Each region is subject to greenhouse gas emission quotas (allowances). To meet the specified emission limits, an economic sector must include energy sources with zero or near-zero CO_2 emissions (e.g., nuclear, renewable energy).

These energy resources must be minimized given the high economic costs (case of renewable energy) or because of the risk factors that limit public acceptability (case of nuclear energy). Pinch analysis involves minimizing the energy resources required to meet the specified emission limits.

Table 2. Inventory data for carbon-constrained energy planning (Tan and Foo 2007)

Energy Resources			**Energy Demands**		
Available Resources		**Emission Factor**	**Expected Demands**		**Emission Quota**
TJ		**$t\ CO_2/TJ$**	**TJ**		**$10^6 t\ CO_2$**
Coal	600,000	105	Region 1	1,000,000	20
Oil	800,000	75	Region 2	400,000	20
Natural gas	200,000	55	Region 3	600,000	60
Others [a]	>400,000	0			

From the data in **Table 2**, the composite curves for energy sources and demands can be plotted as shown in **Figures 4** and **5**, respectively. To plot the supply composite curve (i.e., source composite curve), the available sources are first arranged in order of increasing emission factors. Zero-carbon energy sources are initially excluded. The product of the available energy and the emission factor of each energy source provides the total CO_2 emissions. Each energy source is plotted on the axis system: total CO_2 emissions ($y-$axis) as a function of the cumulative available energy ($x-$axis). The slop of each source is equal to its emission factor.

The composite curve of energy demands is obtained similarly, with the $x-$axis representing cumulative energy demands and the $y-$axis representing the total allocated CO_2 emissions (i.e., total emission quotas). Note that the three regions can be taken as a single demand without regard to their individual, disaggregated emission limits, resulting in the composite curve indicated by the continuous line (**Figure 5**).

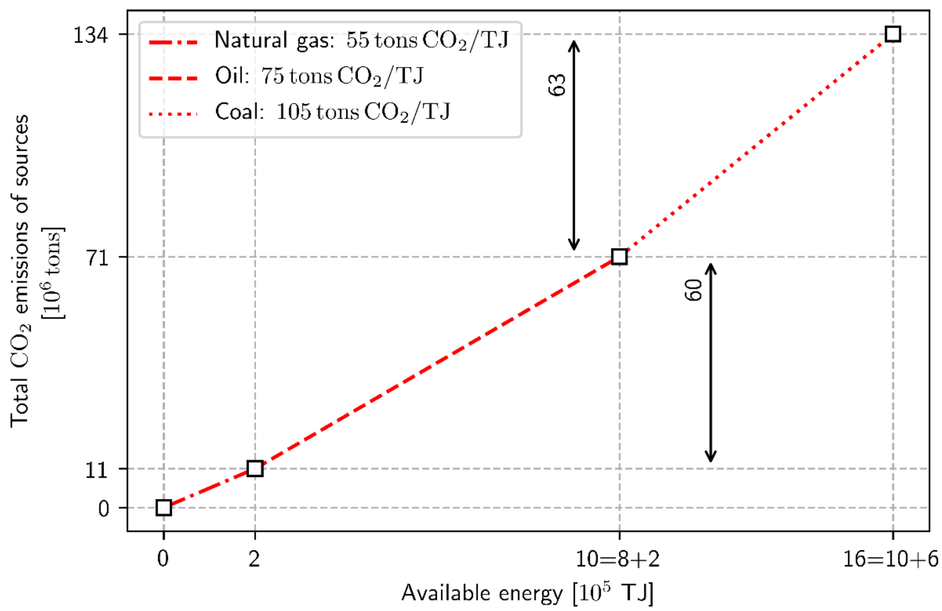

Figure 4. Energy supply composite curve

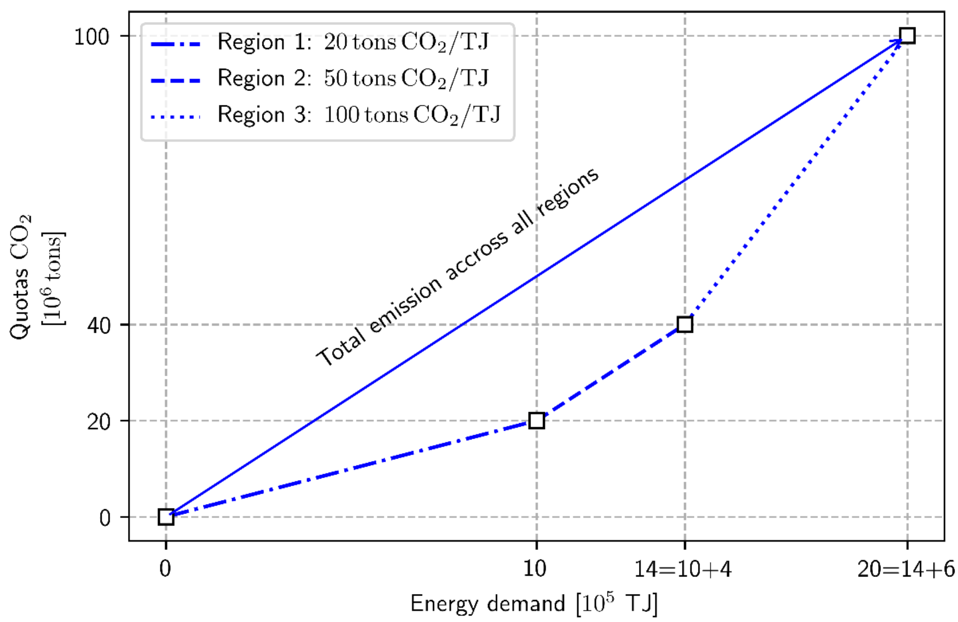

Figure 5. Energy demand composite curve

Emission targeting via pinch analysis can be investigated by combining the two composite curves (**Figure 6**). To provide the required energy sources, the source composite curve is shifted horizontally to the right, until the two curves touch each other at the pinch point. The horizontal distance between the origin and the composite source line represents the amount of zero-carbon energy required for the economic system, in this case approximately $7.2 \times 10^5\ T$.

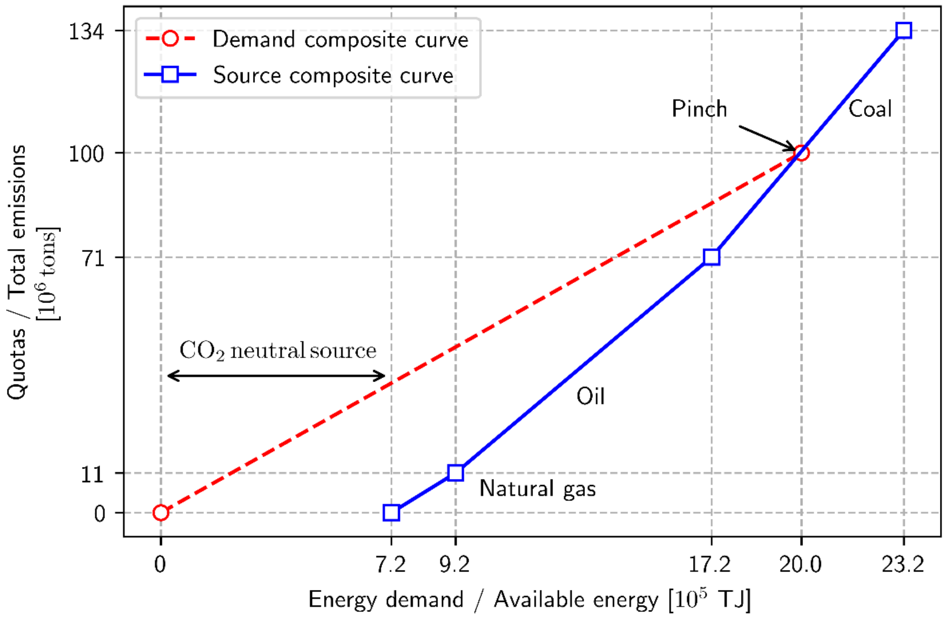

Figure 6. Targeting demand for CO2 neutral energy

1.2.3.3 Design of hydrogen networks

Hydrogen networks play an important role in refineries and large amounts of hydrogen are used for fuel production. Hydrogen networks involve consuming (sink), producing (source) hydrogen operations (Hallale and Liu, 2001). The management of the hydrogen network can be performed through pinch analysis by providing a good understanding of the mass balance of sink and source units and the system limitations. Further developments of hydrogen pinch belong to add some details like pressure constraint (Ding et al., 2011), demand uncertainty (Kim et al., 2008), and test the different solving approaches, like solving the MINLP model with different mathematical formulation to improve the accuracy of answers (Jiao et al., 2012a, 2012b)(Zhou et al., 2013). Recently, Hydrogen network design based on mathematical modeling and also considering reuse and recycle proposed by Deng et al. (2017). To illustrate the pinch procedure, hypothetical data was reported from Alves and Towler's (2002) study. **Table 3** shows a set of sinks and sources of a fictive hydrogen network:

Table 3. Inventory data of sinks and sources of a fictive hydrogen network (Alves and Towler 2002)

Sinks		**Sources**	
Flow Rate (Nm³/h)	**H_2 Purity (%)**	**Flow Rate (Nm³/h)**	**H_2 Purity (%)**
2495.0	80.6	350.0	95.0
180.2	78.9	623.8	93.0
554.4	77.6	415.8	80.0
720.7	75.1	1940.5	75.0
		346.5	73.0
		457.4	70.0

The mass balance of each source and sink can be represented through a two-dimensional plot of total gas flow rate versus hydrogen purity. **Figure 7** shows the composite curves of sinks (dashed line) and sources (solid line). The two composites' profiles start at a zero flow rate, with a horizontal line determined by the flow rate of the specific source or sink. The next source or sink in the order of purity is then plotted in the diagram, also as a horizontal line. Once again, the length will be determined by the flow rate of the specified source or sink, which starts at the same gas flow rate as where the previous source or sink ended. This is repeated until all sources and sinks are presented in the diagram. The area above the sink profile and below the source profile indicates the surplus where sources provide more hydrogen than is required by sinks. Vice versa, the area indicates a deficit of supply. **Figure 8** allows good visualization of the hydrogen surplus by calculation the net cumulative balance between sinks and sources. The minimum hydrogen utility can be determined by horizontally moving the curve toward the purity axis until the vertical segment between sink and source touches the purity axis.

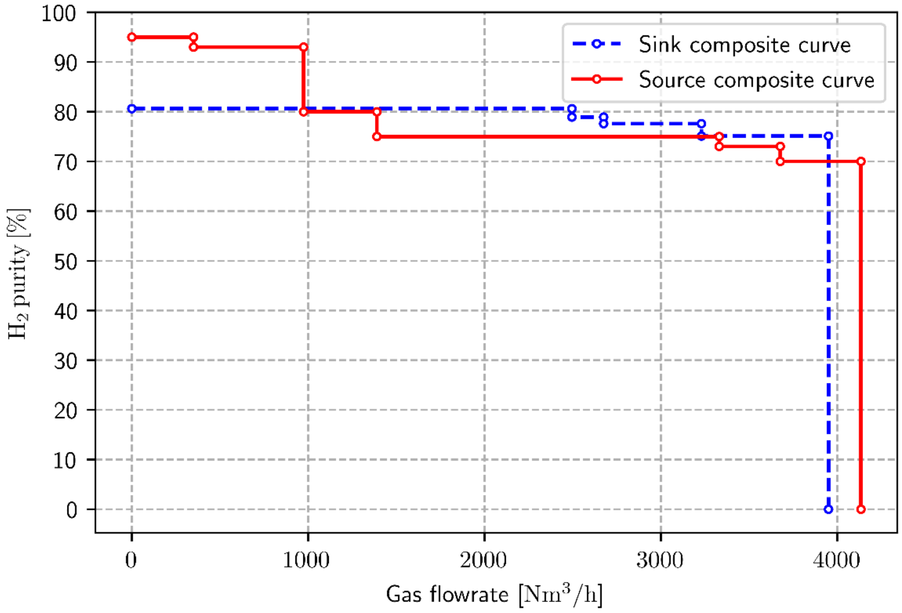

Figure 7. Composite curves of hydrogen network

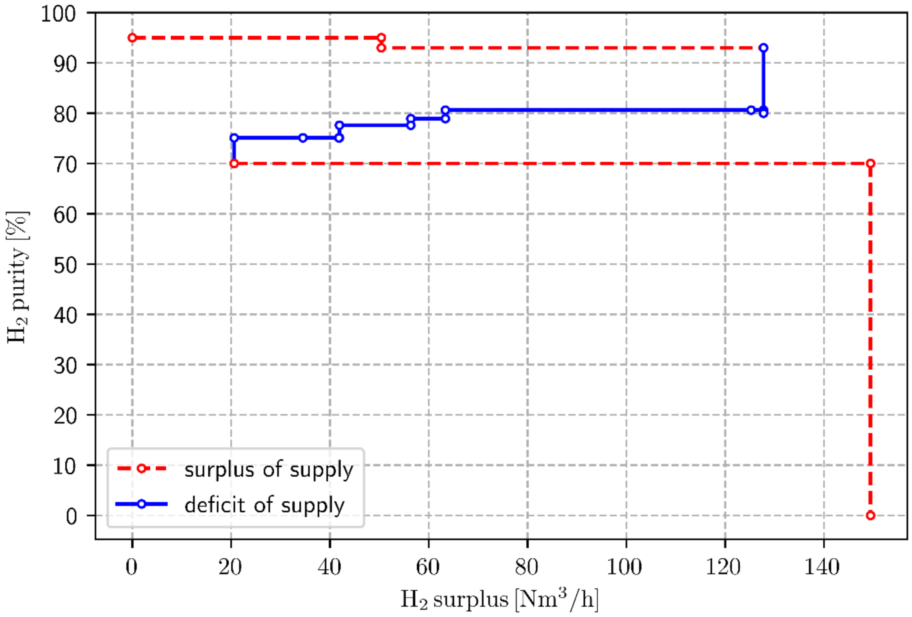

Figure 8. Hydrogen surplus diagram

1.2.3.4 Oxygen Pinch analysis

In a wastewater treatment plant, oxygen is essential for the oxidation reactions of carbon and nitrogen pollution (removal of COD and nitrification). To improve energy performance, it is essential to minimize the supply of oxygen, which is a very energy-intensive operation. For this purpose, oxygen pinch analysis has been developed by Zhelev and Ntlhakana (1999). This method aims to help with designing the wastewater treatment systems with cost efficiency. The method consists first in establishing composite curves using water pinch analysis. The curves are established individually by drawing the concentration of COD as a function of the mass flow rate of COD. After that, all the streams are aggregated within a resulting composite curve. The oxygen required is then calculated by plotting the line between the origin and the pinch point. The inverse of the slope of the limiting oxygen line is the flow rate of the required oxygen (Zhelev and Ntlhakana, 1999). With the implementation of the new method, about a 30 percent decrease in the costs of wastewater treatment plants has been obtained (Zhelev and Bhaw, 2000). Mass pinch transfer concept is the heart of oxygen pinch analysis but potentially oxygen pinch oversteps the targets of the classical pinch. There are some quantitative and qualitative targets within the oxygen pinch. The quantitative targets like oxidation energy load, residence time, oxygen solubility, and qualitative targets like growth rate that presents the micro-organisms age and health (Zhelev and Bhaw, 2000). The last detailed work about this method backs to Zhelev (2002) article, developed a hybrid method named Water-Oxygen-Thermal Pinch Analysis applied to manage the treatment system of wastewater in the industry. This technique almost mixed with other pinch methods like water and not used a lot in literature.

1.2.3.5 Emergy Pinch

Emergy is the solar energy that is available for utilization directly or indirectly to produce a product or service (Odum, 1983). Emergy was used as an environmental indicator to perform life cycle assessments of different ecosystems goods and services, e.g., human labor, trucks (Marchettini et al., 2007). Emergy can be used in energy pinch analysis as cost criteria. The objective is to provide an economic capturing of human demand and values to the analysis (Seider et al., 1999). In Hau and Bakshi's (2004) work, challenges and problems of emergy pinch are considered in detail. In addition, the relation between emergy and engineering concepts like exergy has been discovered. Zhelev and Ridolfi (2006) tried to integrate pinch and classical emergy and propose an integrated concept for the management of resources in a better way. In recent years, some real applications of emergy in different industries like steel companies (Pan et al., 2016) and power plants (Zhang et al., 2018) have been considered.

1.2.3.6 Budget-Time-Income

With inspiration from integrated management for different sources like steam, fresh water, electrical energy, etc. budget-time-income techniques help to increase profits and decrease investment costs. It's possible to use the pinch principles for the amalgamation of finances in the resources management sector. Like other classical pinch methods, in this method, the cost composite curve has also been developed to help for targeting optimal profitability. This helps the experts with trade-offs and decision-making. To do the targeting for combined resources, cost composites (combined composites in classic methods) has been developed as curves of all resource like water, energy, etc. Based on the water pinch analysis diagram, a plot has been developed to present the flow rate of money to guaranty the meet of targets. This method makes the vital amalgamation between businesses and industrial resources management. This flow diagram (money management FD) is an important tool for targets the min of repayment periods, borrowing timetables, commissioning, money management, and also it would be helpful for budgeting actions, etc. (Zhelev, 2005). This variation of pinch applied for resource allocation in stochastic problems (Arya and Bandyopadhyay, 2019), and also it's known as financial pinch analysis, which is a tool for financial aspects of projects (Roychaudhuri et al., 2017), and also it can combine with mathematical modeling concept to solve more complex problems (Roychaudhuri and Bandyopadhyay, 2018).

1.2.3.7 Summary and discussion

The pinch concept is an optimization procedure to find the best tradeoff between demand and present sources. The pinch can apply for different cases even far from the scope of its first development like emergy, oxygen, hydrogen and also in some researches pinch applied to find tradeoff in Budget-time-income sector which explained in the previous section.

Within these variations, different objectives have been followed to obtain. In energy, the pinch goal is to understand the most possible heat exchange between different hot and cold streams. For this reason, normally some data like input and output temperature and heat capacity are required, which not hard to measure. Thanks to B. Linnhoff and Hindmarsh (1983), different works based on real cases published and reliable results in the economic and environmental aspects presented. Other variations of pinch developed To meet the specified emission limits with zero or near-zero CO_2 emissions (Tan and Foo, 2007). This variation of Pinch analysis which called CO_2 emission targeting involves minimizing the energy resources required to meet the specified emission limits. Based on the industry's needs about managing hydrogen networks, especially in refineries, hydrogen pinch developed (Hallale and Liu, 2001). It can be performed through pinch analysis by providing a good understanding of the mass balance of sink and source units and the system limitations. Oxygen pinch was developed by Zhelev and Ntlhakana (1999) to improve the energy performance as it is necessary to minimize the supply of oxygen, which is a very energy-intensive operation. In other variations of a pinch like emergy and budget-time-income, the aim is optimizing some resources. These methods were applied already to real cases and have shown good results and impressive amounts of resource savings. Collecting the required data (temperature, flowrate, measurement of chemical combinations, etc.) is not easy always, and sometimes based on the real-world situation the measurements can be hard, challenging, or even impossible.

Based on these experiences, it seems the application of this known optimization procedure to water networks can have an impressive effect, which we will study about these details in the next sections. One of the most important applications of the pinch concept, called water pinch analysis, refers to water. The pinch concept tries to find an optimal tradeoff between different water sources (fresh, reused, recycled, etc.) and water demands in different industrial sectors. The concept of energy pinch has been explained before and water pinch will explain comprehensively in Section 2. Firstly, an introduction about water pinch is presented and after the literature on water pinch is reviewed and finally, an example of mono-contaminant water pinch analyses based on Wang and Smith (1994b) has been presented to make this method more understandable.

1.2.4 Water Pinch analysis

The first version of the pinch method proposed by B Linnhoff (1978) was called energy pinch analysis and after that different pinch variations have been developed. One of these variations is named process mass integration pinch. This method aims to design a global and systematic approach for minimizing water consumption and discharges, especially for the most water-consuming and energy-intensive factories. Wang and

Smith (1994) first applied this method to water and named it water pinch analyses. After that, different researchers have tried to improve the efficiency of this method by developing new variations of water pinch or proposing new approaches. For example, M. M. El-Halwagi, F. Gabriel, and Harell (2003) and Prakash and Shenoy (2005) obtained good results concerning water consumption reduction using water pinch analysis. There are also different works with the same point of view but focusing on food industries (juice, brewery, and corn refinery) like Almató et al. (1997), Thevendiraraj et al. (2003), Tokos and Novak Pintarič (2009), and (Bavar et al., 2018).

In the following section, we mainly focus on different aspects of water pinch analysis. First, the history of different developments of water pinch has been reviewed to know more about the details. After, to present the water pinch procedure for a mono-contaminant water system, the data of Wang and Smith (1994) has been considered.

1.2.4.1 History of water Pinch development

Superstructures were presented using the concept of the general system structures by Takama et al. (1980). They looked at the reduction of water level within the whole system of water-using and wastewater-treatment units. In the total system, optimizing water allocation was considered as an issue for maximizing water reusability. Programming based on mathematical approaches was utilized, as it allows transforming the problem into a series of sub-problems. Elimination of the initial problem of searching for attainable points was done employing a penalty function without imbalance limitations. This work set the stage for the application of pinch technology to minimizing the water and wastewater treatments either through graphical or numerical methods.

To minimize the wastewater used for water re-use, a graphical method based on the concept of the constraining composite curve and minimum water supply line was reported by Wang and Smith (1994) and Wang and Smith (1994) to target and design the regeneration re-use and regeneration recycling. This method also searches the multi-contaminant processes. The following work of Wang and Smith (1995) was later expanded to processes that required a fixed flowrate, processes with water losses, and multiple sources of freshwater. The design method proposed by Wang and Smith (1994) includes complex breaking loops in the design network (Bagajewicz, 2000).

To bring the difficulty of loop breaking under control, a new design procedure was introduced by Olesen and Polley (1997) continuing the work of Wang and Smith (1994) for single contaminant problems. Also, to make the previous design methods more comprehensible a new graphical approach was explored by Kuo and Smith (1998). This new methodology results in better constructions for regeneration re-use and recycles designs.

Distributed effluent treatment systems were designed by Wang and Smith (1994a). They aimed to minimize cost by keeping the flow treated to a minimum. Comparable in certain respects to the developed method by Wang and Smith (1994b), they fitted an effluent treatment line based on an effluent composite curve to find the minimum treatment volume target. They presented design rules for the achievable treatment target and developed a method for designing a distributed effluent network. The method was also extended to multiple contaminant systems. The distributed effluent treatment design was first reported by Wang and Smith (1994b) and further expanded by Wen-Chu Janice Kuo and Smith (1997). They also handled superstructure and mathematical techniques to find a solution for multi-contaminant issues. However, the superstructure is simplified with a deep intuitive understanding using graphical targeting.

The methods introduced by Wang and Smith (1994b), Wang and Smith (1994a), and Wang and Smith (1995) were then re-worked by Castro et al. (1999) and the concept of multiple pinches was created. This filtered the design of networks that do not lead to the treatment systems with the minimum-cost distributed effluent.

Furthermore, the concept of the two composite plots was introduced by Dhole, Ramchandani, Tainsh, and Wasilewski (1996), which plotted the water sources and water demands with the purity on the y-axis and flow on the x-axis. This useful way to utilize the plot to find freshwater and wastewater targets was explained, as well as the network design. Water pinch, the name of this process, was combined with numerical techniques to solve the problem.

Hallale (2002) reassessed the method of Dhole et al. (1996) and paid particular attention to the equivalency of two-composite plot representations and the true reflection of the target because both the shape of the source composite plot and the targets can be altered by mixing of water sources. The two-composite plot is consequently not an accurate targeting approach, but rather a graphical representation of the particular design that has been acquired using mathematical programming.

The concept of a Water Surplus Diagram was introduced by Hallale (2002) as an alternative targeting approach to that previously presented by Dhole et al. (1996). For this targeting method, a design procedure was also developed. It was mentioned that it is probable to use mathematical programming techniques for solving multiple-contaminant problems (Hallale, 2002). Linear (LP) and non-linear (NLP) mathematical formulations were presented by Doyle and Smith (1997) for targeting the re-use of water with multiple contaminants. It was able to dominate the difficulty of non-linear programming by combining the LP and NLP approaches. They suggested that the NLP problem can be solved using a solution for the linear model and provide the initial values for the NLP optimization.

According to Doyle and Smith (1997), Alva-Argáez, Kokossis, and Smith (1998) reported a developed and automated method for the synthesis of industrial systems for water regeneration. Through this method, the maximum outlet concentrations were chosen and the treatment unit concentrations were set to zero. Both the sum of the model errors in the objective function and capital and the operating cost were considered in the design. That is, running the linear program will reduce the error to zero. The series of linear optimizations will consequently converge to the NLP solution.

A mathematical model was developed by B. Galán and I. E. Grossmann (1998) and utilized for distributed wastewater networks. Rather than discovering a global optimum that leads to convergence difficulties, this model can identify local optima for a non-linear, non-convex obstacle. A search procedure was then proposed involving the sequential global or near-global optimum solutions within a relaxed linear model (MILP) and a non-linear model (MINLP). To set up and solve the MILP and MINLP models, GAMS is utilized throughout the approach. Ching-Huei Huang et al. (1999) followed a similar NLP procedure for determining the capacity of wastewater treatment and the freshwater consumption at the minimum contents. Synthesizing the resulting water usage and treatment network, the method is a good candidate. The MILP method for rapid screening of designs was developed by Jödicke, Fischer, and Hungerbühler (2001) to minimize the total operational and investment costs, even where the contaminant concentration is probably not available. When data are limited, this approach can be used, however, the well-known system and its limits should be available.

Assessing the economic performance of industrial wastewater reuse systems, Feng and Chu (2004) presented a methodology for wastewater treatment. Compared to the cost of wastewater regeneration and reuse, the saving costs of freshwater and wastewater disposal need to be balanced. Pinch analysis applied to water makes it possible to identify projects leading to a minimal use of water in the overall plant and the minimization of liquid effluents. Economically, it is interesting to reduce the investments required to increase the plant production rate by saving water and by reducing the effluent to be treated. Such analysis can be applied to most processes in the agro-food industries including high consumption of water and production of wastewater.

The use of new numerical techniques like water cascade analysis (WCA) instead of graphical approaches like water surplus diagrams has been proposed by Manan, Wan Alwi, and Ujang (2006), who find impressive savings (up to 40% for freshwater and 30% for wastewater with considering reuse and up to 60% for freshwater and 40% for wastewater with considering reuse and regeneration) as results. In another work of Y. L. Tan, Manan, and Foo (2007), they focused on proposing a new technique to retrofit and redesign water networks based on water pinch analysis. They consider the possible regeneration in these water networks.

The applications of water pinch in oil refineries are impressive too. Considering a multi-contaminant system in oil refineries water savings reaching up to 15% resulted from Mohammadnejad, Bidhendi, and Mehrdadi's (2011)'s work. Considering recycling, reuse and regeneration is another point of their work. In the same area of research, Mughees and Al-Ahmad (2015) proposed a tool based on water pinch analysis for a refinery in Tehran. They found almost 40% water savings by considering a multi-contaminant system and tested both graphical and mathematical tools.

Based on two comprehensive review papers (Bagajewicz, 2000)(Ahmetović et al., 2015), in recent years the application of the mathematical models mixed with the water pinch concept for managing water networks has grown. Boix et al. (2011) proposed a mathematical model to handle multi-contaminant systems, with a solving procedure based on Multiple Criteria Decision Making (MCDM) methods for MINLP models. Later, De-León Almaraz et al. (2016) completed the previous work by considering more details and complete databases. These two works (Boix et al. 2011) (De-León Almaraz et al. 2016) led to the development of an extensive water network allocation network for different types of industries by handling multi-contaminant systems. In the oil refinery sector mathematical models have been developed as well (Mohammadnejad et al., 2011) (Mughees and Al-Ahmad, 2015a) to handle multi-contaminant systems while considering regeneration, reuse, and recycling, and good reductions in water consumption are also found by applying this method. Some studies have focused on reuse opportunities (Buabeng-Baidoo et al., 2017), some on the regeneration process (Li and Guan, 2016) and some others on regeneration and recycling together (Feng et al., 2008), and after they proposed their MINLP mathematical model to manage water networks in different sectors like the dairy and chemical industry, etc.

Recently, Skouteris et al. (2018) performed research in the brick-manufacturing industry. To manage water systems in this industry, they used two techniques which they named water pinch analysis and water footprint. The results demonstrate that using an integrated tool based on these two methods improves the efficiency of the water management system.

Based on the energy pinch definitions and according to the flexibility of this method to be applied in different cases like water, oxygen, etc. it's necessary to find the analogies of each element in new variations of pinch to apply this method. There are some analogies between energy and water pinch which are presented in **Table 4**; these analogies help us to apply this method in the water sector. For example, heat exchanger network design is equal to water network design in water pinch and heat capacity flowrate is equal to the water flow rate in the water pinch method and the definition of the hot and cold stream in energy pinch can be compared with the sink and source concept in water pinch techniques.

Table 4. Analogies between process heat and mass integration

Heat Transfer-Based (Energy Pinch)	Mass Transfer-Based (Water Pinch)
Heat Exchanger network design	Water network design
Temperature	Purity of water
Heat capacity flowrate	Water flowrate
Heat flow	Pollutant flowrate
Cold stream	Sink water
Hot stream	Source water
Heat-Pump	Purification Unit (Regeneration)

1.2.4.2 Method description

To illustrate the water pinch procedure for a mono-contaminant water system, hypothetical data were reported in the study of Wang and Smith (1994b). **Table 5** shows the inventory data of a water-using operation.

Table 5. Data set for water pinch analysis (Wang and Smith 1994)

	Pollutant Threshold		
Unit	$C_{in}\ (ppm)$	$C_{out}\ (ppm)$	$\dot{m}_w (t/h)$
U1	0	100	20
U2	50	100	100
U3	50	800	40
U4	400	800	10

The inventory includes water mass flow rate $\dot{m}_w$ and the pollutant threshold at the input and the output of each unit operation (C_{out} and C_{in}). The first step consists of establishing a global water demand of all units (called composite curve demand). **Figure 9** shows the individual demand line of each unit. The demand is represented in a two-dimensional plot: water purity ($y -$ axis) versus pollutant mass flow rate ($x -$ axis). The mass flow rate of pollutant $\dot{m}_C$ is the product of the supplied water and the water purity difference between the input and output of each unit (Equation (2)):

$$\dot{m}_C = \dot{m}_w \cdot (C_{out} - C_{in}) \tag{2}$$

To establish the composite curve, the individual demands of units of the same purity interval are accumulated. The result of the procedure is presented in **Figure 10**. According to **Figure 11**, the minimum water supply can be obtained by drawing the first intersection with the demand line (90 t/h of water at 0 ppm). This first water resource will be used to ensure the transfer of 9 kg/h of pollutants. To transfer the remaining pollutants (up to 41 kg/h), the second source of water is required. The second water source is obtained by recycling the available water. Similar to freshwater, recycling can be deduced by drawing the second intersection with the demand curve (45.7 t/h of wastewater at 100 ppm).

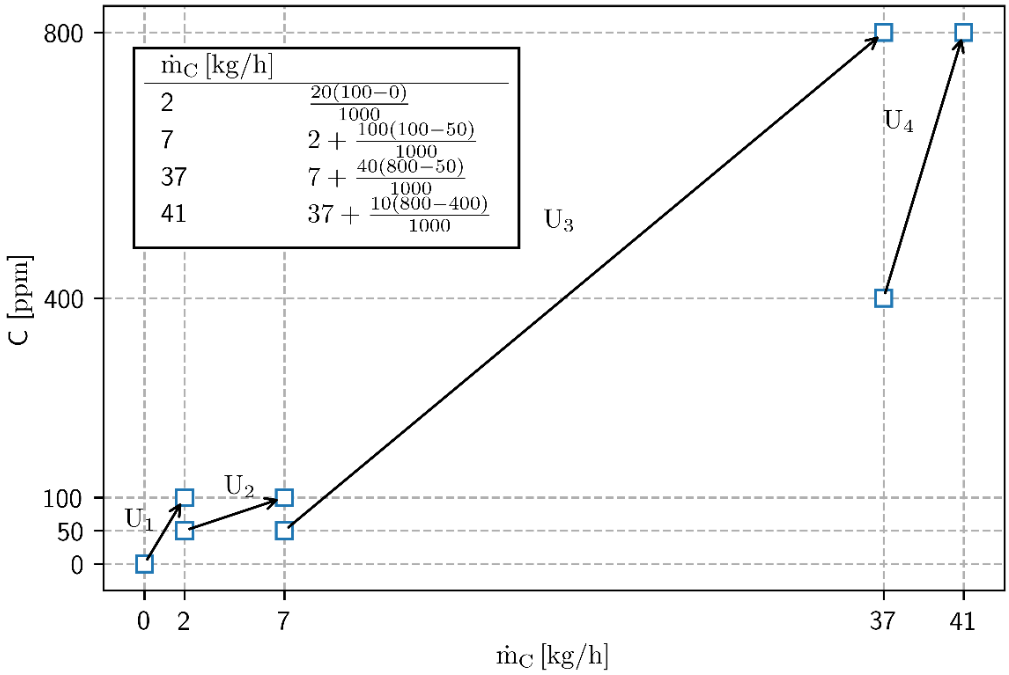

Figure 9. Limiting water profiles for each unit

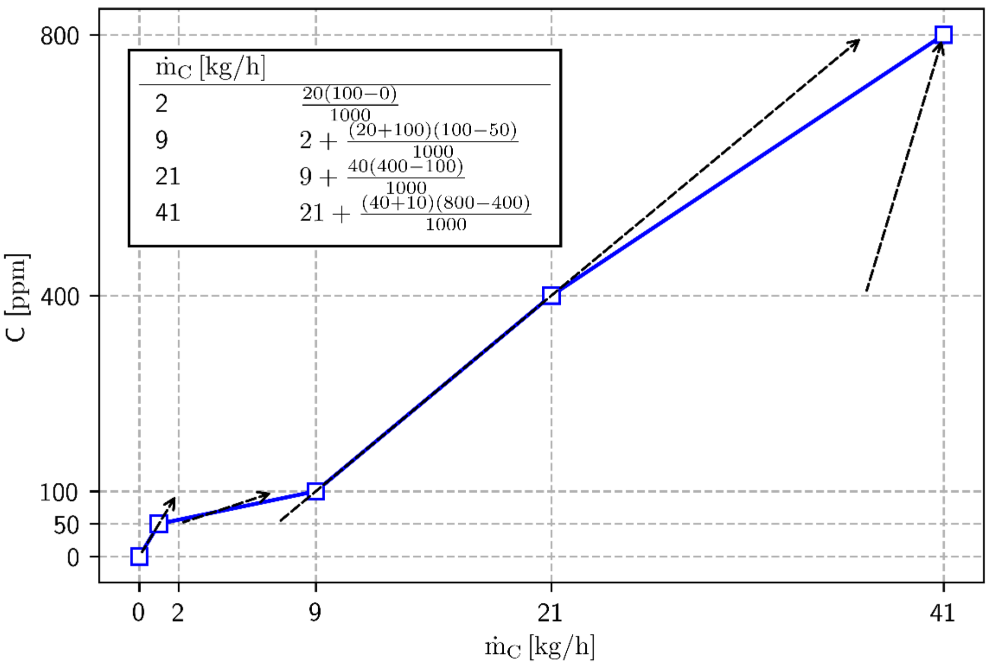

Figure 10. Composite line of water demand

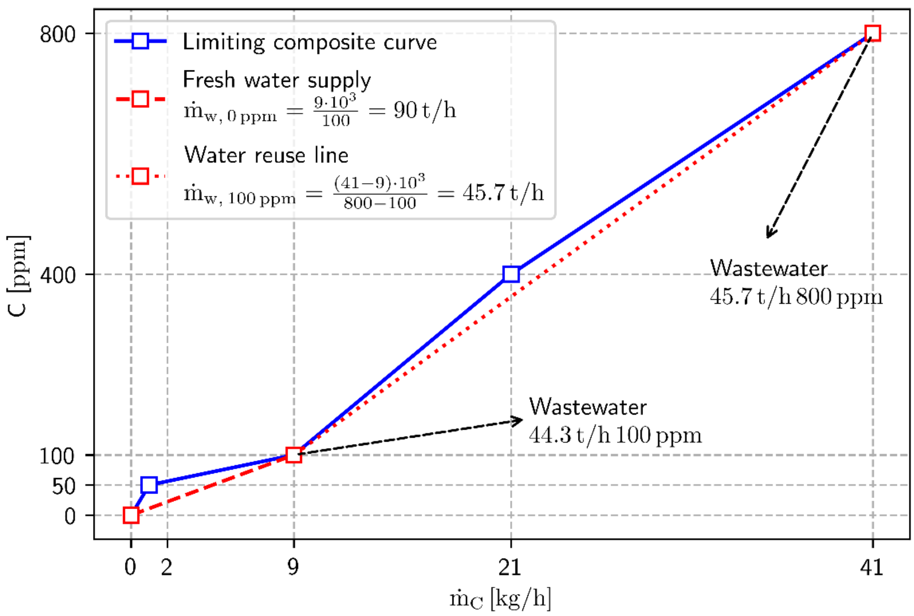

Figure 11. Combination of water demand line and water supply line

1.2.5 Water Pinch analysis in the food industry

In the following section, we mainly focus on different aspects of water pinch analysis as implemented in the food sector. First, a review of current practices for water management in the food industry is mentioned. The aim is to know more about the current methods used for water management in food industries. After that, the potential of water pinch analysis in the food industry has been considered and examples of this method are presented as well. Finally, R&D needs and challenges are discussed to find the research gaps.

1.2.5.1 Current practices for water management in the food industry

Based on the literature about water management practices in the food sector, Casani and Knøchel (2002) were the first to develop a generic model based on hazard analysis critical control point (HACCP) for the implementation of water reuse in the food industry to solve the main barrier of reuse opportunity which was called risk of microbiological contamination of food and environment. After that Casani, Rouhany, and Knøchel (2005) discussed reuse challenges in food industries, where on the one hand food safety and consumers' health is a critical issue and on another hand, there is the limited opportunity of water reuse in the food industry, thanks to regulations that lead to the loss of any big water saving capacity. They discussed different water treatment methods in two main categories: chemicals like chlorine, etc. and physical methods like membrane processes, etc. and they already collected opportunities of reuse within different food industry processes like egg, milk, production, etc. Finally, they categorized all reuse issues in food industries into eight sections: environmental, economic, legislation, technological, water quality assessment, social, food industry, and academia and counted the drivers, barriers, and solutions in the way of water reuse opportunities in food industries. As a result, using HACCP in food systems is highly recommended by the authors. Implementation of HACCP management systems in a dairy plant was already proposed in the work of Lu et al. (2013). Using this technique leads to the identification of critical control points (freezing and pasteurization) and in parallel guarantees food safety and provides improvements at the managerial level. Wujie et al. (2011) considered the effect of water quality on food quality, taking into account treatment opportunities in parallel. Various treatment methods like filtration, water softening, etc. have been reviewed.

In other work, Compton et al. (2018) studied the food processing industry from energy, fuel, and water consuming perspectives. Because of the nature of this type of industry they consume huge amounts of energy and water. In Compton and his colleague's opinion, to stay in the market and be economic, it seems necessary to implement some high-tech technologies like membrane separation, high-pressure processing, microwave assistance, etc. as these technologies help industries increase their efficiency and save them money in dynamic markets. Grobicki (2008) presented a comprehensive report about water's future in the industry. In this work, Grobicki presents a classification of the main strategies of water consumption reduction. She proposes two main groups of opportunities for reuse, the first group named "increasing industrial water productivity" which contain different strategies to increase the efficiency of reuse like "water auditing", "water recycling and reuse on-site", "matching water quality to use requirements", "using reclaimed water", "policy instruments and economic incentives" and the concept of the "virtual water trade in manufactured products". The second group is named" closing to the loop with zero discharge" and within this group four different technique have been proposed to facilitate reaching goals like "stream separation", "raw material recovery from waste", "energy recovery from waste", and "reuse of waste". The main goal of this work was to present different strategies to attain the final goal of zero discharge in industries like the food sector.

In the work of Lee and Okos (2011) the authors tried to propose strategies for food processing industries to achieve zero discharge and reductions in the use of energy and freshwater in parallel. In this way, they consider three different food industries (edible beans, dairy, and corn), and three approaches are proposed to reach the goals: first is plant-scale audit data collection, the second is laboratory-scale experiments, and the third computer-aided simulation to design systems. Implementation of these approaches in food case studies leads to a considerable reduction in water and energy use and also wastewater generation. Buabeng-Baidoo et al. (2017) worked on reuse opportunities in the dairy industry where they focused on process integration tools. Based on their case study, the cleaning-in-place (CIP) phase uses a significant volume of water (more than 70%) in the factory, so for this reason they focused on CIP operations. In this article techniques like reverse osmosis (RO) membranes and parallel mathematical programming (mix-integer nonlinear (MINLP)) techniques have been applied. As a result, a 33% reduction in water and 85% reduction in wastewater production have been reported. Meneses, Stratton, and Flores's (2017) work reviews water reuse challenges in the food industry. They believe that in the food sector, irrigation is the highest water-demanding stage. It mentioned that food processing uses a huge percentage of high-quality freshwater and produces a big amount of wastewater because of its nature, so it’s a key step in the food supply chain. As a result, comprehensive evaluations considering all aspects like cost, risk, and environmental performance are highly recommended.

Suárez, Fidalgo, and Riera (2014) and Suárez and Riera (2015) did two separate research studies in the dairy industry, where the main technique which was implemented was RO to recover wastewater and produces high-quality water. In the first article, they considered three main parameters: pH, COD, and conductivity as pollutant indicators. In the end they proposed a post-treatment to adjust the pH, and a 2.2-year payback period has been considered for treatment instruments. In the other work the main focus was on milk dairy condensates, and they considered COD and conductivity as indicators. A 90% recovery rate with a 1.16-year payback period has been reached as a main result.

Based on the literature, there are different groups of articles with different points of view. In some of them, methods to reduce freshwater consumption and wastewater generation in parallel are presented, and in other groups of articles, they count the challenges in the way of reuse, recycle and regeneration of water in the food industry by considering the limitations, regulations, and hazards due to food safety and the importance of using high-quality water in these special kinds of industries. In this review, a lack of implementation of the water pinch method for food industries seems obvious (or there is no comprehensive work with a pinch as its main focus). In the next section, the potential of water pinch analysis in the food industry has been considered and an in-depth discussion presented based on applying water pinch studies to this sector.

1.2.5.2 Potential of water Pinch analysis in the food industry (new tools for new approaches)

Water is a unique resource for the food processing industry for which there are no alternatives. To ensure food safety, food and drink processes require a stable and high-quality water supply. Given the diversity of organic processed products, a large amount of liquid effluent is produced. The management of effluent is of the highest importance because of the environmental impact of the wastewater. The most important environmental impacts include eutrophication and asphyxiation of aquatic environments, due to highly polluted effluents with organic carbon, nitrogen, and phosphorus. For example, the BOD and COD levels in food industry wastewaters can be 10–100 times higher than those of domestic wastewater. Therefore, food industry water use and wastewater discharge are both subject to stringent environmental regulation and require appropriate treatment. In addition to the cost of feed water, the treatment cost is the most important operating cost. The annual cost of these integration techniques is on average three million euros (J Klemes et al., 2010).

Each process in the food industry has its own unique and specific features. Some processes are intermittent and highly dependent on the availability of a feedstock (e.g., sugar factories, fruit, and vegetable processing). In contrast, the dairy industry operates seven days a week for the whole year. Some other processes operate continuously or nearly continuously (e.g., breweries, wineries, etc.). All these features involve diverse using-water operations and sources of fresh water. In food production, water is used for general purposes, such as cleaning, soaking, blanching, chilling; cooling/heating, or also as an extracting agent (e.g., extraction of sugar from sliced beet). Generally, in the food industry, only properly treated potable water should be used. Often, the source of water comes from municipal plants (public water), or sometimes it comes from in-situ drilling, rainwater, and recycled water to different levels for various operations. In all cases, the water must satisfy the standards required for drinking water, but additional treatments are required to meet the strict quality specifications of food production. For example, in breweries, process water must not contain any organic substances to avoid microbial growth and, consequently, affect the quality of the beer. In a sugar refinery, the presence of inorganic substances is not allowed (e.g., hydrogen carbonates, iron, manganese, nitrates, nitrites, and sulfates).

The pinch analysis applied to water makes it possible to identify ways leading to a minimal use of water in the plant and the minimization of water effluents. Economically, it is interesting to reduce the investments required to increase the production rate of the plant by saving water and by reducing the effluent to be treated. These analyses can be applied to most of the processes in the agro-food industries that involve high consumption of water and the production of wastewater. Despite the development of pinch mass analysis in many studies, this technique still occupies a small place in the industry, particularly in the food sector. There are different challenges in the implementation of this method in the agro-food industry sector. Normal food industries are large scale and have a complex water system, in addition to this, the number of pollutants is not just one, and scientists are faced with multi-contaminant systems. By taking into account the purity constraints for several pollutants the pinch method requires the use of mathematical tools such as multi-objective optimization. This means that the implementation of this method in the real case of agro-food industries normally requires complex mathematical work and optimization tools that are hard to use in nature. Development of a new generic method for water/wastewater minimization and water network design, based on water pinch analysis seems necessary. It has to be suitable for agro-food processes and should therefore be able to handle either single or multi-contaminant flows.

For the implementation of the water pinch method in agro-food industries, it’s necessary to know the nature of each operation in different case studies. This information helps us to have more accurate results. To understand the situation of this categorization and find the type of operations in different case studies three types of food industries have been considered (brewery, citrus, and sugar industries). Generally, there are two types of water-using operations: mass transfer-based operations and non-mass transfer-based operations. In mass transfer-based operations, the bulk pick-up of contaminants in the water occurs through direct contact between the water, the equipment walls, and/or the processed material. Vessel washing operations and wet scrubber operations are two examples of mass transfer-based operations. In non-mass transfer-based operations, the water is used as an energy utility, reactant, or product of a chemical reaction. Using water in cooling towers and evapo-concentration are two examples of non-mass transfer-based operations. As a result, in breweries and the citrus industries, most of the operations are mass transfer-based operations and in the sugar industry, the two categories have approximately the same contribution. Detailed information is presented in the next paragraphs.

Based on Tokos and Novak Pintarič's (2009) work in the brewery industry, there are different operations of which 18% are non-mass transfer-based operations and 82% are mass transfer-based operations. Each of these categories presents some operations and each operation consumes a certain amount of water. In the non-mass transfer-based section four main operations need water, namely water preparation (about 14%), air compressors & CO_2 (less than 3%), evaporative cooling towers (up to 32%) and boilers (about 9%), and in the mass transfer-based section five main operations need water which are keg washing (about 12%), bottle washing (up to 33%), maturation (about 11%), fermentation (about 26%) and CIP (about13%).

To understand the exact categorization of mass and non-mass transfer-based operations in a citrus plant, it's necessary to explain the operations and schematics of this kind of industry. This information was already presented in the work of Thevendiraraj et al. (2003). In terms of a typical citrus plant, there are three main steps which are named selection and cleaning, extraction plant, and treatment operations which contain three subsections (peel, juice, and emulsion). This schematic presents the principle of a citrus plant, but to be more aware of the type of operation (mass or non-mass transfer-based operations), a real case from Thevendiraraj et al.'s (2003) work is considered. The main operations are aligned in the real order of the plant: packing, treatment plant (potable) & boiler, selection/cleaning, APV condenser & green tank, vacuum pump, screen, finisher, distiller, screen 1, distiller condenser &

washing spiral 1 and centrifuge. Based on the explanation about the categorization of mass and non-mass transfer-based operations in the citrus plant, the results show that most of the operations (64%) are mass transfer-based ones and the rest are non-mass transfer-based operations.

To understand the exact categorization for mass and non-mass transfer-based operations in the sugar industry, it is necessary to explain the operations and schematics of this kind of industry. This information was already presented in the work of Ensinas et al. (2007). There are seven main steps in the typical sugar industry. The main operations are sorted in the real order of the plant: sugarcane preparation and juice extraction, juice treatment, juice evaporation, sugar boiling, crystallization, centrifugal separation and drying, fermentation, distillation, condensate tank, and water cooling system. Based on the explanations about the categorization of mass and non-mass transfer-based operations in the sugar industry, the results show that most of the operations (up to 55%) are mass transfer-based ones and the rest are non-mass transfer-based operations.

Applying water pinch analysis has some economic aspects in addition to saving freshwater. Based on the results for four types of food industries (citrus, sugar, fruit juice, and brewery) which are presented in **Table 6** there are economic savings in investments ranging from 23% to 69% with different attractive payback periods ranging from 5 days to 4 months which show the economic benefits of using this method in addition to environmental and other benefits. In the following table different types of operations (continuous and batch) have been considered to demonstrate the flexibility of the applicability of this method for different types of operations. Another issue is the number of indicators used in each case study. Both single and multi-contaminant systems have been considered to do this analysis.

Table 6. Examples of savings identified by applying mass pinch analysis

	Operation	Indicator	Freshwater	Savings	Payback	Reference
Citrus plant	continues	COD	2500 à 4000 m3/month/2500 à 4000 + water from pressing	30%	4 months	(Thevendiraraj et al. 2003)
Beet sugar factory Capacity: 200 t/h beet sugar	continues	pH, COD, Brix	240/246 t/h	69%	5 days	(Žbontar Zver & Glavič 2005)
Fruit juice	Batch	PINCH monocontaminant	96 m3/35 m3	64%	-	(Almató et al. 1999; Li & Chang 2006)
Brewery	Batch	PINCH monocontaminant	653 300 m3/year	23%	4 months	(Tokos & Novak Pintarič 2009)

Based on the literature, applying water pinch to different food sectors like dairy, beverage (including the citrus and food juice industry), etc. has an impressive effect on the reduction of freshwater use and wastewater production. The average reduction range of freshwater use in the different food sectors is between 27% and up to 65% for the beverage sector and palm oil mill industries, respectively. In parallel, information concerning the average amount of wastewater produced in different food sectors is presented in **Figure 12**. The average reduction ranges of wastewater produced in the different food sectors are between 28% which corresponds to the beverage sector up to 75% in the dairy industries.

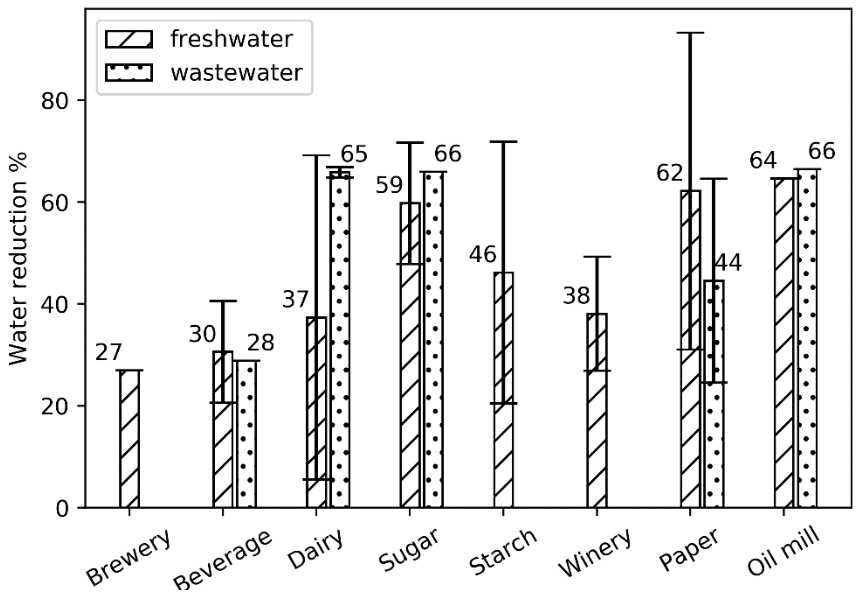

Figure 12. Average freshwater/wastewater consummation/production reduction based on different food sectors

Based on the discussion in this section, the importance of using water pinch in the food industry has been shown clearly. There are different challenges to face to implement this method and obtain impressive savings of water and reduction of wastewater production. In the next section, the discussion will be on R&D needs and challenges for implementing water pinch in agro-food industries.

1.2.5.3 R&D needs and challenges

In the previous section, a comprehensive literature survey about the milestones of water pinch, functions, graphical examples, an in-depth discussion about using water pinch in the food industry has been presented. In addition, some useful information about the type of operation (mass transfer-based operations and non-mass transfer-based operations) in different case studies like brewery, citrus, and sugar industries has been extracted. Thanks to the examples about the implementation of water pinch in the previous section and also the challenges mentioned before, it’s necessary to obtain by measurement or simulation the required data for this method. Some of this information can be obtained directly from industrial site measurements and some of them are standards and specific data from the literature. The required data can also be obtained by numerical simulation. Normally, it is necessary to know the type and number of pollutant indicators, limiting water data like limiting concentration, the minimum and maximum water flow rate in input and output, and threshold values of pollutant indicator for each operation, etc. while another issue is about the type of process. There are different process types like batch, continuous or semi-continuous. To implement the pinch method in the food sector finding the process type is vital. A big part of industries has continuous process operations and the pinch method is normally developed for this type of process in the literature, but in reality, there are also batch or semi-continuous type processes in the food sector. One of the challenges is to propose an adapted model for all types of processes which can be a good subject for further researches.

Based on the information extracted from database articles, some results are obtained and presented below. The frequency of use for different pollutant indicators in different sectors of the food industry is collected in **Table 6**. This table gives useful guidelines about the utilization of indicators in each industry, for example, in the dairy industry, the most used indicator is microbial count which is used five times, followed by electrical conductivity (EC) three times and also COD and turbidity, each used twice. For the sugar industry, the most frequent indicator is COD and four other indicators like pH, BOD, microbial count, and turbidity are in the next level of importance. For the meat processing industry, the microbial count is the most important one and for the paper industry, it is the TDS. For other industries the priorities are aligned in the following order: in the brewery industry COD, pH and EC, in the citrus industry COD, pH, and TSS, in the ethanol sector COD, pH, BOD, and OG, for the starch industry TSS, TDS, TOC and the winery industry COD and TSS are the most important indicators that have the same priority based on their frequency of use in the literature. Based on the information presented in **Figure 13**, it's easy to find which indicator will be more effective to develop a water pinch method considering the pollutant indicators.

The choice of one or more pollution indicators is in itself an important challenge given the variety of processes in the food industry. Often, various constraints are merged, including the consideration of food safety, too strict regulations, and environmental issues. Process management in this sector is not as flexible as regulatory constraints often prohibit the reuse of water of lower quality, despite the availability of water and the potential of water reuse within factories. The development of pinch analysis must take into account these considerations by determining the minimum required water quality and by screening solutions that integrate risk assessment. Pinch analysis should also be considered as a means of promoting advantageous solutions and why not a means to argue changes in the standards and guidelines in the food industry (up to now too strict and not flexible).

Another challenge is how to provide not only effective and safe food security solutions but also sustainable solutions. A fundamental challenge of sustainable development is to provide a water network without any further unacceptable levels of environmental degradation. For example, if the water network proposed by the pinch involves regeneration steps, in this case, some inputs are required (e.g., chemical solvents, energy resources, etc.). It is, therefore, necessary to analyze the environmental efficiency of the solutions provided by the pinch by integrating LCA or water footprint analysis.

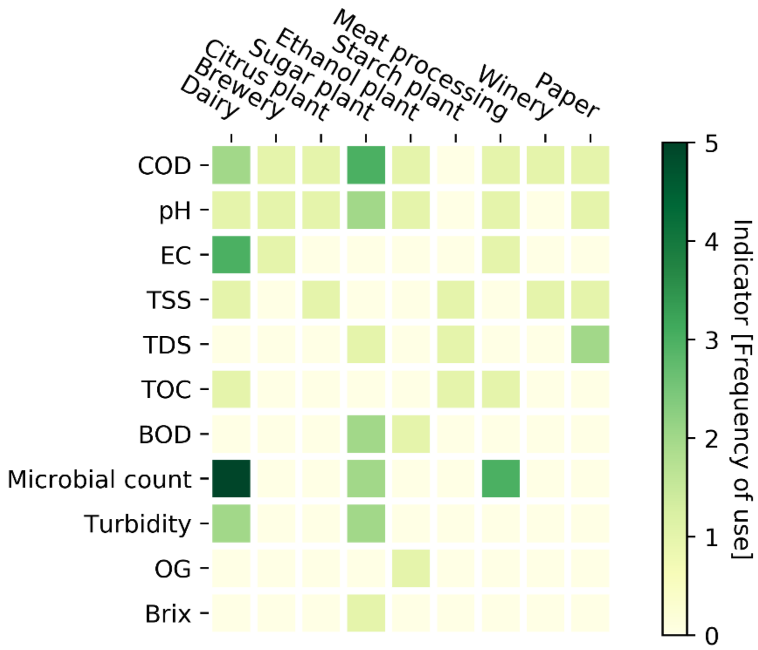

Figure 13. Detailed analysis of the frequency of use indicators

1.2.6 Conclusion

There are some reasons why the food industry faces the challenge of reducing water consumption. These are environmental problems, investment, regulation, sanitary safety (and thus water quality), as well as social problems. Water consumption and wastewater generation in the food industry could be minimized by replacing the existing technologies with new ones. However, setting up innovative equipment will require a lot of investment and R&D time. In addition, regarding the low price of water, investment in purification equipment is unjustified. Optimizing water networks through pinch analysis is an opportunity to increase the efficiency of water use in the food industry with lower investment costs. The pinch analysis applied to water provides a reduction of water consumption ranging from 20 to 40% at a reduced cost. Its development and availability for the food industry should encourage manufacturers to adopt this approach and achieve water savings. The key idea for minimizing water with pinch analysis is to identify streams of water that can be reused in an operation for which water quality is acceptable. Minimum water requirements can be targeted using graphical tools or automated design methods. The earlier graphical targeting methods provide conceptual insight into the problem and highlighted the proper designs. Although, when other components are added to the problem and consequently the need for cost optimization rises, these problems become too complicated for these graphical targeting procedures. As a challenge, data extraction is the most critical step for performing an optimal analysis. Most of the methods discussed in the literature are based on single-contaminant water systems. Considering single water contaminants and the limited number of water sources with a simple framework is suitable to present how water pinch analysis work, however, many contaminants must be taken into account.

In the food industry, it is almost impossible to include all the components that influence water chemistry, the microbiological aspect, and the quality of the food product. In some food processing sectors, it is common to select representative contamination indicators. The application of the graphical method for multi-contaminant water systems is not easily manipulated. For this, the development of numerical tools seems a crucial step for the development of pinch analysis and its application in the food industry. It seems that the trend is towards using methods such as mathematical programming to solve complex problems. Mathematical programming is not without difficulty as non-linear problems are often non-convex. It means that global optima are often not obtained. Recently, a large amount of research has been devoted to this area. In this dissertation, some software like MATLAB® or PYTHON®, etc. rely on mathematical programming techniques and offer graphical insights that provide easy-to-understand solutions. When considering the nature of multi-contaminant mathematical models to solve these models normally the development of multi-criteria optimization methods seems necessary. Multi-objective and multi-constraint optimization tools, especially evolutionary methods (GA, PSO, etc.) seem helpful to solve this kind of problem.

As a further research proposition, the development of an integrated tool that includes water pinch analysis, energy pinch analysis, and also life cycle assessment (LCA) seems necessary. Within this integrated tool, it’s would be possible to improve the energy and water use efficiency and also consider the environmental aspects by taking to account the LCA technique. Another proposition is about new solving procedures. As mentioned before, to solve multi-contaminant system models, the use of evolutionary methods seems necessary. Testing new evolutionary methods instead of traditional ones (GA, PSO, etc.) could be interesting

Chapter 2: Model development - Mathematical model and solving algorithms

To optimize the water networks in real case industries graphical methods are not suitable. Because the real industries are large scale and also with different contaminants which is hard to manage. the necessity of using numerical tools and mathematical modeling is already explained in previous sections. In the following section, two different numerical approaches have been proposed. The core logic of both roots from the water pinch algorithm but expanded to the mathematical models. the approaches toward the optimum answers are different in these two articles. The first article proposes an algorithmic procedure to find the best manual trade-offs for reuse opportunities in industrial water networks. It leads to helps the operator to find the best answer by taking into account the different considerations. The second article facilitates some steps of previous work and proposed a different way to find the optimum point. In this work, the mathematical model is defined as a multi-objective model to be solved by an evolutionary algorithm like NSGA-II. The embedded procedure within this method automates the optimization algorithm. Feed the tool with the requested data and adjust some parameters of the tool would be enough to have the initial results.

This chapter is built based on two different articles. The first one is entitled" *A Novel User-Friendly Tool for Minimizing Water Use in Processing Industry*". This article is *accepted (2021)* in the journal of "*Cleaner Engineering and Technology*" as the second outcome of this chapter. The second one is entitled" *Industrial water reuse and preservation strategies: Generic optimization based on NSGA-II algorithm*". This article is *submitted (2021)* in the journal of "*Process Integration and Optimization for Sustainability*" as the third outcome of this thesis. In this chapter and for each of these articles; firstly, a short French summary of each article has been developed. This summary contains the main contents and results, and, the order of topics within the article. Secondly, the original text of the published article is embedded within the chapter.

2.1 Développement d’un nouvel outil interactif pour optimiser les réseaux d’eau industriels

Mots-clés : Minimisation de l'eau, Modélisation, Réutilisation, Eaux usées, Durabilité, Industrie de transformation

Cet article propose un outil interactif pour étudier les stratégies de réutilisation et de réduction de l'eau dans l'industrie de transformation. L'outil est basé sur une nouvelle approche simple pour minimiser la demande d’eau avec un seul ou plusieurs contaminants. L'étude de la récupération de l'eau convient aux nouvelles conceptions ou au réajustement de réseaux d’eau existants. Selon les exigences de qualité de l'eau, les options de réutilisation de l'eau sont limitées. Chaque opération utilisant de l'eau implique un transfert inévitable de polluants, ce qui augmente les concentrations dans le flux d'eau. En favorisant les options de réutilisation, la quantité d'eau propre diminue, mais les concentrations de polluants augmentent davantage. L’objectif de l’outil consiste à identifier un compromis entre la réutilisation maximale de l'eau, respecter les concentrations maximales de contaminants et respecter le transfert de masse minimal des polluants impliqués dans chaque opération. Une procédure algorithmique d’optimisation manuelle est développée et mise en œuvre dans le langage Python. Cette méthode permet de trouver toutes les possibilités de réutilisation et laisse les experts décider d’une bonne stratégie sur la base de considérations techniques. Cet outil peut être utilisé pour des problèmes mono et multi-contaminants. Une étude de cas de système multi-contaminant issue de la littérature a été appliquée pour le déploiement de cette méthode. Le schéma du réseau donne aperçu détaillé et automatisé du nouveau réseau d'eau modifié.

Dans la pratique, la méthode proposée aide les industries, en particulier les industries alimentaires, à utiliser toutes leurs possibilités de réutilisation pour réduire la demande en eau et rendre le réseau d'eau plus efficace et plus économique. De plus, cette méthode est l'une des moins chères et des plus faciles à appliquer. Cet outil proposera les réutilisations possibles et même de nouveaux réseaux d'eau modifiés en prenant en compte des contraintes industrielles supplémentaires. Dans cet article, pour justifier l'efficacité de cette méthode, un exemple de simulation est présenté. Tout d'abord, la première section explique le développement du modèle, la formulation mathématique, les bilans de masse et l'organigramme de l'algorithme. La section suivante présente la simulation conçue en cinq étapes ainsi qu'une étude de cas issue de la littérature. Les résultats finaux et le diagramme du réseau d'eau sont également présentés dans cette section. Dans ce travail, seul l'effet des flux de réutilisation a été considéré. Il est possible d'allouer manuellement des unités de régénération pour améliorer le réseau. La collecte des données auprès des industries est l'étape la plus critique pour trouver les résultats. Il y a différents défis dans les mesures et la recherche des indicateurs de polluants critiques.

The Second Article General Text

2.2 A novel user-friendly tool for minimizing water use in processing industry

2.2.1 Abstract

This article proposes a user-friendly tool for investigating water reuse and reduction strategies within the processing industry. The tool is based on a new, simple approach to targeting minimum freshwater systems with single or multiple contaminants. This method can be applied to the processing industry in general and in particular the food industry, which presents significant challenges for water-saving. The investigation of water recovery is suitable for the new design or revamping of the water network of continuous processes. According to the water quality requirement, the options for water reuse are limited. Each operation using water involves an inevitable transfer of pollutants, which increases the concentrations in the water flow. By promoting the reuse options, the freshwater decreases, but the contaminant concentrations increase further. The optimum design targets result from a tradeoff between the maximum water reuse, the maximum possible concentrations of contaminants, and the minimum mass transfer of pollutants involved within each operation. An algorithmic procedure for tradeoffs is developed and implemented in Python software language. One case study is used to demonstrate this targeting method.

Keywords: Water Minimization, Modelling, Reuse, Wastewater, Sustainability, Processing Industry

2.2.2 Introduction

Water is a unique and essential resource for the processing industries, and it isn't easy to replace. Minimizing the production of wastewater reduces the environmental impact and therefore reduces production costs. Applying all possible recycling, regeneration, and reuse opportunities in a sustainable water management framework is a crucial idea to reach this goal (Nemati-Amirkolaii et al., 2019). Climatic hazards and lack of fresh water and new European rules which aim to reach zero discharges (like Carbon, Nitrogen, Phosphorus, Acid, etc.) (2455/2001/EC and 2000/60/EC) show the importance of energy efficiency, which aims to improve the environmental and economic performance of industries.

The processing industry should apply the most economical and efficient methods and tools. Using high-performance water purification equipment is strongly recommended by the European Integrated Pollution Prevention and Control (IPPC) Directive (96/61/EC). However, the use of this equipment involves very high costs. (J Klemes et al., 2010). Therefore, it is necessary to apply systemic and strategic optimization methods to find the potential for minimizing water consumption and wastewater production by using reuse and recycling opportunities before integrating purification equipment. To reduce the use of water, in addition to the possibility of making major changes to the production system (renovation, advanced technology), there are less costly possibilities, such as water reuse, reuse with treatment, direct recycling, and recycling with treatment. Water can be reused directly in other operations for which the level of contamination is tolerable. Otherwise, reuse may require mixing the wastewater with freshwater to reduce the level of contamination. The reused water can be treated to partially remove contaminants. Reuse after treatment may require a supply of freshwater to reduce further the level of contamination. Recycling with treatment consists of reintegrating water into the operations in which it was previously used. For this, water treatment or mixing with freshwater is essential to respect the required concentration limit of contaminants.

Mathematical optimization methods can be applied to water network design. Optimization can be used to find the best available water network. The optimization procedure consists of minimizing or maximizing one or more objective functions. (Friedler et al., 1996). The recent work of Chen et al. (Chin et al., 2021) proposed a methodical resource targeting technique that takes care of water reuse and recycling by considering more than one contaminant. In parallel and to find the optimum point, a resource-allocation model is proposed as well. They tried and test several industrial case studies to shows the efficiency of the proposed method. Chen et al. (Chin et al., 2020) proposed another similar method that takes care of the cases by several contaminants. This method provides the graphical representation of the network in parallel with the minimum resource target search.

To increase the water use efficiency in the food sector with lower investment costs, optimization of water network systems through mathematical optimization strategies is interesting to achieve interesting water-saving with low investment costs. The water pinch method can reduce 20 to 40% of freshwater consummation and reduce production costs (Nemati-Amirkolaii et al., 2019). The range of reduction for freshwater use is 65 % in the palm oil mills sector (Chungsiriporn et al., 2006), and in beverage industries is around 27 % (Tokos and Novak Pintarič, 2009b). The range of reduction for wastewater produced in the dairy sector is 75 % (Buabeng-baidoo et al., 2017) (Peng et al., 2008) (Peng et al., 2001), and beverage industries are around 28% (Thevendiraraj et al., 2003a). These examples can encourage manufacturers to apply these methods. Identifying the water streams with the possibility of reuse and recycling is the key idea for minimizing water with these methods. In this article, a novel approach to reduce water use in the food industry has been developed and presented and the results are widely interpreted.

Within the reviewed literature, the mathematical models are one of the most reliable methods to be used. This work also focused on the development of an interactive tool based on a mathematical model. To develop the current model, different mathematical models are reviewed. (Buabeng-baidoo et al., 2017) proposed a multi-contaminant mathematical model based on superstructures, (Ahmetović et al., 2015) reviewed the different methods and models by clustering their different aspects, (Li and Guan, 2016) presented mathematical models by a stepwise optimal design for water networks, (De-León Almaraz et al., 2016) developed a two-stage methodology by the combination of water allocation network and heat exchange networks, (Mohammadnejad et al., 2011) presented a pinch based method by considering different combinations of contaminants, (Mughees and Al-Ahmad, 2015b) used graphical and mathematical integration techniques to have minimum waste and maximum direct recycle, (Boix et al., 2011) proposed a multi-objective optimization model to have an optimal industrial water network. This study provides an optimal design of multi-contaminant industrial water networks that brought some of these considerations from reviewed models by considering different goals.

In actual work, the proposed model is categorized as one of this group of methods. This proposed method helps the industries, especially food industries, use all their reuse possibilities to decrease freshwater consummation and set the water network in a more efficient and economic situation. There is no regeneration and no recycling opportunities in this method because they are costly, and our goal is to reduce the costs. Wastewater treatment processes can be integrated once the minimization step is performed. This method will find all reuse opportunities by considering the concentration limits of each pollutant. As a result, this method is one of the cheapest and also easiest ways to apply. This method will propose the possible reuses and even new modified water networks after using this method by considering all real-world limitations in a whole industry (piping limits, safety limits, distance limits, technical limits, etc.).

In this article, to justify the effectiveness of this method, an example of simulation is presented. First of all, the first section explains the development of the model, the mathematical formulation, the mass balances, and the algorithm's flowchart. The following section presents the simulation steps as well as a case study from the literature. The final results and the water network diagram are also presented in this section.

2.2.3 Model development

The optimization problem can be specified according to its objective type (minimization or maximization). Optimizing water networks involves minimizing the use of freshwater and the production of wastewater. There are constrained versus unconstrained problems; the water network consists of the formulation of equality and inequality constraints (upper concentration limits, the minimum number of interconnections, etc.) In linear versus nonlinear problems, non-linearity can be considered as a specificity of the water network optimization. Indeed, the behavior of decision variables on the objective functions does not necessarily satisfy the principle of proportionality. For example, the formulation of mass balances involves the product of mass flow rates and concentration differences. For continuous and discrete domains, the number of interconnections that present the recycling/reuse of water only makes sense if it is an integer or boolean. The other variables (flow, concentration) are continuous. In such cases, the problem is referred to as MINLPs, which involves nonlinear relationships with both integer (or boolean) and continuous variables.

The water network properties, which determine the objective function (s), are of two types: parameters and variables. Parameters refer to a set of characteristics that do not vary according to the choice to be made (e.g., maximum concentration thresholds). Variables refer to a collection of factors that may vary depending on the option to be made (e.g., water flowrate, recycling/reuse of water, water regeneration, etc.). The site manager's expertise can specify some variables. For example, for technical reasons, certain integration options can be decided before the optimization procedure (distance, difficulty in the coupling, health risk). Except for these exceptions, the variables manipulated by the optimization tools are called decision variables. The objective function (s) can be formulated in terms of a combination of decision variables. Indeed, the value of the objective functions can be modified by adjusting the decision variables.

The proposed model aims to identify the minimum consumption of freshwater and the minimum production of wastewater. The objective also consists of providing a final water network design while respecting the minimum of freshwater and the constraints of the maximum concentrations allowed in each operation.

2.2.3.1 Hypothesis

For the development of the model, first of all, the following assumptions are considered:

- a set of I water-using processes involving a set of K contaminants is assumed.
- the water network can be represented by three types of streams:
  - Freshwater (F_i) supply from a water source to process (i), with $i = 1 \cdots I$
  - Water-reuse (R_{ij}) from the process (i) to process (j), with $i, j = 1 \cdots I$ and $i \neq j$
  - Wastewater release (W_i) from the process (i), with $i = 1 \cdots I$
- water regeneration units are not included. Therefore, wastewater is not reintegrated into the operation in which it is previously used because wastewater treatment is required for this case.

- the operating regime of water use in each process is assumed to be continuous.
- the respective units of water and pollutant flow rates are m3/h and kg/h. So, it is easier to interpret the numerical results by limiting the number of decimals.

2.2.3.2 Material balances

The material balances are applied for each process and include overall (i.e. water) and component balances. Overall water balances are simplified in continuous mode since the accumulated water is negligible. For a process (i), The inlet and the outlet mass flow rate of water should be equal. the overall balance can be written as follows:

$$m_{i,in} \approx m_{i,out} \approx m_i \quad (3)$$

Where m is the mass flowrate of water, expressed in m^3/h.

The input stream includes a fraction of freshwater and possibly reused water from neighboring processes:

$$m_{i,in} = F_i + \sum_{j=1}^{I} R_{ji} \quad (4)$$

A fraction of the output water can be used in neighboring processes by respecting the limits concerning the concentration of the pollutants, and the remaining water is sent to the wastewater discharges:

$$m_{i,out} = W_i + \sum_{j=1}^{I} R_{ij} \quad (5)$$

For one contaminant (k), the material balance can be written as follows:

$$m_{i,in} C_{ki,in} + 1000 \times Q_{ki} = m_{i,out} C_{ki,out} \quad (6)$$

Where $C_{ki,in}$ and $C_{ki,out}$ are the concentrations of contaminant (k) at the boundaries of the process (i). The concentrations are expressed in ppm. Q_{ki} is the mass load of the contaminant (k) from side to side of the process (i). The mass load is expressed in *kg/h*. The mass load of pollution can be considered as a specific property of given water use. For example, a cleaning operation necessarily induces a minimum of the mass load, either from the equipment or the material to be washed. Below a certain mass load Q_{ki}, the washing operation can be considered imperfect. It is therefore essential to respect a minimum transfer of pollution within each process.

The input stream $m_{i,in}$ may combine two or more water reuses with different compositions. The mixing of flows can induce interference between the components (e.g., solubility, reaction), as it can also induce neutral behavior. To simplify the calculation, an equivalent mean concentration in the mixture is considered:

$$C_{ki,in} = \frac{\sum_{j=1}^{I} R_{ji} C_{kj,out}}{\sum_{j=1}^{I} R_{ji} + F_i} \quad (7)$$

2.2.3.3 Constraints and conditions for global optimization

To minimize the overall flowrate of freshwater, the possibility of water-reuse between the different processes must be maximized. Therefore, the supplying water of a given process must have the highest possible input concentration. The specification of the maximum pollution depends on several considerations, namely technological constraint (necessity to avoid fouling, corrosion), environmental constraint (odor problem), sanitary constraint (food safety risk), and also process safety considerations (water-reuse from or to ATEX zones). The determination of the maximum concentration allowed on the inlet and the outlet of each unit operation requires a risk analysis. Simple monitoring of pollution during the operation of the process is insufficient for estimating the maximum concentrations. Their determination requires expertise with several technical, regulatory, environmental, safety, and sanitary considerations. This analysis can be specific to each sector of the manufacturing industry. As with HACCP analysis, guidelines can be set at an industry level, but it is up to the company to determine its own thresholds based on its processes. Finally, these maximum thresholds will not necessarily be the thresholds used in the design of the new network. Any water supply line below these thresholds will meet process requirements. Even if some highest concentration thresholds at each process's boundaries are accepted, the final concentrations selected in the water network design may be below the limits. If a maximum concentration of a contaminant (k) at the input of an operation (i) accepted, the final concentration will be selected within the following interval:

$$0 \leq C_{ki,in} \leq C_{ki,in}^{max} \quad (8)$$

Where $C_{ki,in}^{max}$ is the maximum possible inlet concentration.

The same logic is also applied at the output. Therefore, by accepting a certain level of pollution at the output of the process, the final concentration will be selected within the following interval:

$$C_{ki,out}^{min} \leq C_{ki,in} \leq C_{ki,in}^{max} \quad (9)$$

Where $C_{ki,out}^{max}$ is the maximum possible outlet concentration. $C_{ki,out}^{min}$ is the concentration obtained at the output when the process is supplied only with freshwater:

$$C_{ki,out}^{min} = 1000 \times \frac{Q_{ki}}{m_{i,out}} \quad (10)$$

Several water flows and several concentrations can solve the problem of minimization. However, for a data set of mass flow rates and concentrations, a minimum transfer of pollution must be respected. For example, an increase in the inlet concentration requires a much higher flow rate than if it feeds with less loaded water. This is explained by the fact that each water use induces an inevitable transfer of pollution and a constant load of pollution for any configuration.

For a given process (i), since the water flowrate changes with the type of pollutant, a maximum value is selected to ensure the mass transfer of all the pollutants is satisfied:

$$F_i = \max_{k=1\cdots k} \left\{ 1000 \times \frac{Q_{ki} + \sum_{j=1}^{I} R_{ji} \times C_{kj}^{out}}{C_{ki}^{out}} - \sum_{j=1}^{I} R_{ji} \right\} \quad (11)$$

2.2.3.4 Procedure for solving water network optimization

The corresponding solution algorithm is presented in **Figure 14**. First of all, the maximum concentrations and the pollution load for each process should be specified. According to the data provided, an intermediate calculation procedure simplifies the recycling matrix (R). This consists of generating a sparse matrix since the recycled flows are not taken into account, and also, operations with freshwater restrictions are not supplied with reused streams. It is also possible to specify the matrix while avoiding: (1) any recycling of excessively loaded-water which risks exceeding the maximum concentrations, and (2) any coupling that could induce sanitary, environmental, or even technical risks. The values of input concentrations are then evaluated from equation 7. Secondly, water-reuse options are specified arbitrarily. It begins first with the estimate of the mass flowrate of freshwater (Equation 11) using the maximum concentration at the outlet ($C_{ki,out}^{max}$).

Finally, the last step consists of a debugging procedure by detecting errors in the material balances (Equations 3, 4, and 5), unexpected mass transfer of pollutants (recalculation by Equation 6), or even exceeding maximum concentrations (Equations 8 and 9). At the end of the third step, complementary routines (developed in Python software) provide a simple interface to display a detailed water-network drawing.

Thanks to the debugging information, the user will be able to refine the water-reuse matrix. For each tuning in the water-reuse matrix, the calculation resumes from calculating the mass flow rate of freshwater (Equation 11, step 2), and the result is updated. After a few iterations, the calculation converges, and the tuning possibilities become negligible.

Each time the user adjusts the reuse matrix, the algorithm provides all irregularities in the water balance, the transfer of pollution, and the exceeding of maximum concentrations. But this alert is not sufficient and must be approved by the user by considering other aspects not handled by the algorithm, such as technical, sanitary, or even safety constraints (e.g., risk of explosion, for example, due to hydrocarbon).

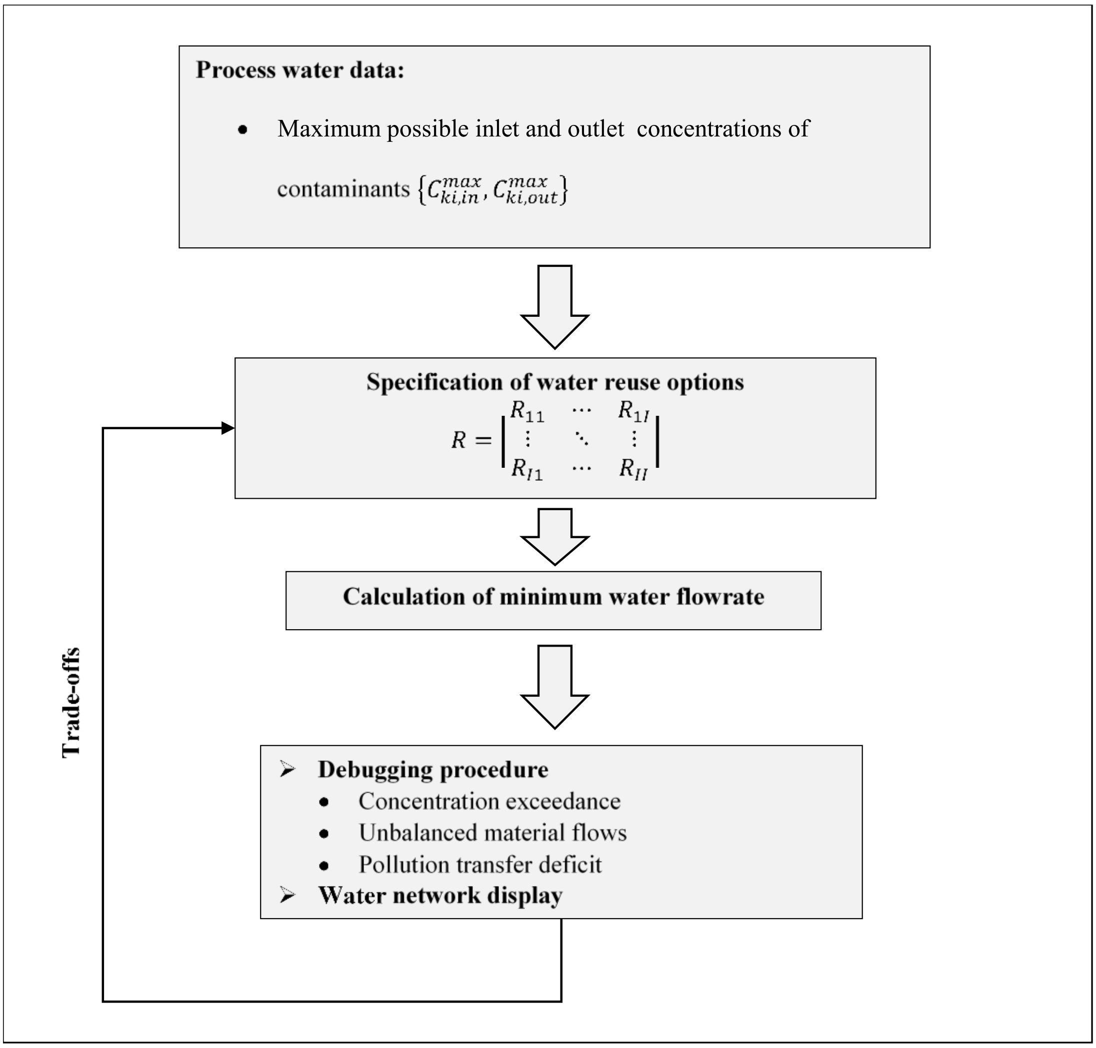

Figure 14. Logical algorithm for targeting minimum freshwater for single or multiple contaminants

2.2.4 Results and discussion

We need to identify and characterize the unit operations that use water, called water using processes, to apply this approach. We can inventory any water use for which water can be supplied from a clean source (freshwater), reused (polluted water), or a mixture of water with different levels of pollution. Once the water has been used, the water produced (loaded with pollutants) can be reused in other operations or sent to the WWTP. We can identify equipment cleaning, washing, or rinsing the product to be transformed or hydraulic transport. Water can also be used as a diluting agent or a lubricating fluid. Some uses of water are not considered, such as cooling or heating utilities. For example, demine water used for the production of hot water or steam constantly circulates in the factory and must return to the boiler. Therefore, this water cannot be reused otherwise. Consequently, we can consider very diverse uses that will be the subject of optimization to reduce water consumption at the plant level. This type of approach is not limited to a particular industrial sector but extends to all manufacturing sectors for which water-using processes are specified.

In this section, a simulation is performed to run the proposed model. A real data set brought from literature was used. The current simulation was performed in several iterations to find the best tradeoff between freshwater and reused water needed to satisfy the demand for operations. Besides the deep investigations in the food sector, this development aims to propose a generic tool to be suitable for different water-consuming sectors. For verifying the tool, benchmarking strategy is used by testing a simple and already tried dataset. In this step, the most important key is to use a dataset with a known result to be comparable. In the absence of these datasets in the food sector, a known and used dataset from the literature selected belongs to the petroleum sector. After this step, the verified tool will implement in food industries case studies as well.

A particular case study for a petroleum refinery (Feng et al., 2008) (Gunaratnam et al., 2005) was considered and analyzed to optimize the water network. The problem included five water processes and three contaminants (i.e., hydrocarbon (HC), hydrogen sulfide (H_2S), and suspended solids (SS)). The given data are the maximum inlet and outlet concentration of each contaminant for each process and the contaminant's mass load for each pollutant and process.

To optimize the water network design, 55 parameters should be identified, including 15 input concentrations, 15 outputs concentrations, a connection matrix with five recycles, and 20 reuses. But the final number of the parameter to be found will be less because, based on inventory data, operations 1 and 4 are supplied exclusively with freshwater. In this case, the water-network includes only 15 connection parameters to be determined.

2.2.4.1 Simulation states

The simulation runs in several steps. Manual and intermediate adjustments are made to respect the various constraints of the problem. The adjustments are made on the water-reuse matrix-like Matrix 12 (considered as the user's dashboard). For each modification of the matrix, a detailed result is instantly displayed. **Annex1** shows all iterations passed by the simulation. The explanation about the errors and debugging procedures is mentioned in the text, but each iteration's updated connection matrix and final information table are presented in detail. The result includes:

- The concentration of pollutants.
- The transfer of contaminants.
- The flowsheet of the water network (graph).
- Additional information to alert the user to certain irregularities (excess concentration, transfer of pollution not respected, or unbalanced flowrates).

First iteration

The first step is to propose the network without using any reuse or recycling opportunity and all freshwater supplies. in this state, the water-reuse matrix is equal to zero (no reuse opportunity):

$$R = \begin{bmatrix} - & 0 & 0 & 0 & 0 \\ 0 & - & 0 & 0 & 0 \\ 0 & 0 & - & 0 & 0 \\ 0 & 0 & 0 & - & 0 \\ 0 & 0 & 0 & 0 & - \end{bmatrix} \qquad (12)$$

This is a useful step to obtain the maximum amount of freshwater required for all operations without considering any reuse or recycling.

As presented in the last line of **Table 7**, the first simulation shows the actual amount of freshwater (153.61 m^3/h) corresponding to the whole process. This solution respects all inlet and outlet concentration limits. But this system is not benefited from possible reuses and even regenerations to save freshwater. This simulation aims to find all possible reuse opportunities to minimize the consumption of freshwater by respecting all considered limitations.

Table 7. Final results of the first iteration of the simulation

Process	Freshwater (m^3/h)	Contaminant	Mass load (kg/h)		Cin (ppm)		Cout (ppm)
			Simulation	**Lower limit***	**Simulation**	**Upper limit****	
Process 1	50.00	HC	0.75	0.75	0	0	15
		H2S	20.00	20.00	0	0	400
		SS	1.75	1.75	0	0	35
Process 2	33.18	HC	3.98	3.40	0	20	120
		H2S	414.80	414.80	0	300	12500
		SS	5.97	4.59	0	45	180
Process 3	54.82	HC	12.06	5.60	0	120	220
		H2S	2.47	1.40	0	20	45
		SS	520.80	520.80	0	200	9500
Process 4	8.00	HC	0.16	0.16	0	0	20
		H2S	0.48	0.48	0	0	60
		SS	0.16	0.16	0	0	20
Process 5	7.60	HC	1.14	0.80	0	50	150
		H2S	60.80	60.80	0	400	8000
		SS	0.91	0.48	0	60	120
Total	**153.61**	-	-		-		-

* minimum transfer of pollution, ** maximum allowed

Second iteration

Based on the literature's input data, processes 1 and 4 accept freshwater without any pollutants, so the amounts of possible reuse to these operations are null. The rest of the operations can accept the quantity of water reused from other processes. The second step is to calculate the approximate upper bound for all possible reuse flows. The calculated upper bound for each process presents the maximum capacity to accept the reused water from other processes. This calculated amounts for the process 2, 3, and 5 are 34 m^3/h, 56 m^3/h, and 8 m^3/h, respectively. These flow rate values are calculated from equation 4, using raw values of the problem provided in **Table 7** (ie, lower limit of pollutant transfers and maximum possible concentrations). These calculated amounts are the highest possible flow rates for each reuse stream (Upper bounds). The searching process to find the best amount of flowrate will start by this amount and will be optimized by considering the limitation of freshwater flow and concentration bounds.

The results of the second iteration do not meet all the input and output concentration limits. All concentration limits are respected, except in process 2 (input concentration of contaminants H2S and SS), in process 3 (input concentration of contaminant H2S), and process 5 (input concentration of contaminant SS).

Simulation continues until all of these errors are debugged, and the tradeoffs meet all upper limits. To improve the results, the simulation continues with further modifications in the following steps.

Third iteration

By applying the previous steps in the 25 possible connections, 13 connections were removed from the reuse opportunities. In this step, all critical reuse opportunities are reminded and carefully considered. Even if a single concentration among the three pollutants exceeds the upper limit, the opportunity for reuse can be considered unfeasible and takes an amount of 0 m^3/h. If the exceedance is very significant, this probability will increase. If the exceedance is minimal, there is the possibility of mixing the wastewater with freshwater for reuse and reducing freshwater consumption.

By considering this rule, six reuse opportunities will have the priority to be considered as the potential reuse interconnections that have more possibility to be optimized as presented in Matrix 13. The $R_{1,2}$, $R_{1,5}$, $R_{4,2}$, $R_{4,3}$, $R_{4,5}$, $R_{5,2}$ are the possible interconnections and reuse flows but not the definite ones because there is the possibility to mix the different streams while respecting the concentration constraint to finalize them as a reuse flow like the stream $R_{1,3}$ that will be used in the last iteration.

$$R = \begin{bmatrix} -\ 34\ 0\ 0\ 8 \\ 0 -\ 0\ 0\ 0 \\ 0\ \ 0 - 0\ 0 \\ 0\ 34\ 56 -\ 8 \\ 0\ 34\ 0\ 0 - \end{bmatrix} \quad (13)$$

It is necessary to mention that the values obtained at this iteration are the maximum possible ones for the nominated reuse opportunities. This means that the potential reuse streams cannot exceed these values, but they can be less or even eliminated, considering the limitations of concentrations. Accordingly, in this step, these values are considered upper limits of reuse opportunities, and these values will be edited step by step with the information on the technical limitations. Also, it is possible to mix the streams and add the new option called partial reuse. This partial reuse can be achieved by combining two used or more streams with fresh water. At first sight, all concentration limits are respected except in processes 2 and 3. These exceedances belong to contaminant HC, H2S, and SS in process 2 and contaminant H2S in process 3. A subsequent change in the maximum amount of reuse is necessary to set and meet all concentration limits to debug these errors.

Fourth iteration

In the fourth state, all six possible reuse opportunities were already obtained. In this step, tuning of reuse for process 3 has been done. There was an error about exceeding the upper limit of concentration (20 *ppm*) in contaminant H2S. By changing the reuse from operation four to process 3 $R_{4,3}$, this problem will be solved. This reuse will strictly respect the concentration limits by decreasing the flow rate from 56 m3/h to 18 m3/h.

In process 2, inlet concentrations of contaminant HC, H2S, and SS are exceeded. The exceeding of contaminant H2S is the most critical compared to HC and SS. By changing the flowrate from process 5 to process 2 ($R_{5,2}$) this problem can be solved. By changing the reuse $R_{5,2}$ from 34 m^3/h to 0 m^3/h, this reuse will strictly respect the concentration limits. in this iteration, all errors concerning the concentration of the pollutants are debugged. Another consideration should take into account about water balance in the input and the output of each operation. For example, process 4 has the inlet flow rate of 8 m3/h. the nominated processes to accept the reuse flow from process 4 can accept 34, 18, and 8 m3/h of water at their maximum, which is not possible (Limit is 8 m3/h). This amount should be allocated to one of these streams in the next and last iteration. The final updated interconnection is presented in Matrix 14:

$$R = \begin{bmatrix} -\ 34\ 0\ 0\ 8 \\ 0 -\ 0\ 0\ 0 \\ 0\ 0 - 0\ 0 \\ 0\ 34\ 18 -\ 8 \\ 0\ 0\ 0\ 0 - \end{bmatrix} \qquad (14)$$

Fifth iteration

By applying previous steps, five final potential reuse opportunities have been found. For some of these streams, the upper limits decreased already to handle the exceedance of concentration limits. The flow rate of process 4 of 8 m^3/h can be used to feed processes 2, 3, and 5. The best option is to use the whole amount to feed the process 2 ($R_{4,2} = 8\ m3/h$). In this case, the reuse opportunities $R_{4,3}$ and $R_{4,5}$ will be eliminated. Because process 1 is supplied with 50 m^3/h, the reuse possibilities to feed processes 5 and 2 are respectively, 8 m^3/h and 24.3 m^3/h. The optimized new values for reuse have been provided. The try and error procedure within the simulation allows the partial reuse, as well as the full reuse, flows to be obtained. For example, process 3 can accept the partial amount (2.6 m^3/h) of reuse from process 1 and mix it with the freshwater. By considering all mentioned tradeoffs, the final table of reuse opportunities and their total amounts *(m^3/h)* are presented in Matrix 15:

$$R = \begin{bmatrix} - \ 24.3\ 2.6\ 0\ 8 \\ 0 -\ 0\ 0\ 0 \\ 0\ 0 - 0\ 0 \\ 0\ 8\ 0 -\ 0 \\ 0\ 0\ 0\ 0 - \end{bmatrix} \qquad (15)$$

Table 8 and **Figure 15** present the final results of the simulation. The total freshwater consummation is 111.93 m^3/h. Also, around 43 m^3/h of required water for all the systems supplied by reuse water. For the same dataset and by using The MINLP procedure (Boix et al., 2011), results reported within the set of 30 answers combined fresh and regenerated water ranged between; [30 m^3/h freshwater + 223.4 m^3/h regenerated water], and [1627 m^3/h freshwater + 30 m^3/h regenerated water]. The different approaches for mathematical modeling and also solving procedures can explain these differences. In parallel, all inlet and outlet concentration limits are automatically respected by the embedded algorithm within the actual method (**Figure**

15). The final water network includes four reuse possibilities, which leads to a decrease in freshwater use.

Table 8. Final results of simulation in optimized situation

Process	**Freshwater (m^3/h)**	**Contaminant**	**Mass load (Kg/h)**		**Cin (ppm)**		**Cout (ppm)**
			Simulation	**Lower limit***	**Simulation**	**Upper limit****	
Process 1	50.00	HC	0.75	0.75	0	0	15
		H2S	20.00	20.00	0	0	400
		SS	1.75	1.75	0	0	35
Process 2	1.70	HC	3.56	3.40	15	20	120
		H2S	414.80	414.80	300	300	12500
		SS	5.11	4.59	30	45	180
Process 3	52.23	HC	12.02	5.60	1	120	220
		H2S	1.43	1.40	19	20	45
		SS	520.80	520.80	2	200	9500
Process 4	8.00	HC	0.16	0.16	0	0	20
		H2S	0.48	0.48	0	0	60
		SS	0.16	0.16	0	0	20
Process 5	0.00	HC	1.08	0.80	15	50	150
		H2S	60.80	60.80	400	400	8000
		SS	0.68	0.48	35	60	120
Total	**111.93**	-	-		-		-

* minimum transfer of pollution, ** maximum allowed

2.2.4.2 Discussion

In the work of (De-León Almaraz et al., 2016) (Boix et al., 2011), the MINLP procedure is applied in a lexicographic strategy, and the resolution is performed in *GAMS* software. For the ranking of the answers, *TOPSIS* and *GEC* methods are used. Furthermore, these methods are usually very time-consuming also require the right expertise in mathematical optimization tools. In the present study, the selection of solutions is performed manually while considering the user targets (i.e., limitations about flowrates, concentration, connections, etc.). Being user-friendly is the main benefit of using the actual method, besides the accuracy and less time-consuming. The method also provides graphical insights with less mathematical calculation. The user can modify the network and flows based on different limits and considerations and obtain new results. In the other aspects, based on the interface design, all of these steps are managed to be done in a graphical environment that makes it easy to use. Finally, the water network's design is reached without the need for in-depth knowledge about mathematical optimization.

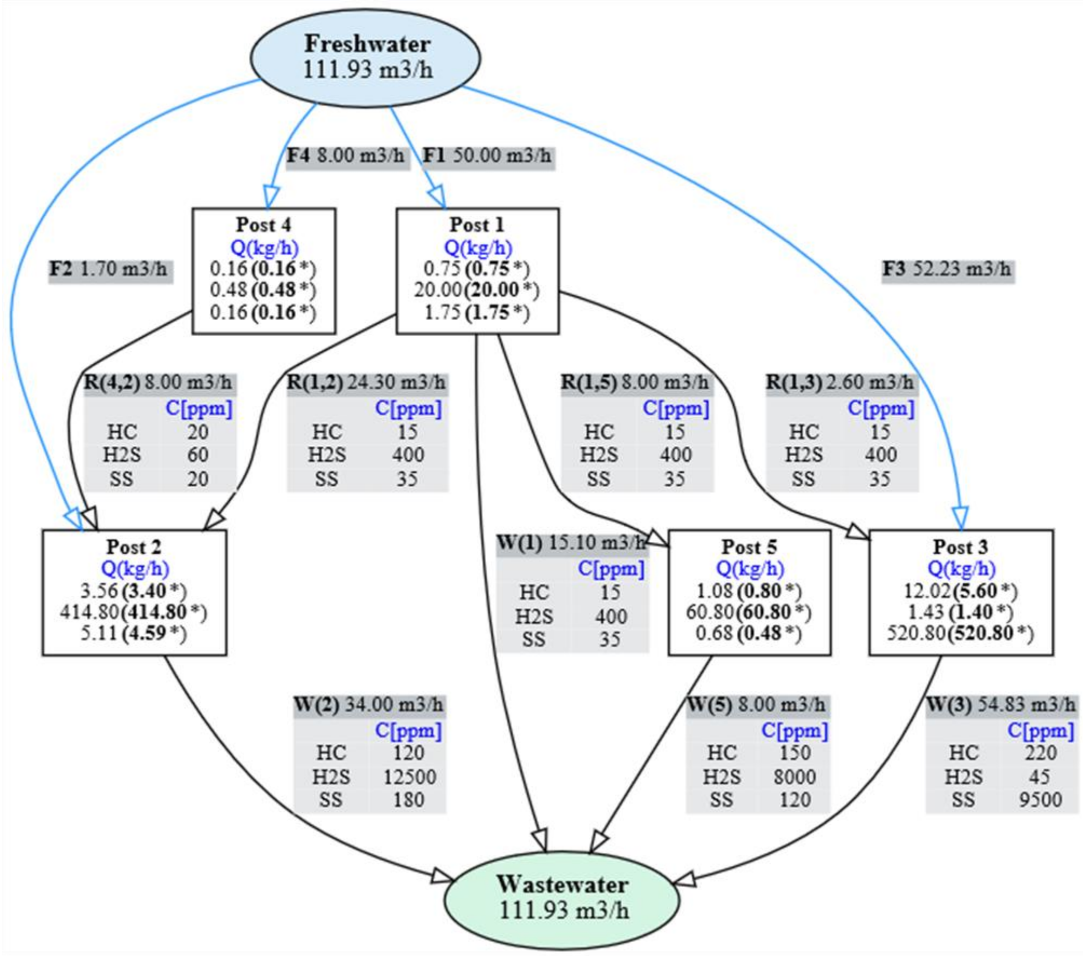

Figure 15. Final schematic of the optimized water network (* minimum transfer of pollution)

In this study, a simple relationship is considered between pollution transfer, water flow rate, and concentration difference between the inlet and the outlet of each water-using process. We also assumed an additivity relation to calculate an average concentration of two or more flows. But in reality, the mixing of flows and the transfer of pollutants could induce more complex phenomena (chemical reaction, interference between contaminants). Therefore, considering these phenomena requires more refined models, particularly in the field of petrochemicals. It is quite possible to integrate analytical relations or even more in-depth calculations into the current tool to obtain a compound matrix consistent with reality.

2.2.4.3 Conclusion

This work aims to maximize the benefits of reuse opportunities in water networks. This leads to different economic and environmental advantages. User-friendly tools and simulation-based procedures have been developed to find the maximum reuse capacity in water networks. This method finds all possible reuse opportunities and lets the experts decide based on technical consideration. This tool can be used for mono and multi-contaminant problems. An example from literature has been applied. The network's schematic provides a good insight into the new modified water network. As a result, the new network is optimized with an optimal water flow rate of 111.93 m^3/h. The network includes 4 reuses, with a total flowrate of 43 m^3/h. In this work, just the effect of reuse streams has been considered. There is a possibility to allocate regeneration units manually to improve the network. Even if the integration of a regeneration unit further reduces freshwater consumption, their technical feasibility, financial profitability, and environmental impact must be justified. Technical difficulties can limit the reuse of flows, such as the lack of space, several pollutants in the water (may require the implementation of several treatment steps), or low flow volumes (without economic interest). The integration of regeneration units requires additional investments in maintenance and operation. These water treatment costs should be compared to the savings on freshwater. When integrating regeneration units, the environmental impacts may be counterbalanced by the possible use of chemicals or excessive use of energy utilities (electricity) and even freshwater use. Collecting the data from industries is the most critical step for finding the results. There are different challenges in measurements, finding the critical pollutants indicators, etc. Manual optimization has several interests compared to automatic optimization. The manual method requires few computer resources, and therefore, fast computing time. Automatic methods require advanced algorithms to solve constrained optimization problems. Often a reconfiguration of the solver and further calculation to track the convergence and constraints violation are needed. The method developed in this work can be deployed quickly without advanced knowledge in optimization. The result of the water network is instantly updated in the form of a dynamic flowsheet. The calculation procedure is simple and provides more calculation flexibility, e.g., an additional economic calculation can be obtained in the same way as the water network design. However, the manual method is limited to small water networks. Optimizing a large number of connections may become a lengthy process and will therefore require an automatic calculation. For further research, using metaheuristic algorithms like NSGA-II for handling the more complicated models seems necessary. It helps to automatize all the steps within this algorithm, be faster and more accurate. Also, considering more limitations like the risks, the distance between operations, technical and engineering limits, etc., can be added to the tool.

2.3 Stratégies de réutilisation et de préservation de l'eau industrielle : Optimisation générique basée sur l'algorithme NSGA-II

Mots-clés : Réutilisation, préservation de l'eau, optimisation multi-objectifs, NSGA-II, industrie de transformation

Un outil de conception de réseaux d'eau industriels est développé. L'outil développé prend en charge les réseaux d'eau avec un ou plusieurs polluants. L'objectif est de concevoir des schémas optimisés de récupération de l'eau afin de préserver la demande en eau propre et minimiser la production d'eaux usées. La procédure d'optimisation est basée sur la résolution d'un problème multi-objectif avec des contraintes. Un modèle mathématique du problème d'optimisation est présenté. Les principales composantes du problème multi-objectif, y compris les fonctions objectives à minimiser, les variables de décision à optimiser et les contraintes à satisfaire, sont développées. Ce problème d'optimisation est résolu avec la méthode NSGA-II. Un algorithme de résolution est implémenté dans l'outil Python. Deux études de cas de la littérature sont résolues et discutées. Les deux études de cas incluent des systèmes mono-contaminant et multi-contaminants.

Des opérateurs personnalisés (échantillonnage, croisement et mutation) sont utilisés dans l'algorithme NSGA-II. Le développement et le test d’une version en régime permanent de l'algorithme NSGA-II ne permet pas d'obtenir les résultats attendus. Par conséquent, une version conventionnelle de l’algorithme a été mise en œuvre. La taille de la population et le nombre de descendants sont configurés à partir de simulations appliquées aux deux études de cas. Une telle configuration permet d'atteindre les résultats attendus avec une taille de population d'environ 100. Une analyse du comportement du programme pendant la résolution a été effectuée pour vérifier la convergence de l'algorithme et la gestion des contraintes. La convergence est vérifiée non seulement pour le résultat final mais aussi pour toutes les générations, ce qui est essentiel pour évaluer les performances de l'algorithme. A partir des solutions faisables, la violation des contraintes et les valeurs de l'espace objectif de la génération correspondante ont été extraites. Des techniques simples de visualisation sont utilisées pour suivre l'évolution des fonctions objectives et de la violation des contraintes au fil des générations. La représentation individuelle des fonctions objectives ou de la violation des contraintes est une procédure basique mais efficace pour vérifier la convergence de l'algorithme. En fonction du réseau d'eau à résoudre, le temps de calcul est plus ou moins rapide. Pour un réseau d'eau avec quatre processus et un seul contaminant, le programme converge en quelques secondes. Pour un réseau d'eau avec cinq processus et trois contaminants, le temps de calcul peut être six fois plus élevé pour une configuration avec une grande taille de population.

L'optimisation des réseaux d'eau pour les deux études montre des bilans de matière précis à la fois sur l'ensemble du réseau et sur une opération individuelle. L'algorithme traite strictement les contraintes pendant la phase de convergence. Ainsi, les limites supérieures des concertations des polluants sont respectées pour la réutilisation unique et les réutilisations multiples (c'est-à-dire les mélanges de plusieurs flux). Le transfert de masse de la pollution induite par chaque opération est également estimé en fonction de la charge minimale requise. Cette charge massique de pollution est considérée comme une propriété spécifique d'une consommation d'eau donnée. Il est essentiel de respecter un transfert minimal de pollution au sein de chaque processus. Pour un réseau d'eau avec un seul polluant, l'estimation du transfert de pollution correspond exactement au minimum requis. Cependant, pour un réseau d'eau avec plusieurs polluants, le transfert de certains polluants peut être estimé avec un léger surplus. Ce surplus est induit par un excédent de l'eau totale, nécessaire au transfert d'autres polluants dans la même opération. Dans le cas de contraintes strictes, qui imposent une limite supérieure pour le transfert de masse d'un ou plusieurs contaminants, il est possible d'ajouter des contraintes supplémentaires au problème d'optimisation. Enfin, l'étude de cas avec plusieurs contaminants montre qu'il est possible d'obtenir plusieurs solutions concurrentes. Les solutions révèlent des débits d'eau plus ou moins élevés correspondant à un réseau avec plus ou moins de couplages entre les opérations. Dans cette étude, le choix se fait en fonction de la solution ayant le minimum de demande en eau et de couplages. Mais ce choix peut être fait différemment en fonction d'autres critères économiques ou environnementaux.

Dans les sections suivantes, tout d'abord, la modélisation mathématique et la procédure NSGA-II sont présentées. Dans la deuxième partie, deux études de cas sont présentées et discutées. Les deux études de cas comprennent des systèmes mono-contaminant et multi-contaminants. L'algorithme évolutionnaire NSGA-II est utilisé comme méthode de résolution du problème d'optimisation. Une procédure de reconfiguration est développée afin d'adapter l'algorithme à l'optimisation du réseau d'eau.

The Third Article General Text

2.4 Multi-objective optimization of industrial water-network using evolutionary algorithms

2.4.1 Abstract

An industrial water network design tool is developed. The objective is to provide water networks with optimized water recovery schemes to preserve freshwater and minimize wastewater production. The developed tool supports water networks with one or more pollutants. The optimization procedure is based on solving a constrained multi-objective problem. Two main objectives are considered: (1) minimization of the quantity of freshwater necessary for the process and (2) the number of interconnections (called also reuses) in the water network. The interconnection minimization provides a simple network and limits the investment costs. According to the water quality requirement, water reuse options are limited for some processes. The restriction of water reuse is managed by constraints implemented in the optimization algorithm. Two case studies from the literature are presented and optimized. The two case studies include mono-contaminant and multi-contaminant systems. The evolutionary NSGA-II algorithm is used as a method of solving the optimization problem. A reconfiguration procedure is developed to adapt the algorithm to the optimization of the water network. Intermediate analysis steps are performed to check the convergence

and the violation of the problem constraints. Finally, two water networks of the two case studies are optimized and discussed.

Keywords: Reuse, Water preservation, Multi-objective optimization, NSGA-II, Processing industry

2.4.2 Introduction

One of the main factors limiting future food production is water. This resource is the basis for food security, livelihoods, industrial growth, and environmental sustainability. In 1995, the global freshwater withdrawal was estimated at 39 cubics (Seckler et al., 1998). By 2025, water withdrawal is expected to increase by at least 50 percent (Rosegrant et al., 2002). Agriculture is the largest water consumer with more than 70%, mainly due to the intensive irrigation of cereals and the intensive farming to produce meat and dairy products (Molden, 2013). Industrial water use is estimated at 20% (Molden, 2013). Unlike agriculture, the water taken by industry is not completely lost. Much is available for reuse in watersheds and rivers. However, industrial water is often polluted. Beyond the direct consumption of water for industrial or agricultural use, the problem is significantly related to virtual water, i.e., the quantity of water used to manufacture a consumer good. This is exactly the case with food products. One kilogram of red meat requires 5,000 to 15,500 liters of water, chicken 4,000 liters, cheese 4,900 liters, and rice 3,000 liters (Hoekstra and Chapagain, 2006). By importing food products, consuming countries subcontract not only food production but also the environmental and economic risks that can arise from the overexploitation of limited water reserves. Much of the water reserves are threatened by both water scarcity and pollution. This imminent crisis can be avoided by regulatory instruments, investment, and good management. Unfortunately, these solutions are not easy and require time, political commitment, and money. In contrast, water management reform in the industry can be rolled out quickly to deal with water scarcity and pollution. Implementing a systematic strategy to reduce water consumption is necessary for industry and, in particular, the food industry. But, regulations represent a major obstacle to the implementation of water conservation strategies in the food industry. Finding techniques for reusing water while respecting constraints related to health safety, food products' requirements, and the protection of processes is a great challenge.

In the food industries, water demand mostly requires high quality like potable water. This demand can be provided from different sources like rainwater, public water, drilling, and recycled/reused water. To meet the high-quality standards of food safety, extra-treatments are required. Because of the wide range of organic processed products in the food industries, a large amount of wastewater is produced. To minimize the environmental impacts of the effluents, the highest priority is to manage them (Nemati-Amirkolaii et al., 2019).

On the one hand, the stringent environmental regulation and the necessary considerations about fresh and wastewater in food industries make the correct treatments inevitable. Minimizing water consummation and wastewater generation is possible by installing expensive purification units. It needs a considerable investment and R&D time. The main challenge is to use extremely expensive processing equipment (J Klemes et al., 2010). Moreover, as the price of freshwater is still low; investment in processing equipment is unjustified. In this case, using cheaper and acceptable methods (water pinch and mathematical medialization, etc.) helps to optimize the water network. Using reuse/recycling opportunities before installing wastewater treatment equipment should be an economic strategy. Water pinch analysis optimizes freshwater use and wastewater production by identifying the potential water flows that can be reused for another process, where this water quality is acceptable. Some previous works in different food sectors like a brewery (Thevendiraraj et al., 2003a), sugar (Žbontar Zver and Glavič, 2005), citrus (Almato et al., 1999), and fruit juice (Tokos and Novak Pintarič, 2009a) shows; besides the environmental aspects, there are economic benefits from the application of water pinch analysis. From 23% up to 69% saving in investment by different fascinating payback periods from less than one week up to 4 months reported based on these four types of the food sector. The water pinch application in food industries shows a decrease in freshwater consummation and effluent production. Based on literature in food industries, the average reduction rate for freshwater ranged from 27% in the beverage industry (Tokos and Novak Pintarič, 2009) up to 65% in palm oil mills industries (Chungsiriporn et al., 2006). In parallel, the average reduction rate for effluent production ranged from 28% in the beverage industry (Thevendiraraj et al., 2003) to 75% in the dairy sector (Buabeng-Baidoo et al., 2017) (Peng et al., 2001). The first development of water pinch was the graphical tool to identify the minimum target for mono-contaminant water networks. Besides, the real case studies in food industries are multi-contaminant, large, and complex systems. In this case, the graphical methods aren't suitable to solve the multi-contaminant real-case problems. Therefore, design numerical tools and applying mathematical optimization for targeting the multi-contaminant system is necessary. In recent years, various mathematical models proposed to handle different water network problems in different industries like starch industry, pulp, and paper mill (Chin et al., 2021) (Chin et al., 2020), dairy industry (Buabeng-Baidoo et al., 2017), petroleum refinery (Li and Guan, 2016) (De-León Almaraz et al., 2016) (Boix et al., 2011), oil refinery (Mohammadnejad et al., 2011), refinery (Mughees and Al-Ahmad, 2015). The main challenge of mathematical programming is that Non-Linear problems are regularly Non-Convex. Therefore, it's hard to find the global optimum point.

Regarding real complex case studies that are multi-contaminant, using software like MATLAB® or PYTHON® is recommended to develop and solve the mathematical models belongs to them. They used to develop multi-criteria optimization methods. multi-constraint and multi-objective optimization algorithms, particularly evolutionary methods (GA, PSO, NSGA-II, etc.), are useful for taking care of these types of problems.

In this work; a tool for optimizing industrial water networks using the NSGA-II method is proposed. It aims to optimize all the opportunities for water reuse to save freshwater and reduce effluents. This tool provides an optimized graphic presentation of the water network. This tool is suitable for complex mono and multi-contaminant systems in the food industry and other processing sectors. In the following sections, first of all, the mathematical modeling and the NSGA-II procedure are presented. In the second part, two case studies are presented and discussed.

2.4.3 Water-network optimization

2.4.3.1 Mathematical formulation

The need to use multi-criteria and multi-objective optimization tools to optimize water-networks is presented in the previous section. Before proceeding to the optimization step, the water network problem must be formulated with mathematical equations. The mathematical equations include several objective functions with possibly several constraints that any feasible solution must satisfy (Deb et al., 2002). This study proposes water-network optimization with two objective-functions. The first objective-function is defined by the demand for freshwater required by the process operations. The second objective-function limits the number of couplings between process operations. The second objective is essential to target only realistic couplings and avoid unnecessary water flow (Friedler et al., 1996) (De-León Almaraz et al., 2016). The two objective-functions must be minimized. Before formulating the equations, we first define the water-network components, their representative parameters, and some hypothesis. We assume a water-network with a set of n water-using processes involving a set of K contaminants. The water-using processes are assumed as continuous operations. Each water-using process (i) is defined by three different parameters (**Table 9**).

Table 9. Parameters of water-using processes

Parameter	Unit
Maximum inlet concentrations	ppm
Maximum outlet concentrations	ppm
Minimum generated pollutant-load during the operating time	kg/h

With $i \in [1, n]$ and $k \in [1, K]$ respectively, for water-using process and contaminants. The Minimum generated pollutant-load can be considered as a specific property of a given water-using process. For example, a cleaning operation necessarily generates a minimum pollutant-load from the equipment or from the material to be washed.

Starting from n water-using processes, the final water network should include adequate interconnections between the different units to minimize freshwater and satisfy the needs in terms of water quality. It should be noted that connections, in general, can include reuse between operations and recycling in an individual operation. But this study is limited only to reuses. Water reuse is represented by the matrix R. One element of the matrix (R_{ij}) represents the reuse from the process (i) to process (j), with $i, j \in [1, n]$ and $i \neq j$.

This optimization problem consists of two antagonists' objective functions about the total freshwater of the network and the number of connections. The objective functions are separate, and there is no particular weight for each of them. In the optimization procedure, objective functions and defined constraints are considered simultaneously to find the set of competitive answers by respecting all limits. Below, we detail the main components of the multi-objective problem, including, objective-functions (to minimize), decision variables (to optimize), and constraints (to satisfy).

Objective Functions: (to be minimized)

For the optimization of the water-network, minimization of two objective functions f_1 (demand for freshwater) and f_2 (interconnection number) are considered:

$$\min \begin{cases} f_1 = \sum_{i=1}^{n} F_i \\ f_2 = \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \left(R_{i,j} \geq \varepsilon\right) \end{cases} \tag{16}$$

Where, F_i is the freshwater supply of process i, expressed in m^3/h. $R_{i,j}$ is the mass flowrate from process i to process j, expressed in m^3/h. ε is a threshold (expressed in m^3/h), below which the reuse is considered negligible.

The individual demand for freshwater F_i is evaluated as:

$$F_i = max\left\{\frac{m_{i,k}}{C_{i,k}^{out} - C_{i,k}^{in}}\right\}_{k=1\cdots K} \times 1000 \ - \sum_j R_{ji} \tag{17}$$

Where $m_{i,k}$ is the mass transfer of contaminant k in process i, $C_{i,k}^{in}$ and $C_{i,k}^{out}$ are the inlet and outlet concentrations of contaminant k in process i, and $R_{j,i}$ is the mass flowrate from process j to process i. The first term on the left side of the equation represents the limiting water profile. Since this profile changes with the type of pollutant, a maximum value is used to satisfy all the pollutants' mass transfer.

Decision variables

The matrix R represents all possible reuse streams between the processes. This matrix act as a space for the decision parameters.

$$[O] \leq R \leq R^U \tag{18}$$

With, R^U is the upper bound of the reuse matrix. The upper bound of the mass flowrate from process i to process j ($R^u_{i,j}$), corresponds to the maximum amount of water that can be supplied by operation i. This flowrate can be estimated from the maximum demand for freshwater:

$$R^u_{i,j} = F^{max}_i \tag{19}$$

Constraints

One of the characteristics of stochastic optimization is that the objective functions constitute a multi-dimensional space. This multi-dimensional space can be represented by a single solution or a set of solutions, called decision variable space (Deb et al., 2002). In the case of an unconstrained optimization problem, the search takes place at any point in large decision space. In water-networks optimization, the research space can include many biased answers with critical features, e.g., unbalanced material flows or exceeding pollution thresholds. To avoid this problem, water-balance constraints and limiting-concentration constraints are considered.

As the total inlet and outlet water flowrate of each process should be equal, Each water-using process (i) is subject to water-balance constraint:

$$F_i + \sum_{j=1}^{n} R_{ji} \geq \sum_{j=1}^{n} R_{ij} \tag{20}$$

Where $F_i + \sum_{j=1}^{n} R_{ji}$ is the total mass flow supplied to process i, and $\sum_{j=1}^{n} R_{ij}$ is the total mass flow available from process i.

Since each operation can be supplied with several flows with different concentrations, the average flow must respect the concentration limit for each pollutant:

$$\frac{\sum_{j=1}^{n} R_{ji} \times C^{out}_{j,k}}{F_i + \sum_{j=1}^{n} R_{ji}} \leq C^{in}_{i,k}\Big|_{max} \tag{21}$$

Where $\frac{\sum_{j=1}^{n} R_{ji} \times C^{out}_{j,k}}{F_i + \sum_{j=1}^{n} R_{ji}}$ is the average concentration of contaminant k in the feed stream of process i. $C^{in}_{i,k}\Big|_{max}$ is the maximum inlet concentrations of process i.

2.4.3.2 Solving method: NSGA-II multi-objective algorithm

The minimization algorithm consists of finding a set of solutions without violation of any constraints. Since the problem can involve several local minima, obtaining a global minimum requires the use of global optimization routines. NSGA-II (Non-dominated Sorting Genetic Algorithm II) provides common routines to global constrained problems (Deb et al., 2002) (Li et al., 2014). Basic routines follow the general outline of a genetic algorithm GA with a modified mating (crossover and mutation) and survival selection (**Figure 16**). The optimization procedure starts with a set of initial solutions (population) from which a new population will be generated. In the beginning, the initial population should be sampled. Using well-distributed sampling increases the robustness and convergence of genetic algorithms (Poles et al., 2009). In this study, the sampling is applied randomly on the decision parameters (i.e., the reuse matrix R) while considering the lower and upper limits of the problem (Equation 18).

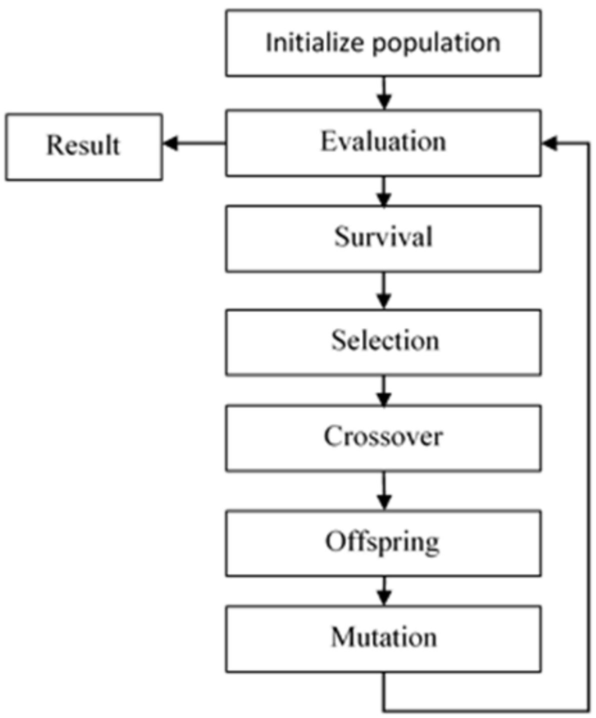

Figure 16. Genetic algorithm Algorithmic steps

The evaluation step consists of associating with each solution a fitness value by using the objective-functions f_1 and f_2. After that, the solutions are ranked according to their fitness level. Since the problem involves constraints, each solution can be either feasible or infeasible. The effect of using constraints is that any feasible solution has a higher non-domination level than any infeasible solution. However, among the two infeasible solutions, the solution with a smaller constraint violation has a better rank. Constraint violation is computed by the normalized violation of all constraints (Equations 20 and 21).

Before the recombination process and the generation of a new population, the current solutions must be selected to participate in the mating step. Different methods of selection can increase the convergence of the algorithm. The solutions can be chosen randomly (random selection) with a permutation procedure to avoid repetitive individuals. To improve convergence, a tournament selection is used instead of random selection (Goldberg et al., 2014). After selection, a crossover operator combines selected solutions into one or several offsprings. Simulated binary crossover SBX is used (Deb et al., 2002) with a probability of 0.9 and a distribution index of 15. Finally, the mutation step is carried out after the creation of offspring by crossing. Each child solution, created by the crossover operator, is then muted with a mutation probability, set at $1/(size(R))$, so that on an average one variable gets mutated per solution (Deb et al., 2007).

This problem formulation is implemented in Python using $pym\infty$ package (Blank and Deb, 2020). The Objective function and inequality constraints have to inherit from $pym\infty - class$. By calling the superclass, lower and upper variable boundaries are supplied. The objective-functions and constraints are overwritten from the superclass and take as an input a two-dimensional array with the number of offsprings as columns and number of rows of 2 and $n(1 + K)$, respectively for objective-functions and constraints.

2.4.4 Result and discussions

In the previous section, the proposed model and the optimization procedure are presented in detail. To justify the performance of the current tool, two case studies from the literature are analyzed. Mono and multi-contaminant water networks are selected to show the current tool's capacity to handle different systems. To solve the optimization problem with the NSGA-II algorithm, it is necessary to configure the optimization method. This configuration of NSGA-II is a challenge in itself, as it requires specifying parameters like population size or even the number of offspring.

The configuration also requires setting elementary calculation methods (also called operators) such as sampling, selection, mutation, and crossover. Such a configuration will influence the convergence and the respect (or violation) of the problem constraints. During the first simulation tests, we found an evident influence in the choice of population size, the number of offspring. For the execution of the NSGA-II method, it is necessary to define a termination criterion. There are two possibilities: (a) a stop after the calculation of a maximum number of generations, or (b) a termination according to a convergence tolerance in the design space (objective functions) and convergence in the constraints. In this simulation, a tolerance of 10^{-6} was defined. A maximum of the generation of 1000 is also provided if convergence is not reached. The tolerance calculation is evaluated not only on the last generation but also on a sequence of n previous generations. In this study, the tolerance calculation is smoothed over the previous 20 generations preceding the nth generation.

The automated optimization tool has been developed in this section. Before all, to validate the tool, it's necessary to test and benchmark it with some known dataset. To check the generality of the tool, two types of the dataset have been selected: one mono-contaminant system and one multi-contaminant system. The most known and frequently used dataset about water networks in the literature belongs to (Wang and Smith, 1994) for the mono-contaminant system and (Feng et al., 2008) (Gunaratnam et al., 2005) multi-contaminant system. These two datasets were tested by the tool, and the results are reported below.

2.4.4.1 First case study: mono-contaminant system

Hypothetical data (Wang and Smith, 1994) are selected as a mono-contaminant water system in the proposed tool. **Table 10** shows the inventory data of a water-network, including four water-using processes and one contaminant. Columns two, three, and four in **Table 10** represent limiting data, i.e., maximum inlet (C_{in}^{max}) and outlet (C_{out}^{max}) concentrations; and the mass load of contaminant through each process. The last column of **Table 10** presents the limiting water flowrates obtained by considering a linear relationship between the mass transfer and the concentration difference (which is still valid for a diluted system).

Table 10. Inventory water data for first case study (Y. P. Wang and Smith, 1994)

Process	Mass load (kg/h)	C_{in}^{max} ppm	C_{out}^{max} ppm	water flowrate (m^3 /h)
Process 1	2	0	100	20
Process 2	5	50	100	100
Process 3	30	50	800	40
Process 4	4	400	800	10

For the optimization of the water network, we consider the minimization of two objective functions f_1 and f_2:

$$min: f_1(R) = F_1 + F_2 + F_3 + F_4 \quad (22)$$

$$min: f_2(R) = \sum_{\substack{i,j=1 \\ i\neq j}}^{4} (R > 10^{-3}\ m^3/h)_{i,j} \quad (23)$$

With, f_1 is the sum of the freshwater flow rates required for the four processes, and f_2 includes the number of interconnections (i.e., reuses). To avoid the presence of micro-flows in the final water-network, only the solutions greater than $10^{-3}\ m^3/h$ are counted in the objective function f_2.

The formulation above defines two-objective optimization problems with 4×4 variables defined in the reuse matrix R. If we consider the freshwater requirement of the first process and if we remove all recycling; the optimization problem will be presented with only nine variables (Matrix 24):

$$R = \begin{bmatrix} 0 & R_{1,2} & R_{1,3} & R_{1,4} \\ 0 & 0 & R_{2,3} & R_{2,4} \\ 0 & R_{3,2} & 0 & R_{3,4} \\ 0 & R_{4,2} & R_{4,3} & 0 \end{bmatrix} \quad (24)$$

Moreover, for each possible reuse stream, variable $R_{i,j}$ with its lower and upper boundaries are defined::

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \leq R \leq \begin{bmatrix} 0 & 20 & 20 & 20 \\ 0 & 0 & 100 & 100 \\ 0 & 40 & 0 & 40 \\ 0 & 10 & 10 & 0 \end{bmatrix} \quad (25)$$

Initially, the above problem is subject to 8 inequalities $(4 + 4)$. Since the first process is supplied with fresh water, its constraint related to the maximum concentration is already satisfied. The number of constraints for this dataset is, therefore, equal to 7 inequalities $(4 + (4 - 1))$. Three constraints belong to the pollutant inlet concentration limits and four constraints belong to the water balances for each of these 4 processes. Process1 don't need the concentration limit as there is an obligation to be supplied by the freshwater:

$$\begin{bmatrix} C_{in,2} \\ C_{in,3} \\ C_{in,4} \end{bmatrix} \leq \begin{bmatrix} 50 \\ 500 \\ 4000 \end{bmatrix}_{\mathrm{ppm}} \tag{26}$$

$$\mathrm{F}_1 \geq \mathrm{R}_{1,2} + \mathrm{R}_{1,3} + \mathrm{R}_{1,4} \tag{27}$$

$$\mathrm{F}_2 + \mathrm{R}_{1,2} + \mathrm{R}_{3,2} + \mathrm{R}_{4,2} \geq \mathrm{R}_{2,3} + \mathrm{R}_{2,4} \tag{28}$$

$$\mathrm{F}_3 + \mathrm{R}_{1,3} + \mathrm{R}_{2,3} + \mathrm{R}_{4,3} \geq \mathrm{R}_{3,2} + \mathrm{R}_{3,4} \tag{29}$$

$$\mathrm{F}_4 + \mathrm{R}_{1,4} + \mathrm{R}_{2,4} + \mathrm{R}_{3,4} \geq \mathrm{R}_{4,2} + \mathrm{R}_{4,3} \tag{30}$$

In this case study, we performed initial simulations to find the best parameters setting for NSGA-II (i.e., population size and the number of offsprings). The result of the simulation is presented in **Table 11**. The first two columns show the population size and number of offspring. Only the final results (i.e., after convergence) are presented, namely the objective space values (f_1 and f_2), the number of generations, and the time required to run the algorithm. Before starting the simulation with a population size equal to the number of offsprings, a steady-state version of NSGA-II was tested by creating a single new member for insertion into the population at each step of the algorithm (Mishra et al., 2016). Despite a rapid convergence of the steady-state algorithm, it is almost impossible to target the expected result. Therefore, we have chosen to set the number of offsprings equal to the size of the population (**Table 11**). The expected minimum of freshwater (90 m3/h) is easily obtained for most of the configurations. However, the minimization of the number of connections is more frequently achieved for the largest populations. The global minimum (90 m3/h, 2 reuses) is reached from a population size of 100. The result shows a clear trend between the increase in population size and the number of generations at convergence.

The increase in the number of generations improves the quality of the result with a slight increase of simulation time which remains globally comparable (a few seconds).

Table 11. NSGA-II runs with different population size and number of offspring (case study 1, *expected minimum)

Population size	**Number of offspring**	**Objective spaces values**		**Number of generations**	**Elapsed time** (s)
		$\mathbf{f_1 (m^3/h)}$	$\boldsymbol{f_2}(-)$		
40	40	90.02	4	25	0.40
40	40	90.55	3	25	0.40
60	60	90.01	4	30	1.08
60	60	90.08	3	30	1.08
60	60	90.23	**2***	30	1.08
80	80	**90.00***	3	45	2.08
80	80	95.61	1	45	2.08
80	80	90.47	**2***	45	2.08
100	100	**90.00***	**2***	74	4.46

After obtaining the results, we carry out post-processing to analyze the program's behavior during the resolution, check the algorithm's convergence, and explore the constraints (supposed to be respected). For such an analysis, intermediate steps of the algorithm need to be assessed. This is achieved by storing a deep copy of the algorithm results on each generation. First, we need to extract the population for each generation of the algorithm. After that, each population is filtered, retaining only the feasible-solutions. Then, from the feasible-solutions, we extract the constraint violation and the objective space values (f_1, f_2) of the corresponding generation. The convergence graph (**Figure 17**) shows the improvement over the generation of the objective space values. The population size and the number of offspring are set at 100. Some generations are not presented since they include non-feasible populations. The individual representation of objective functions is a basic but efficient procedure to check the algorithm's convergence.

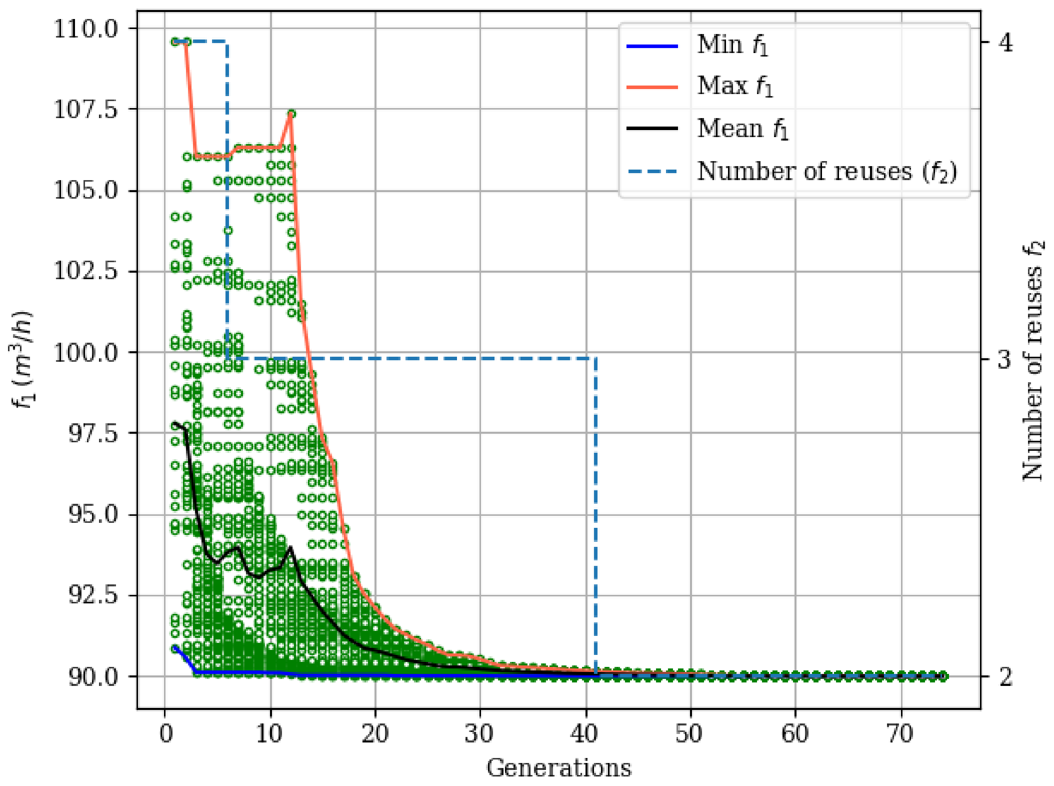

Figure 17. Variation of objective-functions throughout generations, case 1, population size = 100, number of offspring =100

So far, we have found the set of converging solutions that are considered as good as possible concerning both objectives (f_1, f_2). The goal is also to find a set of solutions that don't have any violation of constraints. According to **Figure 18**, the first generation with a feasible solution is identified at the tenth generation level. The constraints of the problem were not respected between the first and the tenth generation, and the constraints are respected during the convergence phase of the program.

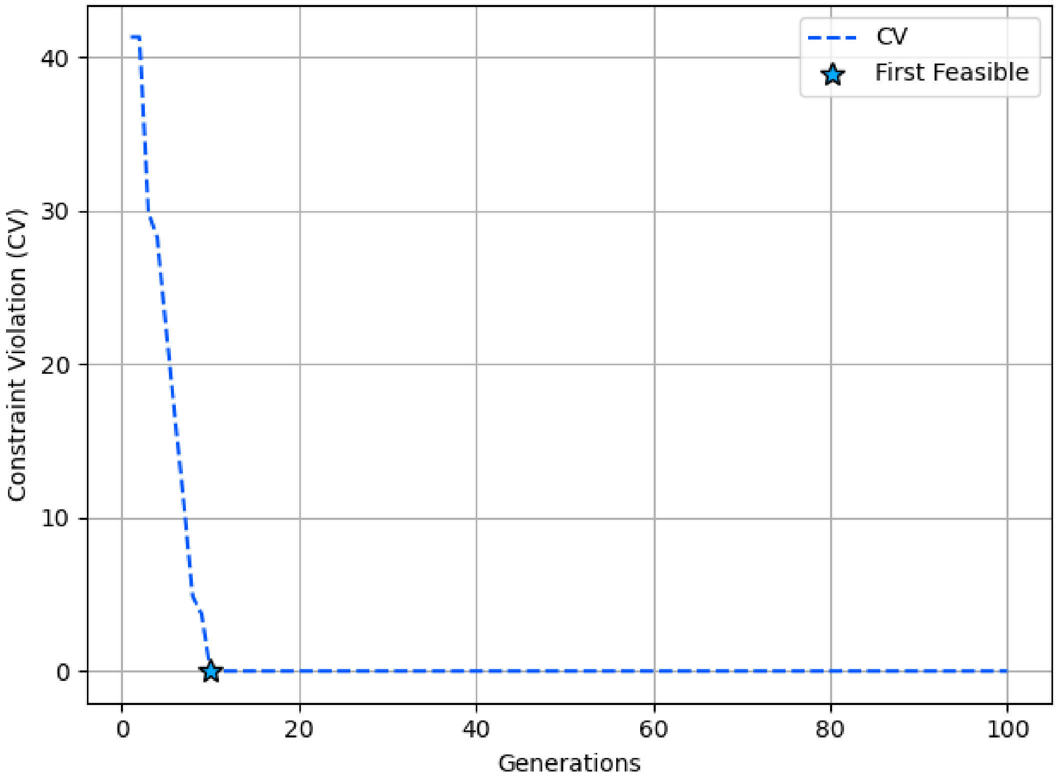

Figure 18. Constraint violation, case 1, population size = 100, number of offspring = 100

Figure 19 shows the water network design, which corresponds to a simulation with population size and the number of offsprings of 100. Water balance is respected with a corresponding freshwater and wastewater of 90 m3/h. Processes 1 and 2 are supplied exclusively with freshwater, with 20 and 50 m3/h, respectively. The estimate of the pollution transfer corresponds to the minimum transfer required by process 1 and process 2, i.e., 2 and 5 kg/h, respectively. Process 3 is supplied with a mixture of freshwater (20 m3/h, 0 ppm) and reused water from process 2 (20 m3/h, 100 ppm). The resulting stream (40 m3/h) has a concentration of 50 ppm, which corresponds to the pollution threshold required by process 3. The estimate of the pollution transfer corresponds to the minimum transfer required by process 3, i.e., 30 kg/h. Process 4 is supplied with 5.71 m3/h at 100 ppm from post 2. The pollution concentration (100 ppm) is below the threshold required by operation 4 (800 ppm) and the calculated mass load of contaminant corresponds to the minimum involved by process 4 (4.00 kg/h).

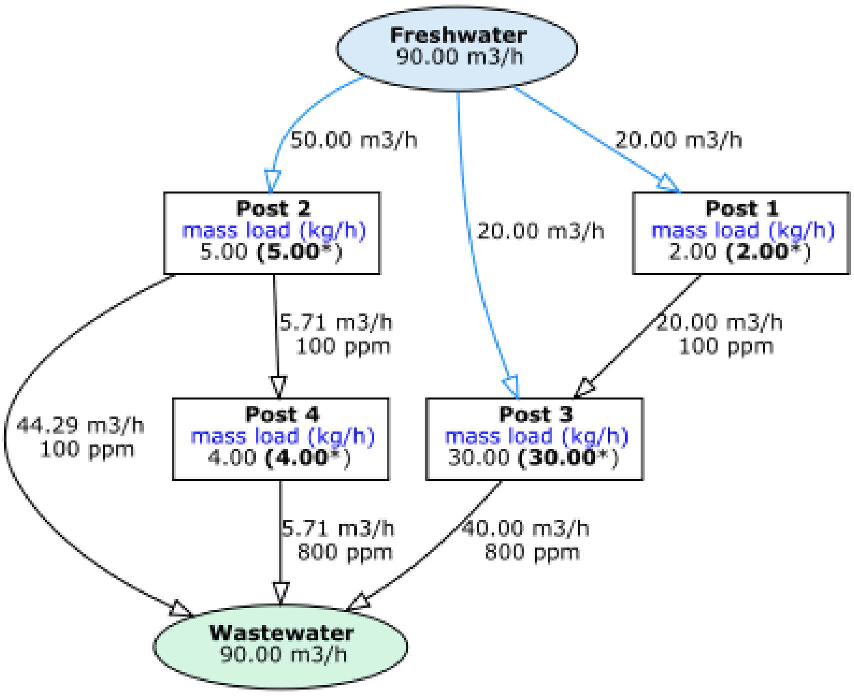

Figure 19. water-network, case 1, population size = 100, number of offspring = 100, *minimum mass load of contaminant

2.4.4.2 Second case study: multi-contaminant system

Case study two shows a multi-contaminant example with five processes representing five water uses and three contaminants. **Table 12** shows the inventory data, i.e., maximum inlet (C_{in}^{max}) and outlet (C_{out}^{max}) concentrations of contaminants (A, B, and C); and the mass load of each pollutant through each process (Feng et al., 2008) (Gunaratnam et al., 2005). The last column of **Table 12** presents the limiting water flowrates obtained by considering a linear relationship between the mass transfer and the concentration difference.

Table 12. Inventory water data for case study 2 (Feng et al., 2008) (Gunaratnam et al., 2005)

Process	Contaminant	Mass load (kg/h)	C_{in}^{max} ppm	C_{out}^{max} ppm	water flowrate (m3/h)
Process 1	A	0.75	0	15	50
	B	20.00	0	400	
	C	1.75	0	35	
Process 2	A	3.40	20	120	34
	B	414.80	300	12500	
	C	4.59	45	180	
Process 3	A	5.60	120	220	56
	B	1.40	20	45	
	C	520.80	200	9500	
Process 4	A	0.16	0	20	8
	B	0.48	0	60	
	C	0.16	0	20	
Process 5	A	0.80	50	150	8
	B	60.80	400	8000	
	C	0.48	35	120	

For the optimization of the water network, we consider the minimization of two objective functions f_1 and f_2:

$$min{:}\, f_1(R) = F_1 + F_2 + F_3 + F_4 + F_5 \quad (31)$$

$$min{:}\, f_2(R) = \sum_{\substack{i,j=1 \\ i \neq j}}^{5} (R > 10^{-3}\ m^3/h)_{i,j} \quad (32)$$

With, f_1 is the sum of the freshwater flowrates required for the five processes, and f_2 includes the number of interconnections (i.e., reuses).

The formulation above defines a two-objective optimization problem with 5×5 variables defined in the reuse matrix R. If we consider the freshwater requirement of the first and fourth processes and if we remove all recycling; the optimization problem will be presented with only 12 variables (Matrix 33):

$$\mathrm{R} = \begin{bmatrix} 0 & \mathrm{R}_{1,2} & \mathrm{R}_{1,3} & 0 & \mathrm{R}_{1,5} \\ 0 & 0 & \mathrm{R}_{2,3} & 0 & \mathrm{R}_{2,5} \\ 0 & \mathrm{R}_{3,2} & 0 & 0 & \mathrm{R}_{3,5} \\ 0 & \mathrm{R}_{4,2} & \mathrm{R}_{4,3} & 0 & \mathrm{R}_{4,5} \\ 0 & \mathrm{R}_{5,2} & \mathrm{R}_{5,3} & 0 & 0 \end{bmatrix} \tag{33}$$

Moreover, for each variable $R_{i,j}$ lower and upper variable boundaries are defined:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \leq R \leq \begin{bmatrix} 0 & 50 & 50 & 0 & 50 \\ 0 & 0 & 34 & 0 & 34 \\ 0 & 56 & 0 & 0 & 56 \\ 0 & 8 & 8 & 0 & 8 \\ 0 & 8 & 8 & 0 & 0 \end{bmatrix} \tag{34}$$

Initially, the above problem is subject to 20 inequalities $(5 + 5 \times 3)$. Since the first and fourth processes are supplied with freshwater, their constraints related to the maximum concentrations are already satisfied The number of constraints is therefore reduced to 14 inequalities $(5 + (5 - 2) \times 3)$. Nine constraints belong to the pollutant inlet concentration limits (except for Process 1 and 4) and five constraints belong to the water balances for each of these 5 processes.:

$$\begin{bmatrix} \mathrm{C}_{\mathrm{in},2}^{\mathrm{A}} \\ \mathrm{C}_{\mathrm{in},2}^{\mathrm{B}} \\ \mathrm{C}_{\mathrm{in},2}^{\mathrm{C}} \end{bmatrix} \leq \begin{bmatrix} 120 \\ 12500 \\ 180 \end{bmatrix}_{\mathrm{ppm}} \tag{35}$$

$$\begin{bmatrix} \mathrm{C}_{\mathrm{in},3}^{\mathrm{A}} \\ \mathrm{C}_{\mathrm{in},3}^{\mathrm{B}} \\ \mathrm{C}_{\mathrm{in},3}^{\mathrm{C}} \end{bmatrix} \leq \begin{bmatrix} 220 \\ 45 \\ 9500 \end{bmatrix}_{\mathrm{ppm}} \tag{36}$$

$$\begin{bmatrix} \mathrm{C}_{\mathrm{in},5}^{\mathrm{A}} \\ \mathrm{C}_{\mathrm{in},5}^{\mathrm{B}} \\ \mathrm{C}_{\mathrm{in},5}^{\mathrm{C}} \end{bmatrix} \leq \begin{bmatrix} 150 \\ 8000 \\ 120 \end{bmatrix}_{\mathrm{ppm}} \tag{37}$$

$$\mathrm{F}_1 \geq \mathrm{R}_{1,2} + \mathrm{R}_{1,3} + \mathrm{R}_{1,5} \tag{38}$$

$$\mathrm{F}_2 + \mathrm{R}_{1,2} + \mathrm{R}_{3,2} + \mathrm{R}_{4,2} + \mathrm{R}_{5,2} \geq \mathrm{R}_{2,3} + \mathrm{R}_{2,5} \tag{39}$$

$$F_3 + R_{1,3} + R_{2,3} + R_{4,3} + R_{5,3} \geq R_{3,2} + R_{3,5} \quad (40)$$

$$F_4 \geq R_{4,2} + R_{4,3} + R_{4,5} \quad (41)$$

$$F_5 + R_{1,5} + R_{2,5} + R_{3,5} + R_{4,5} \geq R_{5,2} + R_{5,3} \quad (42)$$

The implementation of the steady-state version of NSGA-II doesn't provide the expected result. So, the algorithm is configured in the same way as the first case study (i.e. population size equals the number of offsprings). The result of the simulation of the second case study is presented in **Table 13**. The global minimum (111.87 m3/h, 4 reuses) is obtained for a population size equal to 100. The result does not show a clear trend between population size and the number of generations, since the number of generations decreases from 392 to 185 as the population size increases from 60 to 80.

Table 13. NSGA-II runs with different population size and number of offspring (case study 2, *expected minimum)

Population size	**Number of offspring**	**Objective spaces values**		**Number of generations**	**Elapsed time** (s)
		$\mathbf{f_1(m^3/h)}$	$f_2(-)$		
40	40	112.59	**4***	205	7.59
40	40	121.91	2	205	7.59
40	40	114.48	3	205	7.59
40	40	112.26	5	205	7.59
60	60	113.24	3	392	20.05
60	60	128.44	1	392	20.05
60	60	120.75	2	392	20.05
80	80	113.26	3	185	13.58
80	80	**111.89***	5	185	13.58
80	80	120.75	2	185	13.58
80	80	111.90	**4***	185	13.58
100	100	**111.87***	**4***	295	24.72
100	100	113.24	3	295	24.72
100	100	121.04	2	295	24.72

In the result proposed by the algorithm, we can identify solutions with several reuses less than 4, but with a higher amount of freshwater. Solutions with three, two, and one connection(s) require more freshwater, approximately 113, 121, and 128 m3/h, respectively. Therefore, the optimization problem presents a conflicting behavior between the objective-functions. A solution with a minimum of freshwater will not necessarily be the ideal solution in terms of the number of reuses. On the contrary, a solution having a minimum number of reuses requires a surplus of freshwater. **Figure**

20 shows this conflicting behavior of the two objective-functions. Initially, **Figure 20** is established to check the convergence of the optimization algorithm. The progress of the two objective-functions during the convergence phase shows three main dominant solutions (111.87 m3/h, 4 reuses), (113.56 m3/h, 3 reuses), and (121.23 m3/h, 2 reuses).

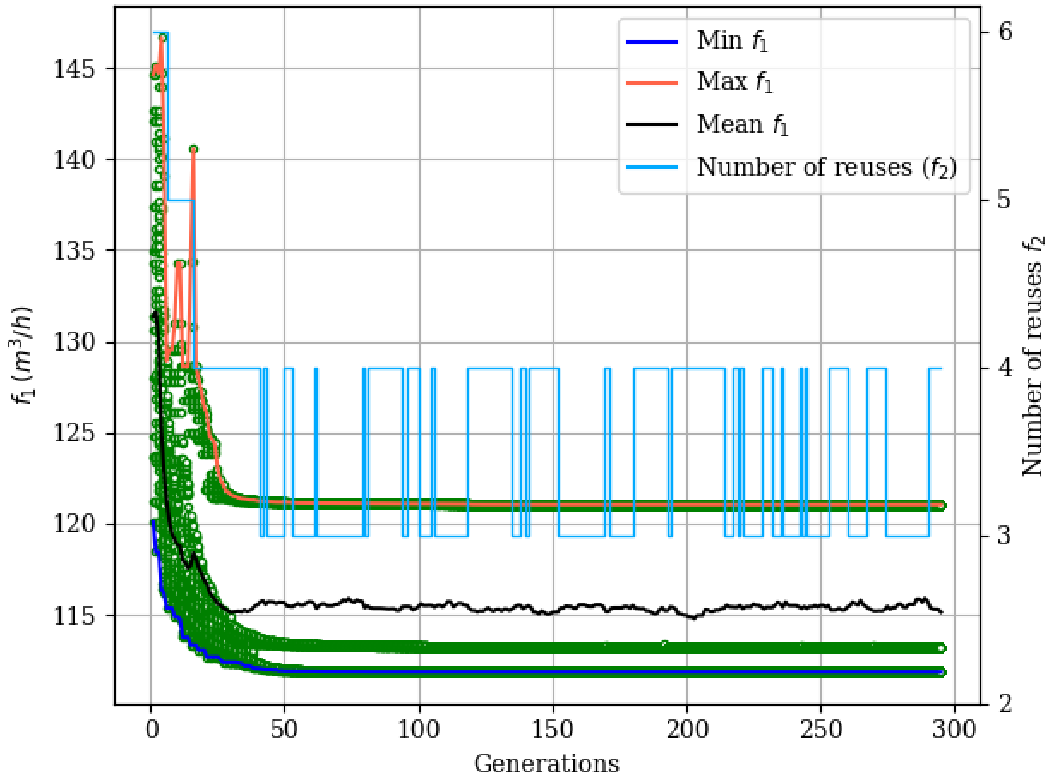

Figure 20. Variation of objective-functions throughout generations, case 2, population size = 100, number of offspring = 100

According to **Figure 21**, the first generation with a feasible solution is identified at the seventieth generation level. The constraints of the problem were not respected between the first and the seventieth generation, and the constraints are respected during the convergence phase of the program. According to **Table 13**, the resolution requires a higher generation number than the system with a single contaminant. The computation time is 5 to 6 times higher for a configuration with large population size (80 to 100), and approximately 20 times higher for a configuration with a smaller population size (40 to 60).

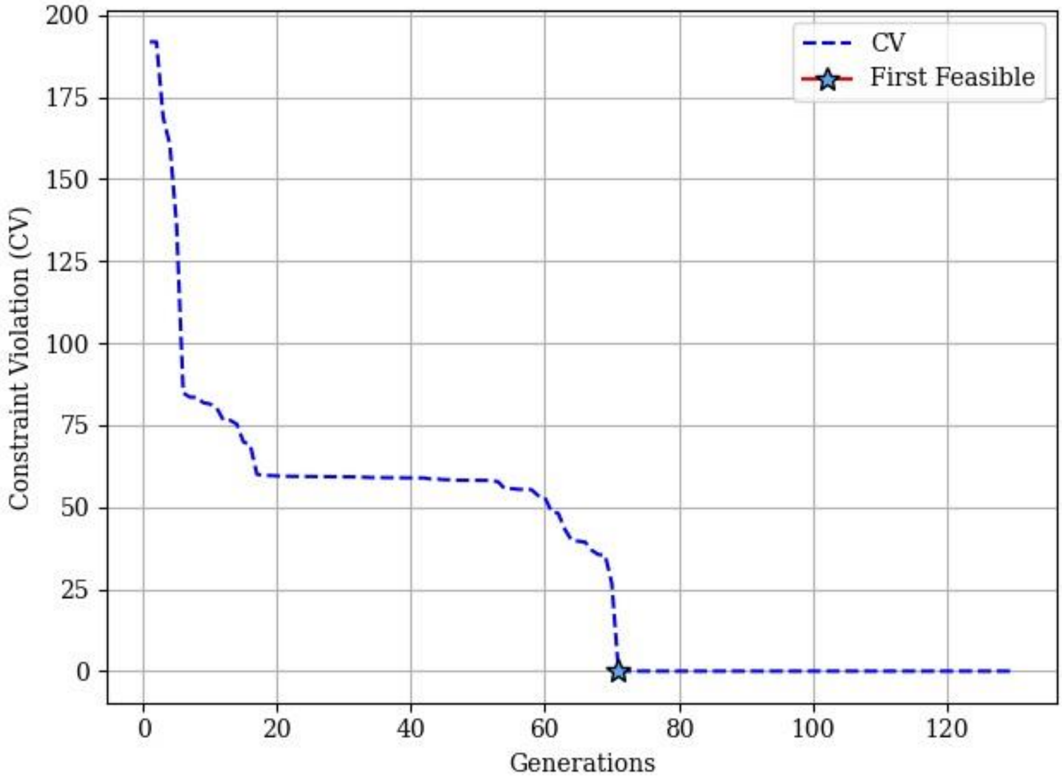

Figure 21. Constraint violation, case 2, population size = 100, number of offspring = 100

Figure 22 shows the design of the network corresponding to a minimum of freshwater of 111.87 m3/h and involving four reuses. Water balance is respected with a corresponding freshwater and wastewater of 111.87 m3/h. Processes 1 and 4 are supplied exclusively with freshwater, with 50 and 8 m3/h, respectively. The estimate of the mass transfer of the three pollutants (A, B, and C) corresponds to the minimum transfer required by process 1 and process 4, i.e., (0.75, 20.00, 1.75) and (0.16, 0.48, 0.16) kg/h, respectively. Process 2 is supplied with a mixture of freshwater (8.48 m3/h) and reused water from process 1 (25.50 m3/h). The resulting water (39.98 m3/h) has concentrations of (11, 300, 26) ppm that correspond to the pollution thresholds required by process 2 (20, 300, 45) ppm. There is a small increase in the transfer of pollutants A and C compared to the minimum required. This surplus is induced by a surplus of total water, which is essential for transferring pollutant B in process 2. Process 3 is supplied with a mixture of freshwater (45.39 m3/h) and reused water from process 4 (7.98 m3/h) and process 1 (1.47 m3/h). The resulting water (54.84 m3/h) has concentrations of (3, 19, 4) ppm that correspond to the pollution thresholds required by process 3 (120, 20, 200) ppm. The transfer of pollution in process 3 is respected, i.e. (11.88, 1.40, 520.80) kg/h, knowing that the required minimums are (5.60, 1.40, 520.80) kg/h. There is a small increase in the transfer of pollutant A compared to the necessary minimum. This surplus is induced by a surplus of total water, which is essential for transferring pollutants B and C in process 3. Process 5 is supplied only with water from process 1. The pollutant concentrations at the outlet of process 1, i.e. (15, 400, 35), are suitable with the upper limits required by process 5, i.e. (50, 400, 60) ppm. The water flow from process 1 (8 m3/h) is sufficient for the transfer of pollution in process 5. The pollutant transfer values obtained are (1.08, 60.80, 0.68), knowing that the minimums required are (0.8, 60.80, 0.48). This water flow presents a surplus regarding the transfer of A and C, but just what is necessary for the transfer of B.

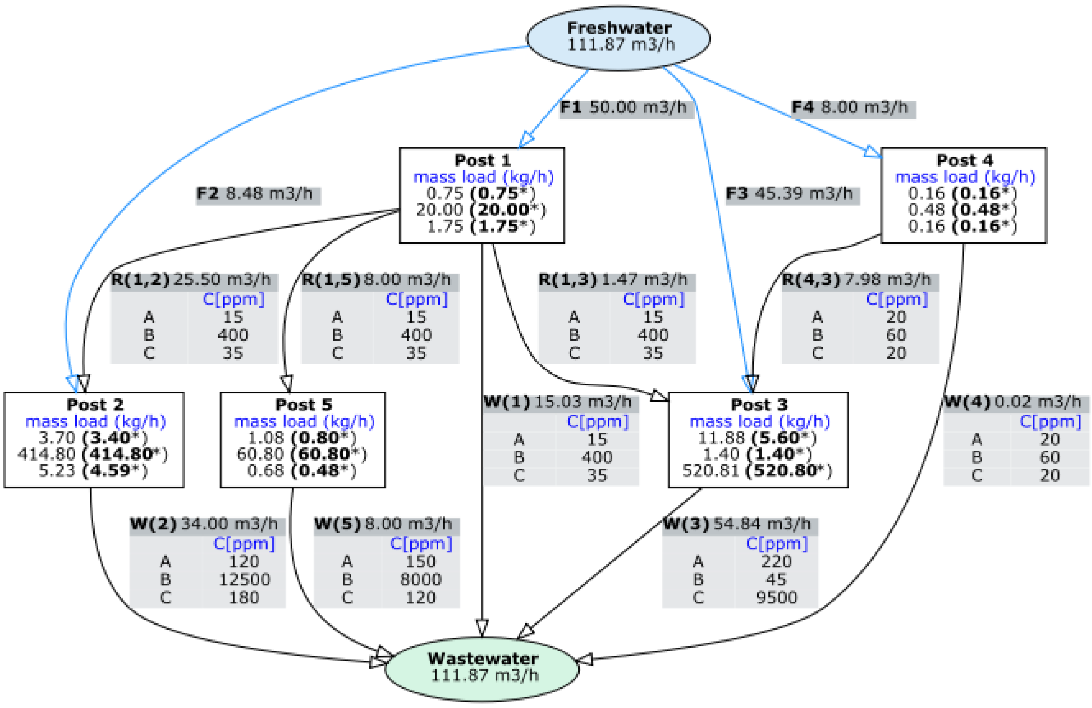

Figure 22. water-network, case 2, population size = 100, number of offspring = 100, *minimum mass load of contaminant, F (freshwater), R (reuse), W (wastewater)

2.4.5 Conclusion

This work proposes a new method of optimizing industrial water networks. The method handles systems with a single or several pollutants. A mathematical formulation of the optimization problem is presented. The main components of the multi-objective problem, including objective functions (to be minimized), decision variables (to be optimized), and constraints (to be satisfied), are developed. This optimization problem is solved with the NSGA-II method. A resolution algorithm is implemented in the Python tool. Two case studies from the literature are resolved and discussed. The two case studies include mono-contaminant and multi-contaminant systems. Customized operators (sampling, crossover, and mutation) are used in the NSGA-II algorithm. A steady-state version of the NSGA-II algorithm doesn't target the expected results. We chose then a population size equals the number of offsprings. The population size and the number of offsprings are configured from simulations applied to the two case studies. Such a configuration reaches the expected results with a population size of 100. An analysis of the program's behavior during the resolution was carried out to check the algorithm's convergence and constraint handling. Convergence is checked not only for the final result but also for all generations, which is essential for evaluating the algorithm's performance. This evaluation consists of storing all the results for each generation and extracting the information necessary for post-processing. From feasible solutions, we extract the constraint violation and the objective space values of the corresponding generation. Simple visualization techniques are used to track the evolution of objective functions and violation of constraints over generations. The individual representation of objective functions or constraint violation is a basic but efficient procedure to check the algorithm's convergence. In the literature, other methods are recommended, such as the Hypervolume method (Fonseca et al., 2006), Generational Distance (Van Veldhuizen, 1999), Inverted Generational Distance, and Inverted Generational Distance Plus (Ishibuchi et al., 2015). These methods require defining a reference point that must be greater than the Pareto front's maximum value. Depending on the water network to solve, the calculation time is more or less fast. For a water network including four processes and a single contaminant, the program converges in a few seconds. For a water network including five processes and three contaminants, the calculation time can be six times higher for a configuration with a large population size (80 to 100). The optimization of the water networks for the two case studies shows accurate water balances both on the whole network and on an individual water-using operation. The algorithm strictly handles the constraints during the convergence phase. Therefore, the upper limits of pollutant concertation are respected for single reuse and multiple reuses (i.e., mixtures of several streams). The mass transfer of pollution-induced by each operation is also estimated according to the minimum required load. This mass pollution load is considered to be a specific property of given water consumption. For example, a cleaning operation necessarily induces a minimum mass load, either from the equipment or from the material to be washed. Below a certain minimum mass load, the operation can be considered deficient. It is therefore essential to respect a minimum transfer of pollution within each process. For a water network with only one pollutant, the estimate of the pollution transfer corresponds exactly to the minimum required. However, for a water network with several pollutants, the transfer of certain pollutants can be estimated with a small surplus. This surplus is induced by an excess in the total water, which is required for transferring other contaminants within the same process. In the case of strict constraints, which impose an upper limit for the mass transfer of one or more contaminants, it is possible to add additional constraints to the optimization problem.

Finally, the case study with several contaminants shows that it is possible to obtain several competing solutions. The solutions have higher or lower freshwater flowrates corresponding to a network with more or fewer interconnections between operations. In this study, the choice is made according to the solution having the minimum flowrate of freshwater. But this choice can be made differently depending on other economic or environmental criteria. This type of optimization will require the definition of new objective-functions or different constraint management strategies such as the penality-based approach (Blank and Deb, 2020). For an optimization problem with at least three objective functions, the NSGA-III solving algorithm is more suitable than NSGA-II because of defining a hyperplane and a few benchmarks to rank the solutions and select the most qualified for the next population. In the penalty-based constraint management approach, violation of inequality and equality constraints penalizes objective value. However, it might create a more difficult fitness to solve.

both developed methods (Manual Trade-Off and automatic tool) use the same core logic, but, in the first one, the optimum point will find manually by trying and error with the guidelines from the tool, and in the second one all these steps are automatized. Based on the cases and the needs of the industries each of these tools can be helpful. Based on their interface design and examples proposed, the tools are easy to use and there is no need to have a deep knowledge of coding and process engineering. One of the main goals of this development, besides the accuracy and speed, was the generality of this tool. That makes it easier to use these tools in real case studies and industries by different technicians from different fields. In parallel, these tools are fast to use and if the standard defined data give to the tools the answer will obtain in a short time.

Chapter 3: Industrial application: case study of a French edible oil processing

Nowadays, Industries are faced with different environmental limits which need to be respected. One of the critical issues is to managing the reduction of freshwater consummation and wastewater release in the environment. The proposed method in this thesis aims to help the industries to reach this goal with an economical approach. As it mentioned before, this method can be implemented in a different type of industries, like food industries. The method had been tested and validated in both mono and multi-contaminant system before by using the data from the literature. In this chapter and to show the applicability of this method a real case study has been selected and tried. The case study is a French edible oil industry that belongs to the food sector. There are different operations and contaminants to be handled by the tool and the results are reported in detail. Besides, an additional discussion about different parameters that can affect decision-making about the optimized network has been done. This chapter is built based on two different articles. The first one is entitled" *Tradeoff Optimization for Industrial Water Systems: Case Study of a French Edible Oil Refinery*". This article is *under submission (2021)* as the fourth outcome of this thesis. The second one is entitled" Water *Reuse Strategies in Edible Oil Plant: Generic Optimization Based On NSGA-II Algorithm*". This article is *under submission (2021)* as well. as the fifth outcome of this thesis. In this chapter and for each of these articles; firstly, a short French summary of each article has been developed. This summary contains the main contents and results, and, the order of topics within the article. Secondly, the original text of the published article is embedded within the chapter.

3.1 Étude de cas d'une raffinerie française d'huiles alimentaires : Méthode d'optimisation manuelle

Mots-clés : Réseau d'eau, huile comestible, optimisation, réutilisation, compromis

Le présent travail porte sur l'application d'une méthode d'optimisation algorithmique du de réseau d'eau industriel. La procédure d'optimisation consiste en un algorithme manuel développé dans le logiciel Python. L'objectif consiste à identifier les réponses optimales et quasi-optimales du réseau d'eau, impliquant une demande en eau minimale. L'étude de cas de ce travail est un exemple d'une usine de transformation des huiles alimentaires. Un jeu de données avec huit usages d'eau, et deux contaminants critiques (basés sur les commentaires de l'expert) ont été collectés. Deux propositions optimales ont été identifiées. Avant l'utilisation de l'outil, le réseau d'eau demande 16,59 *m3/h* d'eau propre. Après l'optimisation, deux réponses avec la même quantité de 15,07 *m3/h* avec différentes options de réutilisation ont été obtenues, montrant la possibilité d'économiser environ 9% d'eau. Dans la première réponse l'eau est réutilisée provient de différentes opérations. Dans la deuxième réponse l'eau réutilisée provient d'une seule opération. Théoriquement, les deux réponses sont faisables et peuvent donc être déployées. Puisque l'eau réutilisée est fournie par les ateliers de production des utilités, la solution actuelle nécessite certainement une étude supplémentaire pour évaluer la faisabilité technique, le risque sanitaire et la sureté du procédé. La solution proposée dans cette étude est basée sur les indicateurs de pollution DCO et MES. Par conséquent, une analyse plus approfondie du flux d'eau est nécessaire. Cette analyse approfondie permettra de confirmer la solution actuelle. L'eau fournie par les ateliers de production des utilités nécessitera probablement un traitement partiel avant sa réutilisation. Si tel est le cas, un investissement supplémentaire est nécessaire. L'intégration d'une unité de régénération nécessite également un coût d'exploitation (utilité, produits chimiques, remplacement et entretien). Enfin, le critère économique pourrait être déterminant si un traitement de l'eau réutilisée semble nécessaire.

Ce travail présente une application de cet outil pour un cas réel de transformation des d'huiles alimentaires. Dans ce qui suit, une première sous-section présente les principaux usages de l'eau d'une entreprise de transformation d'huile alimentaire ainsi que la collecte des données. Ensuite, une deuxième sous-section rappelle les principales étapes de la procédure d'optimisation. Enfin, dans une troisième sous-section, nous discutons des résultats de l'optimisation.

The Forth Article General Text

3.2 Trade-off optimization for industrial water systems: case study of a French edible oil refinery

3.2.1 Abstract

This study shows the application of an optimization tool for industrial water networks. The optimization procedure consists of a manual tradeoff algorithm developed in Python software. The objective consists of targeting the optimal and near-optimal answers of the water network, involving a minimum water consumption. The case study of this work is an example of an edible oil processing plant. The dataset was collected on eight processes, including the transformation of edible oils, packaging, and production of energy utilities. COD and TSS were selected as pollution indicators. The results show two different possibilities of reuse with about 9% water saving.

Keywords: Water network, edible oil, optimization, reuse, tradeoff

3.2.2 Introduction

Limited freshwater sources and increasing water consumption in different sectors (municipal use, agriculture, industries) can lead to serious environmental challenges. Based on (Helmer and Hespanhol, 1997)(Lehr et al., 1980)(Nemerow and Leonard, 1978), the agricultural sector consumes 70% of water demand, 22% concerns the industrial sector, the rest 8% is mainly municipal uses. The rapid growth of industries has increased the demand for freshwater, and the volume of industrial effluents has risen rapidly. Releasing these effluents that contain different pollutants creates different environmental problems.

The edible oil market demand predictions by Persistence Market Research *(PMR, 2016)* show that the total market share from 83.4 billion dollars in 2015 will exceed 130 billion dollars in 2024 (Ahmad et al., 2020). The growing market of edible oil leads to an increase in the number of edible oil companies worldwide. Consequently, the number and volume of effluents released by this sector can be increased impressively (Ahmad et al., 2020). Sustainable water management involves different approaches like recycling, reuse, and water treatment. These approaches may not perform their best and have their optimum efficiency. Reuse opportunities in the industrial water networks are one of these mentioned approaches that can be optimized. Besides the different treatment techniques, it seems necessary to benefit from all the reuse potentials to reduce water consummation and wastewater release.

Several ecological issues like highly contaminated water with oil and grease content, odor problems, watercolor changing, phytotoxicity (Ma et al., 2015), and de-oxygenation of water (Lee et al., 2019) constitute a challenge for food industries effluents. The pollutants contained in the effluents from the edible oil sector can be characterized by indicators such as chemical oxygen demand (COD), biological oxygen demand (BOD), lipids (fats, oil, and grease), total suspended solids (TSS), total dissolved solids (TDS), high nutrient content and organic/inorganic contents (Nweke et al., 2014)(Ahmad et al., 2020). The main treatments mentioned for these effluents are categorized into electrochemical, biological, and Physico-chemical methods (Louhıchı et al., 2019)(Ohimain and Izah, 2017). However, they are generally complex and costly to apply. Therefore, it's interesting to find all possible reuse opportunities within the water network of edible oil companies. This water reuse strategy uses partially polluted water from one operation to another according to the concentration limits. This leads to minimizing the total freshwater use and, in parallel, decrease the effluents release. As a result, the effluent volume and the related wastewater treatment cost decrease. By considering the environmental issues and the difficulties of treating edible oil effluents, developing the tool to optimize the reuse opportunities before treatment is challenging.

Mass integration methods such as water pinch analysis (Wang and Smith, 1994) are suitable for targeting and finding reuse opportunities. However, their use is limited to the water network with a single pollutant. But in practice, industrial water networks contain more than a single pollutant. It is, therefore, almost impossible to optimize real networks with traditional methods. Recently, different researchers proposed numerical tools and mathematical models for minimization of water consumption and effluents and water network optimization in sectors such as oil refinery (Mohammadnejad et al., 2011)(Mughees and Al-Ahmad, 2015), petroleum refinery (Boix et al., 2011)(Li and Guan, 2016)(De-León Almaraz et al., 2016), pulp and paper mill, starch industry (Chin et al., 2021)(Chin et al., 2020) and dairy (Buabeng-baidoo et al., 2017). The development of numerical tools and mathematical modeling is a logical procedure for handling multi-contaminant systems. The basic logic of numerical tools is inspired by the traditional water pinch method by giving more flexibility to solve more significant problems. However, it is also necessary to apply a systemic and generic method to provide rapid and practical solutions.

A novel tool aiming to overcome the challenges of water network optimization and benefits from reuse streams was proposed and developed by our research team (Chapter 2). The designed tool follows the manual tradeoff mode. In general, the manual mode gives more flexibility and control to the user to apply different considerations. Numerical and graphical information of the water network is detailed and dynamically updated throughout the optimization procedure. The updated data include the freshwater for the whole network and each operation, the material balances (water and pollutants), the flowsheet of the water network, and a set of instructions to alert the user to calculation errors (unbalanced stream) and exceeding pollutant concentration. This work aimed to apply this tool to a real case study of edible oil in France to prove its applicability. In the following, a first sub-section presents the main water uses of an edible oil processing company as well as the data collection. After that, a second subsection reminds the main steps of the optimization procedure. Finally, in a third subsection, we discuss the optimization results.

3.2.3 Edible oil processing presentation

3.2.3.1 Plant description

This work presents a case study of a French edible oils industry, including oil-processing steps, packaging, and production of energy utilities. The processing steps include seed-pressing, solvent extraction from the pressed cake, and refining crude oil. Two workshops for the production of energy utilities (steam and cooling water) are considered. The packaging step includes the bottling of edible oils. **Table 14** summarizes the main water uses for each workshop and provides key information on water demand or water availability for each unit operation. Water is mainly used as a solvent, both for preparing seeds and the extraction of oils. Water is also used for cleaning operations. The cooling and heating water typically circulates in a closed hydraulic circuit. The heating water is returned to the boiler workshop, and the cooling water circulates between the air-cooling tower and the plant. However, the production of these two utilities requires a surplus of water and a continuous water evacuation. In the air-cooling tower, water is used to replace the evaporated and the purged water. In the production workshop for hot utilities (hot water and steam), a surplus of water is used to cooling evacuation screws ash (ashes come from a hull-burning boiler).

Table 14. A detailed description of processes in the edible oil sector

N°	Section	Workshop	Unit operation	Description
1	Oil processing	Crushing	Washing / Drying of pressure oil	Injection of water into the pressure oil to facilitate separation of impurities followed by an evaporation operation to dry the oil
2		Extraction	Dissolventing and toasting	The hexane-containing meal is treated in the Dissolventing toaster with the help of indirect heating and steam.
			Removing of solvent by distillation	The miscella, a mixture of oil and solvent, is separated by distillation into two components, oil, and solvent.
3		Refining	Neutralization	The oil is treated with an alkali solution (caustic soda) that reacts with the free fatty acids present and converts them into soap stock. The mixture allows them to separate the oil phase freed from a fatty acid that floats on top from a layered phase of soap, alkali solution, and other impurities drawn off. The oil is then washed with water to remove the soap, alkali solution, and other impurities.
4			Deodorization	Deodorization is simply a vacuum steam distillation process that removes the relatively volatile components that give rise to undesirable flavors, colors, and odors in fats and oils. This is feasible because of the significant differences in volatility between these undesirable substances and triglycerides.
5		Lecithin	Lecithin drying	Water from the drying of the vacuum gums separated from the oils in the first washing stage
6	Packaging	Packaging	Bottling	Process water from the bottling process
7	Utilities	Hot utility	Boiler	Water from boiler blowdowns
8		Cold utility	Air-cooling tower	Water from Air-cooling tower blowdowns

The current process diagram shows the consumption of freshwater for several representative water-using operations (**Figure 23**). Generally, in the industrial site, several water sources are used, such as drill water, water from the public network, or treated river water. In this study, the optimization procedure targets all water resources. However, for simplicity, a single source of water called freshwater is considered.

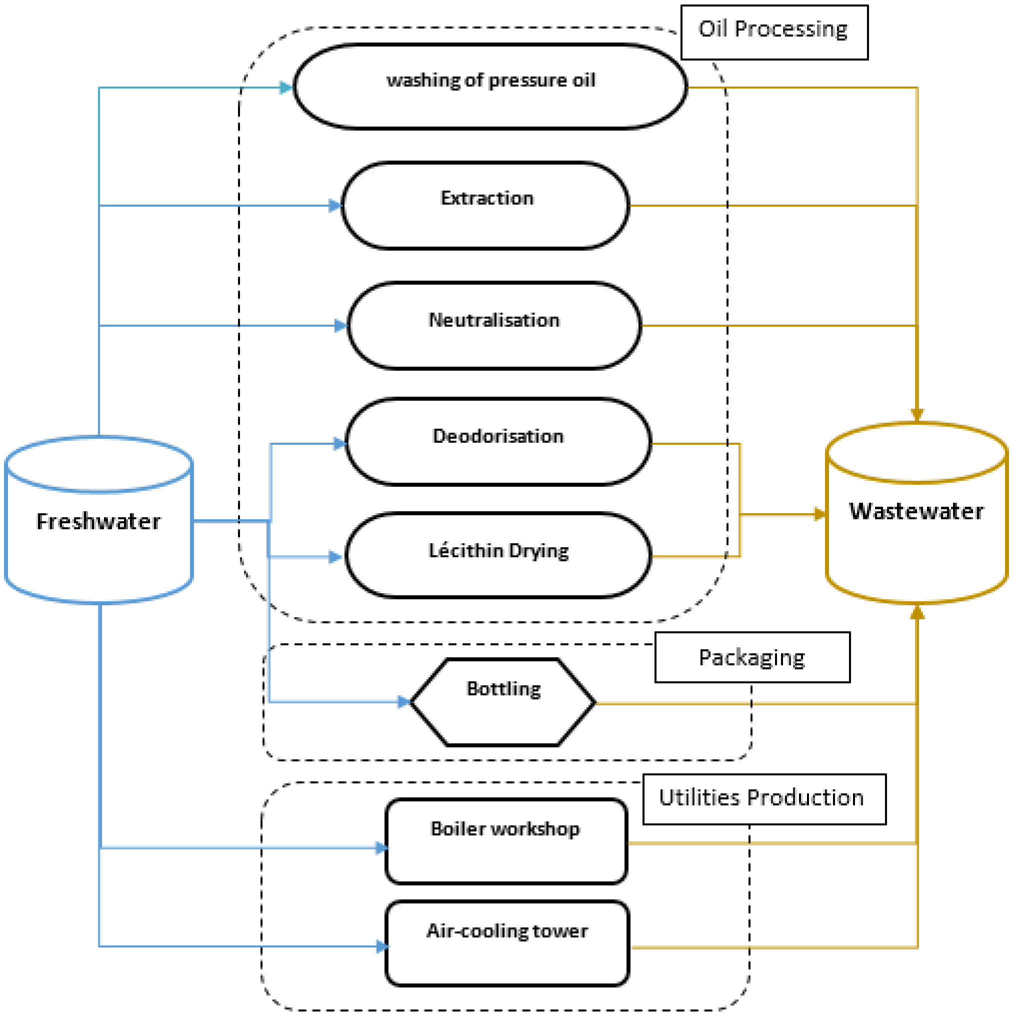

Figure 23. Schematic of water-using processes

3.2.3.2 French edible oil dataset

Based on the data set, the current case study includes eight main water-using processes. Each of these processes has different considerations to accept fresh or reused water. Besides, there are different pollutant indicators within the edible oil sector. Based on the accessibility of the data and the comments of experts about this site, COD and TSS were selected as the two main pollutant indicators. The detailed necessary data to implement the tradeoff optimization tool is provided in **Table 15** and include:

- *Water flowrate* (m^3/h): This data was obtained from direct measurements in the site. The freshwater consumption of these eight operations was measured and reported around 16.59 m^3 in each hour on average.

- *Maximum inlet and outlet concentration of each contaminant for each process* (*ppm):* The outlet concentration was obtained from direct sampling from the outlet streams of processes in the site and analysis in the laboratory. The inlet concentrations were obtained from the expert's comments by knowing the limits for each process.
- *Mass load of contaminants (kg/h):* Calculated from linear relation of concentrations and water flowrate.

Table 15. Real data set from a French edible oil sector

N°	Process	Contaminant	Mass load *(kg/h)*	C_{in}^{max} *ppm*	C_{out}^{max} *ppm*	water flowrate *(m³/h)*
1	**Washing of pressure oil**	COD	0.052	1160	1370	0.25
		TSS	0.003	17	29	
2	**Extraction**	COD	8.920	0	2230	4.00
		TSS	0.232	0	58	
3	**Neutralization**	COD	29.250	24900	48300	1.25
		TSS	2.703	17	2180	
4	**Deodorization**	COD	48.600	0	24300	2.00
		TSS	0.004	0	2	
5	**Lecithin drying**	COD	0.580	0	2320	0.25
		TSS	0.001	0	7	
6	**Bottling**	COD	0.374	0	1630	0.23
		TSS	0.010	0	44	
7	**Boiler**	COD	0.050	0	30	1.67
		TSS	0.007	0	4	
8	**Air-cooling tower**	COD	0.381	0	55	6.94
		TSS	0.057	0	8	
Total Water Flowrate						**16.59**

3.2.4 Water-network optimization

The diagram of the current water network does not show any strategy for water reuse or recycling. This work aims to reorganize the existing water network and benefit from the maximum possibility of reuse opportunities. The applied approach follows the logic of water pinch analysis but improved to be suitable for complex, multi-contaminant systems as a numerical tool. The details of the current approach are presented in (Chapter 2). The current approach uses the manual tradeoff possibilities to find the optimum and near-optimum answers for the water network. At first, the methodology is presented briefly, and the next part shows the result obtained from applying this method to the current case study.

3.2.4.1 Manual tradeoff procedure

The manual tradeoff method aims to minimize the total freshwater and effluents of the water network by using the reuse streams in the continuous system. This method also provides the graphical design of an optimized water network with numerical results. The algorithm within this proposed method instantly compiles the user data, updates the graph of the water network, and warns the user of any pollution exceeding or unbalanced mass transfer. Based on (Chapter 2), the algorithm is defined in four steps as below. *Step I* will handle once; then, *steps II, III,* and *IV* will repeat till finding an optimum answer:

I. *Process water data*

The first step of the algorithm belongs to the specification of the necessary input data, which is:

- Maximum inlet and outlet concentrations of contaminants
- Minimum mass transfer of contaminants

Table 15 presents the input data belongs to the current case study. Collecting this information (collected from the site by the measurements and expert's comments) is necessary to pass the first step of the algorithm. It's also possible to calculate the limiting water flow rates by the classic formula of mass transfer (linear relationship of the mass load transfer and the concentrations).

II. *Specification of water reuse options*

In the second step, we try to simplify the matrix of all possible flows. This matrix includes all reuse and recycling options within the network. **Table 16** is an example of this matrix for the current case study. It proceeds by using the data from the previous step and some intermediate calculations as well as some considerations. For example, as recycling was not considered (it means that water cannot re-enter the process in which it has previously been used), these flows are not considered in the optimization procedure. And, of course, the processes which have at least one pollutant with a zero threshold will not be supplied with reused water. There are also more considerations to simplify the matrix as much as possible: *a)* any mixing between two or more streams that can impose technical, environmental, or sanitary risks; *b)* considering the extremely polluted streams for reuse that leads to exceeding the allowed concentration limits.

III. *Calculation of minimum water flowrate*

After eliminating incompatible streams in the previous steps, the estimation of possible reuse streams will continue in this step. Finally, a trial and error procedure will recognize the optimal reuse amounts with some tool guidance. For example, the first estimation of all reuse streams can be the mass flowrate of freshwater estimation by considering the maximum outlet concentration.

IV. *Debugging procedure and water network results display*

The last step of the algorithm belongs to debugging process related to the two main challenge:

- Concentration exceedance: exceedance of maximum concentrations, finding errors in material balances, unforeseen mass transfer of pollutants
- Specify the feasible and non-feasible reuse opportunities

After performing all the steps and thanks to the designed tool, the detailed results appear for the user. It shows different information, such as the graphical presentation of the water network and numerical representation of flowrates and concentrations. The debugging alerts will appear at the end of each simulation as well. That is how the user can modify the reuse streams to respect all the limits and eliminate the errors related to the concentration exceedance. After each debugging of the water-reuse matrix, the tool will update the results and recalculate the total freshwater for the network. The tradeoff between steps two, three, and four will continue up to finding the optimum answer. Tuning potentials become limited, and the calculations converge after few iterations.

3.2.5 Result and discussion

After extracting the required data from the edible oil case study and setting it up into the tool, the outcomes and discussions are presented in this section. Based on (Chapter 2), an algorithmic simulation was designed in some iterations. The iteration steps can be merged or separated based on each database. The main important point is to respect the tradeoff procedure presented in the previous section. In the first step, the water network without any reuse streams is considered within the tool. As an outcome of this step, the network uses 16.42 *m3/h* of water without modification or integration of new reuse streams, as shown in **Figure 24**.

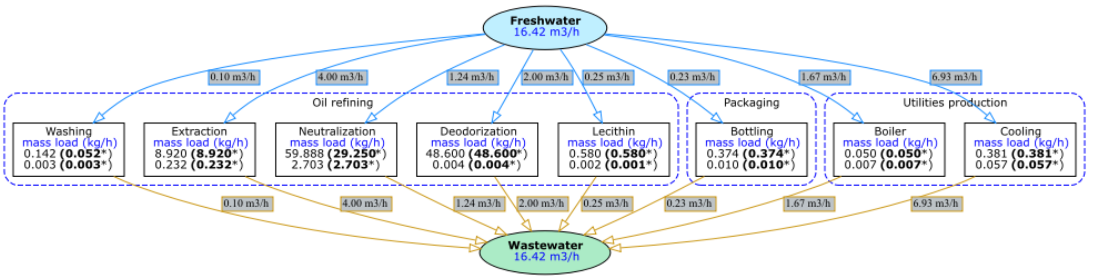

Figure 24. The water network without reuse (* minimum mass load of contaminants)

Based on the maximum concentrations data from **Table 15**, it is understood that only operations numbers 1 and 3 can accept the reuse streams from other operations. The other operations should be supplied with freshwater as their maximum inlet concentration is zero. **Table 16** presents the (8×8) flow matrix of this case study. This matrix will be updated in each iteration. Within **Table 16,** operations that should be supplied with freshwater sources appear with blue zeros. In addition, recycling is not allowed in this approach and is presented with red zeros in the matrix. The possible reuse opportunities are presented by black color. In conclusion, 16 potential reuse options exist. The rest of the operations can be used as a source of reuse streams.

Table 16. Potential reuse opportunities within the current case study

↓ Output Input →	**Post 1**	**Post 2**	**Post 3**	**Post 4**	**Post 5**	**Post 6**	**Post 7**	**Post 8**
Post 1	**0.00**	0.00	**0.25**	0.00	0.00	0.00	0.00	0.00
Post 2	**4.00**	**0.00**	**4.00**	0.00	0.00	0.00	0.00	0.00
Post 3	**1.25**	0.00	**0.00**	0.00	0.00	0.00	0.00	0.00
Post 4	**2.00**	0.00	**2.00**	**0.00**	0.00	0.00	0.00	0.00
Post 5	**0.25**	0.00	**0.25**	0.00	**0.00**	0.00	0.00	0.00
Post 6	**0.23**	0.00	**0.23**	0.00	0.00	**0.00**	0.00	0.00
Post 7	**1.67**	0.00	**1.67**	0.00	0.00	0.00	**0.00**	0.00
Post 8	**6.94**	0.00	**6.94**	0.00	0.00	0.00	0.00	**0.00**

The next steps of the simulation belong to the possible tradeoff, eliminations, and tunings of the possible reuse streams. These steps can handle simultaneously by considering the different guidelines of the tool, like concentration exceedance warnings. In addition, If the reuse flow rate is set higher than the limits, the tool warns to adjust that flow. Based on these steps, the problem may have different near-optimum and optimum answers. After eliminating non-feasible streams and adjusting the flow rate with possible reuse streams in the current case study, two optimization possibilities with one optimum amount were obtained. The first possibility benefits from different reuse opportunities from the three operations (Posts 1, 2, and 8). The second possibility is using reuse streams from a single operation (Post 7). **Table 17** belongs to the first optimum answer that contains four reuse streams with different flow rates. Operation 1 accepts one reuse stream from operation eight equal to 0.15 *m3/h*. Besides, operation 3 receives three reuse streams from operations 1, 2, and 8 with 0.05, 0.1, and 1.1 *m3/h* flowrates, respectively. As a result, the total freshwater required for all networks decreases to 15.07 m3/h, which means more than 9% saving in freshwater. Moreover, at the tool's output, the detailed graphic presentation of the new modified network is provided in **Figure 25**, which shows that all the concentration limits are respected.

Table 17. First state of the optimal results by using reuse steams of different processes

↓ **Output** **Input** →	**Post 1**	**Post 2**	**Post 3**	**Post 4**	**Post 5**	**Post 6**	**Post 7**	**Post 8**
Post 1	**0.00**	0.00	**0.05**	0.00	0.00	0.00	0.00	0.00
Post 2	**0.00**	**0.00**	**0.10**	0.00	0.00	0.00	0.00	0.00
Post 3	**0.00**	0.00	**0.00**	0.00	0.00	0.00	0.00	0.00
Post 4	**0.00**	0.00	**0.00**	**0.00**	0.00	0.00	0.00	0.00
Post 5	**0.00**	0.00	**0.00**	0.00	**0.00**	0.00	0.00	0.00
Post 6	**0.00**	0.00	**0.00**	0.00	0.00	**0.00**	0.00	0.00
Post 7	**0.00**	0.00	**0.00**	0.00	0.00	0.00	**0.00**	0.00
Post 8	**0.15**	0.00	**1.10**	0.00	0.00	0.00	0.00	**0.00**

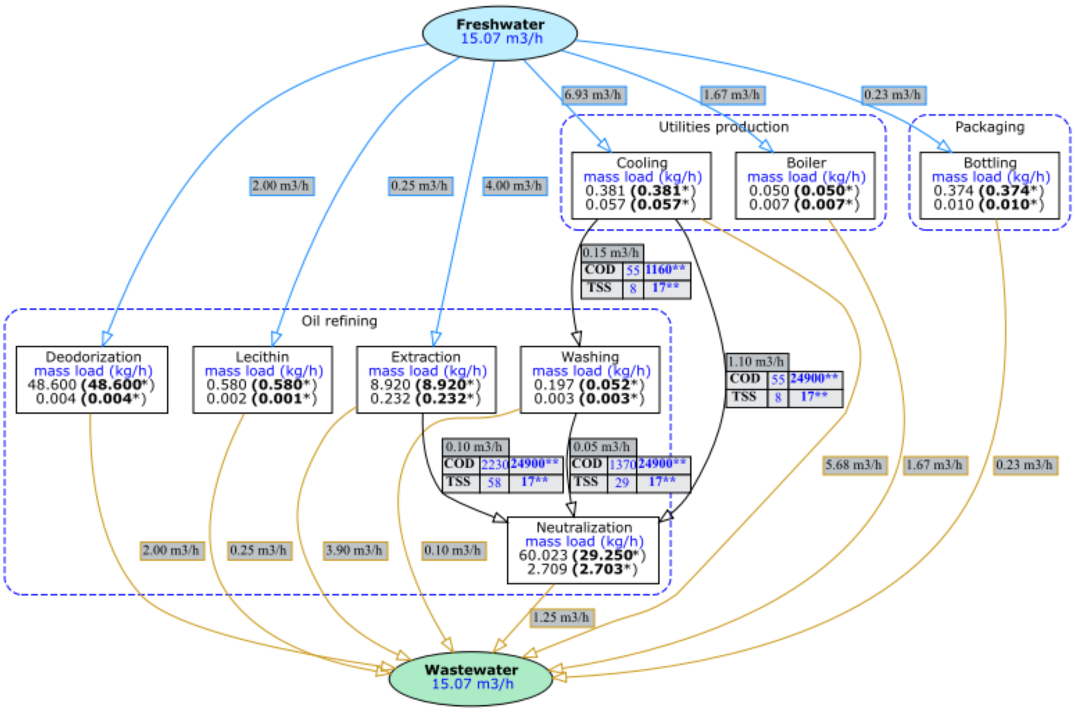

Figure 25. Schematic of the optimized network (* minimum mass load of contaminants, ** maximum allowed concentration)

The flow matrix of the second optimum answer is presented in **Table 18.** This answer benefits from two reuse streams from *Post 7*. Operation 1 accepts a reuse stream from operation seven equal to 0.13 *m3/h*. Furthermore, operation 3 accepts a reuse stream from operation seven equal to 1.3 *m3/h*. In this state, the total required freshwater for all the networks is reduced to 15.07 *m3/h*, as in the previous answer. In parallel, the detailed graphical presentation of the new modified networks is provided in **Figure 26,** which shows that all concentration limits are respected.

Table 18. Second state of optimal answer by using the reuse streams from post 7

↓ Output Input →	**Post 1**	**Post 2**	**Post 3**	**Post 4**	**Post 5**	**Post 6**	**Post 7**	**Post 8**
Post 1	**0.00**	0.00	**0.00**	0.00	0.00	0.00	0.00	0.00
Post 2	**0.00**	**0.00**	**0.00**	0.00	0.00	0.00	0.00	0.00
Post 3	**0.00**	0.00	**0.00**	0.00	0.00	0.00	0.00	0.00
Post 4	**0.00**	0.00	**0.00**	**0.00**	0.00	0.00	0.00	0.00
Post 5	**0.00**	0.00	**0.00**	0.00	**0.00**	0.00	0.00	0.00
Post 6	**0.00**	0.00	**0.00**	0.00	0.00	**0.00**	0.00	0.00
Post 7	**0.13**	0.00	**1.30**	0.00	0.00	0.00	**0.00**	0.00
Post 8	**0.00**	0.00	**0.00**	0.00	0.00	0.00	0.00	**0.00**

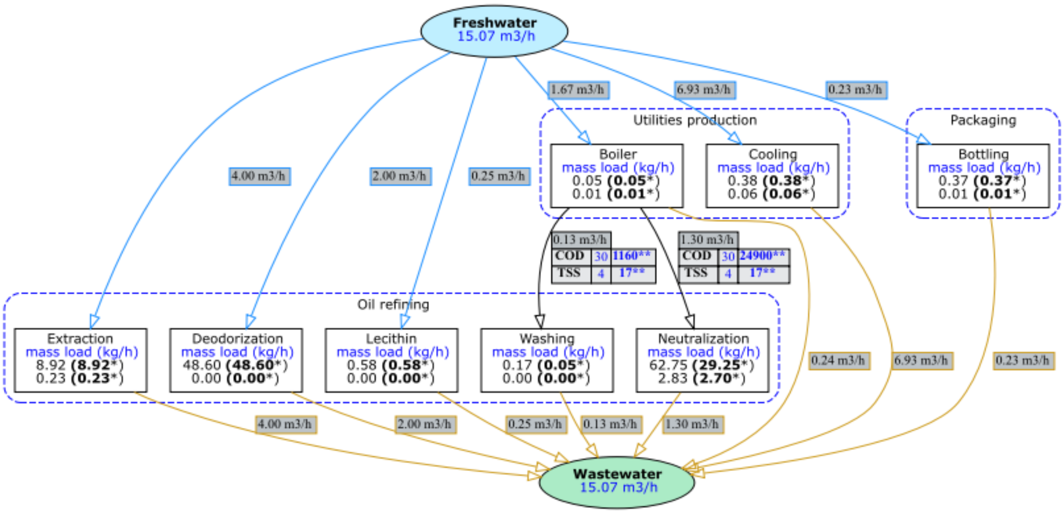

Figure 26. Schematic of the optimized network - the second state (* minimum mass load of contaminants, ** maximum allowed concentration)

In this case study, two optimal answers with one amount equal to 15.07 m3/h but with two different designs were obtained with 9% total water saving compared to the existing situation.

In the first answer, four reuse streams from three different operations (washing, extraction, and air-cooling tower) were obtained. In the second answer, two reuse streams from the boiler workshop were identified. To find which solution is most suitable for the case study (or even feasible in practice), and, as the criteria used in the tool don't include all the limitations, it makes sense to consider other criteria. For example, in this work, two critical parameters (COD and TSS) are considered. Besides the chemical considerations, other aspects like cost, safety, and physical limits within the site are important, especially for the four water using processes (washing, extraction, air-cooling tower, and boiler workshop) as reuse water suppliers. For both answers, it should be checked if, in practice, adding reuse streams between suppliers and receivers of reuse is possible or not. For example, based on different factors like the location, complexity of piping between the operations, and safety issues, a feasible solution can be found. In this case, it seems necessary to review all these reuse streams in the mentioned aspects by the experts in the company to see which answer is suitable for the site. At first glance, it seems the second answer is more logical because it has fewer reuse streams and more simple (just two reuse streams from the boiler workshop). But, on the other hand, it can't be the best choice because of less flexibility (lack of alternative operation or streams) compared to the first answer.

In economic aspects, 1.52 m3/h of water-saving was obtained in the optimized water network compared to the actual state. By considering around 7200 working hours per year in this industry, applying the current tool leads to 10944 m3 of water-using in each working yea. If we consider an average water price of 3.45 euros/m3, the annual saving is 37 k€. This saving varies by country and can be twice as high in regions with higher water costs. If we consider a typical gross income between 2 and 3 M€, the company's economic efficiency can increase by up 1.2-1.8 point. It shows that, in long periods, the water network is sensitive about even small changes in water flow rates. The extra financial analysis also needed to check the tradeoff between the costs for adding the new reuse streams and the economy by using these new streams. If the net balance is positive even in the long term, it’s useful to add the new reuse streams (by being aware of all other above-mentioned considerations).

3.2.6 Conclusion

This study provides an algorithmic water network tradeoff optimization in a real case study from the food sector. A data set includes eight main processes, and two critical contaminants (based on the expert’s comments) have been assessed. The dataset is implemented in the tradeoff procedure, and as a result, two optimum propositions have been obtained. The existing water network requires 16.59 m3/h of freshwater. After the optimization, two answers with the same amount of 15.07 m3/h with different reuse options have been identified, showing the possibility of around 9% water-saving. The first answer uses different operations and reuses streams to satisfy the water demand of other operations. The second answer supply all reuse demands by using only one operation (post 7). Based on the tool’s considerations, both answers have the feasibility and possibility of their deployment. Since the reused water is provided from the utility workshops, the current solution certainly requires an additional study to assess the technical feasibility, the health risk, and the safety of the process. The solution proposed in this study is based on the COD and TSS pollution indicators. Therefore, a more in-depth water flow analysis is needed. This in-depth analysis will confirm the current solution. Water provided from utility workshops will likely require partial treatment before its reuse. If that is the case, additional investment is needed. The integration of a regeneration unit also requires an operating cost (utility, chemical, replacement, and maintenance). Finally, the economic criterion could be decisive if treatment of reused water seems necessary.

3.3 Stratégies de réutilisation de l'eau dans une usine de transformation des huiles alimentaires : Optimisation générique basée sur l'algorithme NSGA-II

Mots-clés : Huile comestible, Gestion de l'eau, Optimisation mathématique, Réutilisation

Cette étude présente une approche d'optimisation pour le revamping d'un réseau d'eau industriel. Le problème d'optimisation est formulé à partir de données collectées sur une usine de transformation des huiles alimentaires. L'étude de cas n'est pas complexe mais représente un exemple éco-innovant qui permettra de diminuer les impacts négatifs de l'industrie alimentaire sur l'environnement et les ressources en eau. Les processus inventoriés comprennent les transformations des graines oléagineuses (raffinage chimique et physique), le conditionnement (embouteillage) et la production des utilités de chauffage et de refroidissement (vapeur et eau de refroidissement). Les processus utilisant de l'eau sont caractérisés en spécifiant les concentrations maximales d'eau à l'entrée et à la sortie de chaque opération ainsi que le transfert minimal de polluants. La DCO et les MES sont choisis comme indicateurs de pollution. L'algorithme génétique basé sur le tri non dominé (NSGA-II) est utilisé pour résoudre un problème multi-objectif avec prise en compte de contraintes. La procédure d'optimisation consiste à minimiser la demande en eau en optimisant le couplage entre les opérations. Deux stratégies d'optimisation sont étudiées. La première stratégie est basée sur la définition d'un problème d'optimisation avec deux objectifs, à savoir, la minimisation de la demande en eau et la minimisation du nombre de couplages. A partir de la réduction du nombre de couplages, on souhaite concevoir des réseaux d'eau simplifiés et moins coûteux. La deuxième stratégie est une extension de la première en intégrant un troisième objectif pour évaluer les surcoûts économiques liés à l'intégration d'unités de régénération des eaux avant leur réutilisation. L'évaluation des coûts comprend suffisamment de détails pour montrer la flexibilité et la capacité de l'outil à traiter les fonctions objectives. Le traitement des contraintes est essentiel pour obtenir un bilan matière correct tant pour l'eau que pour les différents polluants. Le traitement des contraintes est également essentiel pour garantir le respect des valeurs limites de concentration. L'interprétation du problème à deux objectifs est assez simple étant donné que les données peuvent être représentées dans un graphe 2D classique. Pour les problèmes ayant plus d'objectifs les diagrammes à coordonnées parallèles sont utilisés pour analyser la façon dont les solutions denses sont distribuées dans différentes plages concernant chaque fonction objective. Dans le cas du problème tri-objectif, l'interprétation du résultat a nécessité une sélection manuelle des solutions. Cette étape peut être automatisée pendant l'exécution du programme.

Cette étude fournit des données représentatives de l'industrie de la transformation des huiles alimentaires ainsi que la procédure pratique pour la reconception du réseau d'eau. Tout d'abord, le problème d'optimisation est résolu en considérant la procédure d'optimisation développée dans le chapitre 2. La procédure d'optimisation implique deux fonctions objectives (débit d'eau propre et nombre de réutilisations). L'optimisation aboutit à une ou plusieurs conceptions du réseau d'eau. Le réaménagement du réseau d'eau peut nécessiter un coût d'investissement supplémentaire lié à l'installation de la tuyauterie et à l'intégration de systèmes de traitement décentralisés. L'impact économique du système de traitement est évalué en définissant une troisième fonction objective. L'impact économique est basé sur l'évaluation du coût total annualisé. Des étapes d'analyse intermédiaires sont effectuées pour vérifier la validité numérique de la procédure d'optimisation (par exemple, la convergence et la violation des contraintes du problème).

The Fifth Article General Text

3.4 Edible oil plant water reuse problem A multi-objective optimization based on NSGA-II algorithm

3.4.1 Abstract

This study shows an optimization approach for the revamping of an industrial water network. The optimization problem is formulated from data collected on the edible oil processing plant. The inventoried processes (called water-using processes) include the transformations of oilseeds (chemical and physical refining), packaging (bottling), and the production of heating and cooling utilities. The water-using processes are characterized by specifying the maximum inlet and outlet concentrations of water and the minimum mass load of contaminants. COD and TSS are selected as pollution indicators. Non dominated sorting genetic algorithm (NSGA-II) is used to solve a constrained multi-objective problem. The optimization procedure consists of minimizing freshwater consumption by optimizing water reuse from one process to

another. First of all, the optimization problem is solved by considering two objective functions (freshwater flow rate and number of reuses). Intermediate analysis steps are performed to check the convergence and the violation of the problem constraints. Secondly, the optimization problem is extended by considering a third objective function. The third objective function refers to the total annualized cost required for the revamping of the water network.

Keywords: Water reuse, multi-objective optimization, NSGA-II, edible oil

3.4.2 Introduction

The reuse of water in the food industry, particularly in the edible oils sector, is an environmental challenge. This is due to industry reforms, growing demand, climate change, and water stress (Ahmad et al., 2020). The edible oil effluents (for ex. palm oil (Ahmed et al., 2015) and soybean oil (Yu et al., 2017)) include a large amount of TSS, COD, BOD, TDS, inorganic and organic contents (Ngoie et al., 2020; Nweke et al., 2014), oils (Saranya et al., 2014). The principle of water reuse consists of using wastewater in processes for which a pollution level is accepted. Unfortunately, food safety regulations represent a major obstacle to applying water reuse strategy in the food industry (OOPEC; 1998; IPPC, 1996).

Usually, wastewater is collected and depolluted in a centralized wastewater treatment plant (WWTP). However, decentralized regeneration of wastewater for reuse or recycling (i.e., before WWTP) is much less common because it requires an investment and additional operating costs. Even if the individual wastewater regeneration practices exist, they are mostly limited to partial treatment by settling, screening, or centrifugation. In certain edible oil companies, both edible oils and diesel fuel are produced. For these companies, the regulations allow the reuse or recycling of wastewater in esterification workshops since there is no risk on the final product. This work is focused only on the optimization of water networks of edible oil production workshops. The objective is to provide safe water reuse opportunities as a primary means of saving water in edible oil processing. The reuse of wastewater from one process to another is supposed without any treatment. In practice, the use of series or parallel regeneration processes is required to avoid any health risks.

Current industrial water management includes two main strategies (Grobicki, 2008) implemented at the plant and national scales. The local measures implemented at the plant scale consist of expertise progressively developed within the company through audits or best practices. National water conservation policy includes obligatory and initiative actions such as the progressive increase in water fees, applying specific taxes on effluents released to the environment, or providing subsidies to encourage innovative water-saving technologies. This work aims to promote applying a reuse strategy in food processing throughout developing systemic and generic optimization procedures.

In the literature, there are pinch-based contributions (Wang and Smith, 1994; Dhole et al., 1996; Feng et al., 2007) and mathematical approaches (Boix et al., 2011; De-León Almaraz et al., 2016). The pinch-based method is limited to water networks with single-pollutant, while water networks in the food industry involve multiple pollutants. Mathematical techniques are developed to solve water networks with multiple pollutants. However, current mathematical methods are based on conceptual design procedures, which require very advanced knowledge to interpret the results and often lack efficiency and optimality in the calculation.

The design method proposed in this work combines both the pinch-based approach but also multi-objective optimization. NSGA-II algorithm is used to solve a constrained multi-objective problem. The technique is systemic and can be applied to common industrial data.

The problem for the food industry is the lack of data on water volumes and pollutant loads. It is possible to obtain one part of the data by measurement or by estimate. However, specifying the maximum possible inlet and outlet concentrations of pollutants is almost impossible by measurement and requires expertise based on experience in process management and risk analyses. This study provides representative data for the edible oil industry as well as the practical procedure for retrofitting the water network. First of all, the optimization problem is solved by considering the optimization procedure developed in Chapter 2. The optimization procedure involves two objective functions (i.e., the flow rate of freshwater and the number of reuses). The optimization results in one or more designs of the water network. Redesigning the water network may require an extra investment cost related to piping installation and integrating series or parallel decentralized treatment systems. The economic impact of the treatment system is evaluated by defining a third objective function. The economic impact consists of assessing the Total Annualized Cost (TAC). Intermediate analysis steps are performed to check the numerical validity of the optimization procedure (e.g., convergence and violation of the problem constraints).

3.4.3 Data inventory

The dataset is presented in Chapter 3 and reminded in **Table 19**. The inventory is performed on an edible oil processing company. Only the water-using processes with the continuous regime are selected for the inventory. The water-use process is supposed as an open system with (1) water circulation between the inlet and the outlet and (2) a transfer of one or more pollutants. The continuous regime represents only the circulation of water. The product (e.g., oils) can be processed either in batch or continuous mode. The main water uses include oil processing steps, packaging, and production of heating and cooling utilities. Oil processing steps include seed pressing, solvent extraction of the pressed cake, and crude oil refining. Packaging consists of bottling edible oils during which water is used for washing bottles and bottling equipment. Two production workshops for energy utilities are considered: (1) boiler workshop to produce steam and (2) air-cooling tower to produce cooling water. The steam production workshop has two water circuits. The first circuit includes the boiler feed water. In the second circuit, water is used to dissipate large amounts of heat (e.g., cooling of ash evacuation screws, ashes come from a hull-burning boiler). In this study, only the water from the second circuit is taken into account. In the air-cooling tower, water is used to balance evaporated water and purged water.

Table 19. Data inventory for edible oil process

i	Process	Pollutant	Mass load (kg/h)	C_{in}^{max} ppm	C_{out}^{max} ppm	water flowrate (m³/h)
1	Washing / Drying of Pressure Oil	COD	0.052	1160	1370	0.25
		TSS	0.003	17	29	
2	Extraction	COD	8.920	0	2230	4.00
		TSS	0.232	0	58	
3	Neutralization	COD	29.250	24900	48300	1.25
		TSS	2.703	17	2180	
4	Deodorization	COD	48.600	0	24300	2.00
		TSS	0.004	0	2	
5	Lecithin drying	COD	0.580	0	2320	0.25
		TSS	0.001	0	6.9	
6	Bottling	COD	0.374	0	1630	0.23
		TSS	0.010	0	44	
7	Boiler	COD	0.050	0	30	1.67
		TSS	0.007	0	4.3	
8	Cooling Tower	COD	0.381	0	55	6.94
		TSS	0.057	0	8.3	

The current process diagram shows no recycling or reuse of water. Remember here that the term reuse means direct or indirect use (after treatment) of water in other operations for which the level of contamination is acceptable. Recycling consists of reintegrating water into operations where it was previously used. For this, the water treatment or its mixture with freshwater is necessary to respect the limit of pollutant concentration. In the existing water network, all water-use processes are supplied with freshwater. The corresponding water flowrate is 16.59 *m3/h*.

Let us remember the objective of this study which consists of providing the less costly solution by promoting any possible reuse of wastewater. Therefore, it is essential to specify for each water-use the maximum inlet and outlet concentrations of water. The limiting process data for this case study are presented in **Table 19**, i.e., maximum inlet and outlet concentrations of Chemical Oxygen Demand (COD) and Total Suspended Solids (TSS), minimum mass transfer of pollutants, and water flowrate. For obtaining the mass transfer of pollutants, we assume a linear relation of concentrations and water flowrate (**Equation 43**).

$$m_{i,k} = \left(C_{i,k}^{out} - C_{i,k}^{in}\right) \times \frac{F_i}{1000} \qquad (43)$$

Where $m_{i,k}$ is the mass transfer of contaminant k (COD or TSS) in process i ($i = 1 \cdots 8$), expressed in kg/h. $C_{i,k}^{in}$ and $C_{i,k}^{out}$ are the inlet and outlet concentrations of contaminant k in process i, expressed in ppm. F_i is the freshwater supply of process i, expressed in m^3/h.

The water flowrate values (shown in **Table 19**) are the values specified at 0 ppm since the processes are currently supplied with freshwater. During the optimization procedure, the water flowrate may increase for processes supplied with wastewater. These flowrates are not necessarily the values to be retained in the design of the new water network. Any water supply line above 0 ppm will require a higher water flowrate to meet the minimum pollution transfer specified in the inventory. The same goes for concentrations. The maximum concentration values are not necessarily the values used in the new water network. Any water supply line below these maximums will meet process requirements.

3.4.4 Optimization formulation

The general formulation of the constrained multi-objective optimization problem is presented in Chapter 3. This subsection provides the mathematical formulation of the optimization problem applied for this case study. The initial optimization problem includes two objective functions (to be minimized), the specification of the decision variables (to be optimized), and the constraints (to be satisfied). The first step in the analysis represents the problem with two objective functions (freshwater flowrate and number of reuses). The optimized water network will include one or more water reuses. This network is assumed to be the most economical solution for which the water can be directly reused in other operations where contamination is acceptable. However, in reality, reused water may require intermediate and partial treatment to remove specific pollutants. Remember that in this case study, only the indicators COD and TSS are considered. However, other minor pollutants (of second-order) can potentially present a major barrier to water reuse. Therefore, water treatment becomes inevitable, with additional investment and operating costs. For this reason, a second formulation of the optimization problem is proposed by considering a third objective function defined by the TAC.

3.4.4.1 Bi-objective problem

In the following, we consider a bi-objective minimization:

$$\min \begin{cases} f_1 = \sum_{i=1}^{8} F_i \\ f_2 = \sum_{\substack{i,j=1 \\ i \neq j}}^{8} \left(R_{i,j} \geq \varepsilon\right) \end{cases} \tag{44}$$

Where functions f_1 and f_2 represent the demand for freshwater and the interconnection number, respectively. R is the reuse matrix that defines the space of 14 decision parameters (**Matrix 45**). ε is the mass flowrate threshold set at 0.001 m^3/h, below which the reuse is considered negligible.

$$[O] \leq \begin{bmatrix} 0 & 0 & R_{1,3} & 0 & 0 & 0 & 0 & 0 \\ R_{2,1} & 0 & R_{2,3} & 0 & 0 & 0 & 0 & 0 \\ R_{3,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ R_{4,1} & 0 & R_{4,3} & 0 & 0 & 0 & 0 & 0 \\ R_{5,1} & 0 & R_{5,3} & 0 & 0 & 0 & 0 & 0 \\ R_{6,1} & 0 & R_{6,3} & 0 & 0 & 0 & 0 & 0 \\ R_{7,1} & 0 & R_{7,3} & 0 & 0 & 0 & 0 & 0 \\ R_{8,1} & 0 & R_{8,3} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \leq \begin{bmatrix} 0.00 & 0 & 0.25 & 0 & 0 & 0 & 0 & 0 \\ 4.00 & 0 & 4.00 & 0 & 0 & 0 & 0 & 0 \\ 1.25 & 0 & 0.00 & 0 & 0 & 0 & 0 & 0 \\ 2.00 & 0 & 2.00 & 0 & 0 & 0 & 0 & 0 \\ 0.25 & 0 & 0.25 & 0 & 0 & 0 & 0 & 0 \\ 0.23 & 0 & 0.23 & 0 & 0 & 0 & 0 & 0 \\ 1.67 & 0 & 1.67 & 0 & 0 & 0 & 0 & 0 \\ 6.94 & 0 & 6.94 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(45)

The right-side term in **Inequality 45** represents the upper bound of the decision parameters. These flowrate values are estimated from the maximum demand for freshwater (**Table 19**).

The optimization problem is subject to 12 inequalities ($8 + 2 \times 2$). Since processes 2, 4, 5, 6, 7, and 8 should be supplied with fresh water, their related constraints about maximum concentrations are already satisfied. Only processes 1 and 3 are subject to conditions about maximum inlet concentrations. Since processes 1 and 3 can be supplied with several flows with different concentrations, the average flow must respect the concentration limit for COD and TSS:

$$\begin{bmatrix} \frac{\sum_{j=1}^{8} R_{j,1} \times C_{j,COD}^{out}}{F_1 + \sum_{j=1}^{8} R_{j,1}} \\ \frac{\sum_{j=1}^{8} R_{j,1} \times C_{j,TSS}^{out}}{F_1 + \sum_{j=1}^{8} R_{j,1}} \end{bmatrix} \leq \begin{bmatrix} 1160 \\ 17 \end{bmatrix}_{\text{ppm}} \quad (46)$$

$$\begin{bmatrix} \frac{\sum_{j=1}^{8} R_{j,3} \times C_{j,COD}^{out}}{F_3 + \sum_{j=1}^{8} R_{j1}} \\ \frac{\sum_{j=1}^{8} R_{j1} \times C_{j,TSS}^{out}}{F_3 + \sum_{j=1}^{8} R_{j,3}} \end{bmatrix} \leq \begin{bmatrix} 24900 \\ 17 \end{bmatrix}_{\text{ppm}} \quad (47)$$

Each water-using process is subject to water-balance constraint:

$$F_1 + \sum_{j=1}^{8} R_{j,1} \geq R_{1,3} \quad (48)$$

$$F_3 + \sum_{j=1}^{8} R_{j,3} \geq R_{3,1} \quad (49)$$

$$\{F_{\text{i}} \geq R_{\text{i},1} + R_{\text{i},3}\}_{i=2,4,5,6,7,8} \quad (50)$$

3.4.4.2 Tri-objective problem

In the following, we study the economic impact of integrating regeneration units. This regeneration unit is used to reduce the pollutant load of reused water. The idea is to develop a tri-objective problem to show the flexibility of the optimization tool. We, therefore, specify, as an example, a membrane process with sufficient design data for demonstration purposes, but not too much to lose the idea of a global evaluation. In practice, if a microbiological risk is suspected from the reuse of water, the regeneration process can be used to remove particles and microorganisms from the water. The integration of this unit requires investment and operating costs. Hence the interest in formulating a third objective function based on the total annualized cost, defined by **Equation 51**:

$$TAC = CRF \times C_{eq} + C_{op} \quad (51)$$

Where TAC is the total annualized cost, expressed in $k€/year$. C_{eq} is the equipment cost, expressed in $k€$. C_{op} is the annual operating cost, expressed in $k€//year$. CRF is the capital recovery factor, obtained from **Equation 52**:

$$CRF = \frac{IR \times (1+IR)^{L_f}}{(1+IR)^{L_f} - 1} \quad (52)$$

Where IR is the interest rate, and L_f is the lifetime expressed in $year$.

The equipment cost includes the pumps and membranes costs:

$$C_{eq} = C_m S + C_p E_p \quad (53)$$

Where, C_m is the membrane unit cost ($k€/m^2$), S is the membrane area (m^2), C_p is the pump unit cost ($k€/kWh$), and E_p is the pump power (kWh).

The annual operating cost includes the electric utility cost, and membrane replacement and cleaning cost:

$$C_{op} = \frac{C_e E_p}{1000} t_y + C_{rc} S \quad (54)$$

Where C_e is the cost of electricity expressed in $€/kWh$, C_{rc} is the membrane replacement and cleaning cost, expressed in $k€/m^2/year$, and t_y is the annual operating time, expressed in h/year.

The idea of this calculation is to provide a marginal value of the total annualized cost. Since this cost is integrated as an objective function, its value must depend on the decision variables, i.e., the flowrate of reused water (F_r), expressed in m^3/h. In this study, only the reuse of water from utility production workshops will be subject to partial treatment:

$$F_r = F_7 + F_8 \quad (55)$$

To simplify the cost assessment while keeping a representative calculation, specific parameters are set for tubular or hollow fiber membranes, i.e., the transmembrane pressure (ΔP_m) expressed in bar, fiber diameter (d) expressed in m, fiber length (L)

expressed in m, water velocity through the fiber (u) expressed in m/s, and water permeability (A) expressed in $m/s/bar$.

The membrane area is evaluated according to:

$$S = \frac{F_r}{3600 \times \Delta P_m \times A} \tag{56}$$

The pump power is evaluated according to:

$$E_p = \frac{F_r}{3600}\left(\frac{\Delta P_m}{10^5} + 4\frac{L}{d}\rho\frac{u^2}{2}\right) \times \frac{1}{1000} \tag{57}$$

Where ρ is the water density expressed in kg/m^3.

3.4.4.3 Optimization procedure and parameter specification

The bi-objective and tri-objective problems, formulated previously, are solved successively using the NSGA-II algorithm. The same basic routines following the general outline of genetic algorithm GA with a modified mating (crossover and mutation) and survival selection are used for both problems. The tri-objective problem inherits from the bi-objective problem routines. The decisive parameters and the constraints are preserved. However, the size of the design space is appended by adding the economic calculation routines. For the NSGA-II setup, we chose a population size of 100 and generate the same number of offsprings. The problem is solved with termination criterion based on the convergence of design space and constraints. In this simulation, a tolerance of 10^{-6} was defined for design space and constraints. A maximum of the generation of 1000 is defined if convergence is not reached. The tolerance calculation is smoothed over the previous 20 generations preceding the nth generation. Customized operators (sampling, crossover, and mutation) are used in this simulation, i.e.:

- Sampling: is applied randomly on the decision parameters by using the upper and lower bound of matrix R (**Matrix 45**)
- Crossover: simulated binary crossover SBX is used with a probability of 0.9 and a distribution index of 15
- Mutation: each child solution is muted with a probability of $1/14$ (14 is the decision parameter size) so that, on average, one variable is mutated per solution.

To solve the tri-objective problem, additional data are required. Process specification and cost data are collected in **Table 20**.

Table 20. Process specification and cost data

Process specification		
A	$10^{-6}\ m/s/bar$	Water permeability
ρ	$1000\ kg/m^3$	Water density
L	$2\ m$	Fiber length
d	$1\ mm$	Fiber diameter
ΔP_m	$10\ bar$	Transmembrane pressure
Data cost		
C_m	$2\ k€//m^2$	Membrane unit cost
C_p	$1\ k€//kWh$	Pump unit cost
C_{rc}	$0.20\ k€//m^2/year$	membrane replacement and cleaning cost
IR	0.08	Interest rate
L_f	$10\ years$	Lifetime
t_y	$7200\ h/year$	Annual operating time

3.4.5 Result and discussion

The result of the bi-objective problem is exactly that obtained by the tradeoff method (Chapter 3). The minimum of freshwater is estimated at 15.07 m3/h. Since the current consumption is 16.59 m3/h, the potential of water-saving is around 9%, i.e., 1.52 m3/h. This economy should be quite significant over a year, especially when the operating regime is continuous. Considering the annual working time of 7200 h/year, approximately 11 thousand m3 of freshwater per year is saved.

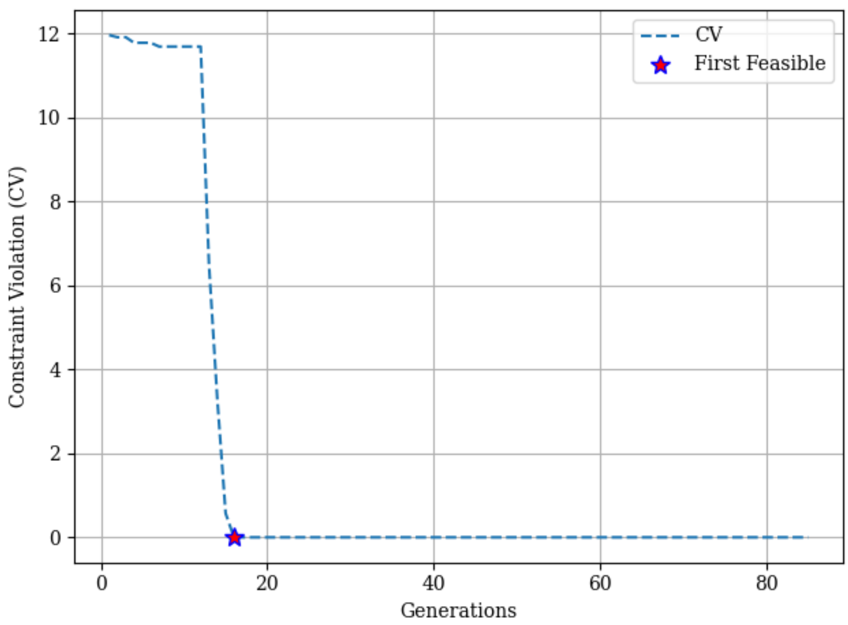

Figure 27. Constraint violation, edible oil case study

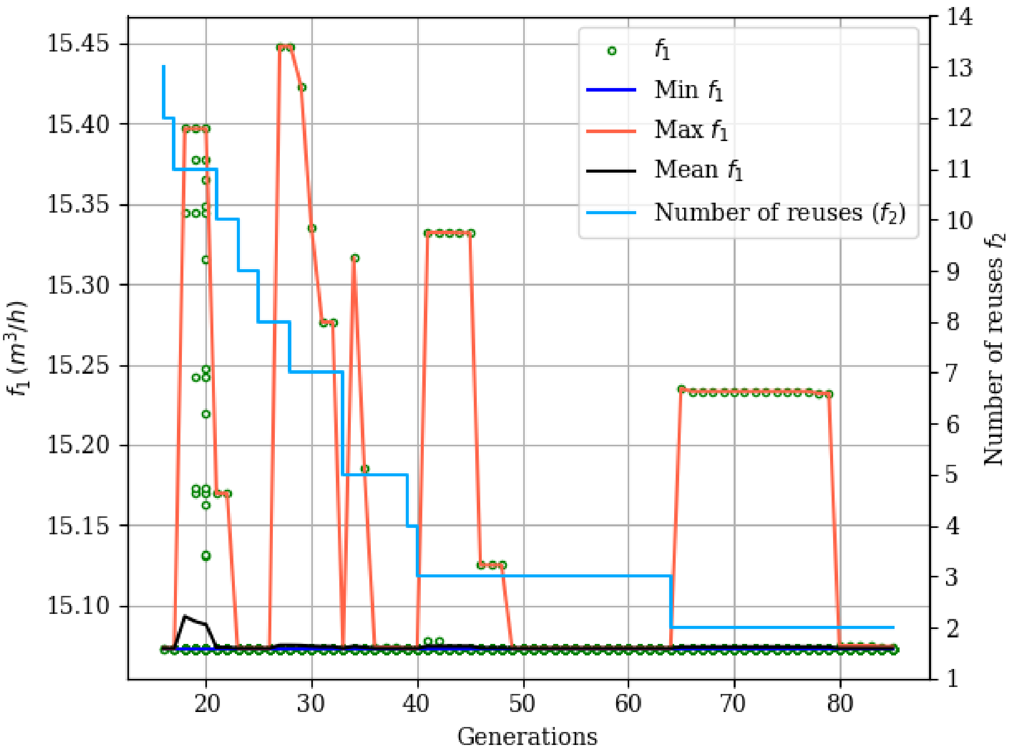

Figure 28. Variation of objective functions throughout generations, edible oil case study

Let's visualize the results and the convergence. This case study can be considered a relatively simple case. The program is executed for a few seconds while iterating 60 generations. To find the best solutions regarding the objective functions and the constraints, a post-treatment of the program's behavior is performed. First of all, we extract the population for each generation of the algorithm. After that, each population is filtered, retaining only the feasible solutions. Finally, from feasible-solutions, we extract the constraint violation and objective functions. According to **Figure 27**, the first generation with feasible solutions without constraint violation is located from the sixteenth generation. According to **Figure 28**, the convergent solutions (identified from approximately the sixty-fifth generation) respect the problem's constraints. **Figure 28** also shows that the first objective function is almost minimized from the sixteenth generation. A minimum of 15.07 m3/h is reached for most of the population. However, the number of connections converges more slowly and does not reach its minimum (i.e., two reuses) until the sixty-fifth generation.

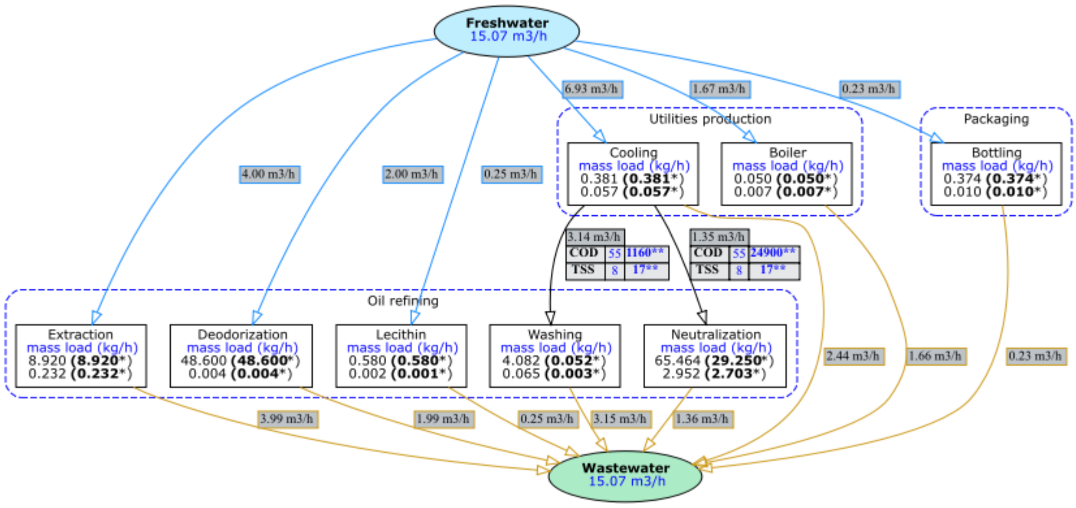

Figure 29. water-network design, edible oil case study

Figure 29 shows the design of the network corresponding to a minimum of 15.07 m3/h of freshwater and involving two reuses. Water balance is respected with a corresponding freshwater and wastewater of 15.07 m3/h. All water uses in the oil processing workshop are supplied with freshwater except for oil washing and neutralization. For extraction, deodorization, and lecithin, the freshwater flowrate is 4.00, 2.00, and 0.25 m3/h, respectively. The estimate of the mass transfer of COD and TSS corresponds to the minimum transfer required by the extraction, deodorization, and lecithin processes, i.e., (8.920, 0.232), (48.600, 0.004) and (0.580, 0.001) kg/h, respectively. The oil washing process is supplied with 3.14 m3/h from the air-cooling tower. The pollution concentration (55 ppm COD and 8 ppm TSS) is below the threshold required by the oil washing process (1160 ppm COD and 17 ppm TSS). The transfer of pollution in the oil washing process is respected, i.e. (4.082, 0.065) kg/h, knowing that the required minimums are (0.052, 0.003) kg/h. The neutralization process is supplied with 1.35 m3/h from the air-cooling tower. The pollution concentration (55 ppm COD and 8 ppm TSS) is below the threshold required by the oil washing process (24900ppm COD and 17 ppm TSS). The pollution transfers in the oil washing process is respected, i.e. (65.464, 2.952) kg/h, knowing that the required minimums are (29.250, 2.703) kg/h. Finally, the utility production and packaging workshops are supplied with freshwater, i.e., 1.67, 6.94, and 0.23 m3/h, respectively, for boiler, cooling tower, and bottling. The estimate of the mass transfer of COD and TSS corresponds to the minimum transfer required by the boiler, air-cooling tower, and bottling processes, i.e., (0.050, 0.007), (0.381, 0.057) and (0.374, 0.010) kg/h, respectively.

Let us now analyze the interest of this optimization procedure. From a technical viewpoint, optimality and the prediction of a good solution is a significant issue. The current algorithm solves the problem without initialization with any feasible solution. We can see that from a fairly simple formulation of the two objective functions and the constraints, the material balance on water and contaminants is correctly established. The application of this case study is relatively simple. But thanks to the generic aspect of the method, it is quite possible to modify the inventory by adding or removing water uses or changing the limiting data for a water-use process (e.g., maximum inlet and outlet concentrations of water). According to the inventory presented in **Table 19**, we see that only two water uses (among 8 processes) are the subject of a water supply with a specific polluting load. To go beyond the 9% of water-saving, it will be interesting to (a) specify higher concentration thresholds for oil washing and neutralization processes or (b) specify non-zero concentration thresholds for other water uses. The safety of edible oils is a strong reason that prevents the reuse of water for extraction, deodorization, and lecithin processes.

The water used in the air-cooling tower is not used in direct contact with edible oils. Therefore, there is not a priori a major health risk on the product. On the other hand, preventive anti-legionella measures require rigorous monitoring of water contamination. Consequently, supplying the air-cooling tower with even slightly polluted water will expose the air-cooling tower to legionella problems.

The cooling water used in the boiler workshop doesn't present a health safety problem for edible oils. The use of good quality water is likely required to avoid technical issues, including corrosion. Specifying maximum concentrations for these workshops requires a risk analysis which is more than ever needed. Indeed, this is as necessary as if the process concerned does not present a health risk. As in the HACCP (Hazard Analysis Critical Control Point) approach used in food safety, guidelines can be established at the level of each water use, but it is the company that must determine its limiting data based on its processes.

The packaging workshop represents the last step for which the health risk must be avoided. However, since the water is used for washing, the possibility of pre-washing and rinsing probably allows the rinsing water to be reused. Therefore, this strategy should be studied even if the water consumption is minimal (0.23 m3/h).

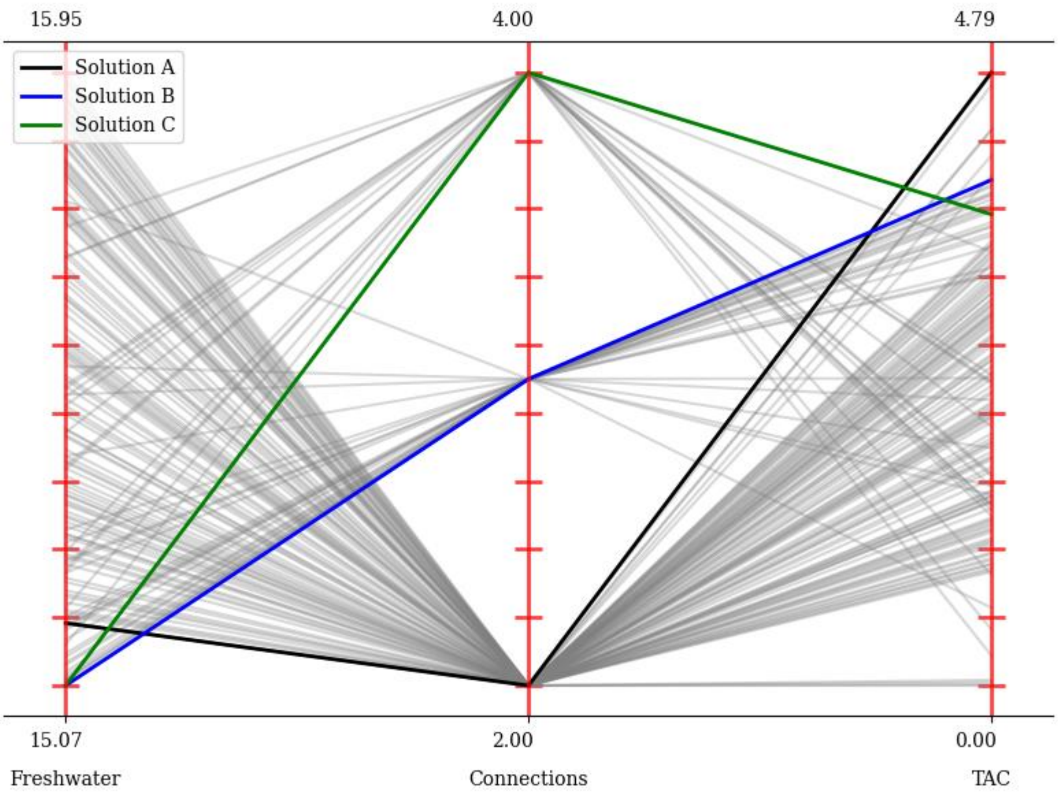

Figure 30. Parallel coordinate plots of tri-objective problem, edible oil case study

Let us now analyze the economic performance of the solution. At this stage of the optimization procedure, the solution provided by the algorithm is assumed to be the most economical since it is characterized by a minimum of water demand and a minimum of connections. This solution is also supposed to be the simplest and does not require major changes within the company. In practice, this solution may depend on several factors, such as the feasibility of the solution, the location, and the required effluent quality. We remind that the reused water is provided from the air-cooling tower (non-food area) and supplied to the oil transformation workshop (food area). The COD and TSS are not necessarily the only indicators to ensure and guarantee the reuse of water. A complete and refined analysis of the purge water from the air-cooling tower is required. We assume that the purge water requires a partial regeneration step. In this case, additional investment is inevitable. This led to the idea of integrating the total annualized cost into the optimization problem. In the following, we investigate the tri-objective problem. The optimization is subject to the same constraints and decision parameters defined in the bi-objective problem. We used the NSGA-II algorithm with the default configuration performed for the bi-objective problem. The results are illustrated in Parallel Coordinate Plots PCP (**Figure 30**). PCP technique is useful for analyzing how dense solutions are distributed in different ranges of objective functions. The three objectives represent the freshwater flow expressed in m3/h, the number of connections, and the total annualized cost expressed in k€/year. We remember that this calculation is very marginal and mainly demonstrates the tool's flexibility to integrate a more refined calculation compared to the bi-objective problem. To simplify the interpretation of the PCP diagram, three solutions are highlighted, corresponding to solutions with two connections (solution A), three connections (solution B), and four connections (solution B). The selection of these three solutions is performed in two steps. The solutions are first filtered according to the number of water reuses, i.e., 2, 3, and 4 reuses. Subsequently, on each group, a second selection is made by choosing the lowest water flowrate solution. Solution A is the closest solution to that provided by the bi-objective optimization. According to the specification provided in **Table 20**, integrating a regeneration process requires a total annualized cost of approximately 4.79 k€/year. The cost breakdown is around 49% for the investment and 51% for the utilizes and maintenance. Solutions A, B, and C have nearly similar water flowrate values. The greater the number of connections and the less expensive the solution. The cost reduction is evaluated at 18 and 23% for solutions B and C, i.e., 3.95 and 3.7 k€/year, respectively. The cost criterion can be decisive for the choice of one of the solutions. However, it must be confirmed in conjunction with equipment suppliers and must correspond to the right technical solution. The solution of a membrane process is considered in this study. Other solutions can be analyzed in the same way, e.g., biological treatment, chemical coagulation, lime treatment, reverse osmosis, etc.

This version of the tool proposed an automatic procedure to optimize the water network. There is only a need to feed the tool by the asked input, and all the procedures will take care of by the tool. Finally, because of these kinds of optimization problems, we will face a set of competing answers. About choosing the answer between a set of competing answers, there is the fact that some manual considerations are inevitable and necessary based on each case study. In the presented PCP plot, there is not only one BEST answer for all cases. Some considerations should take into account manually by managers and experts of each industry to select the best possible answer for each case based on their limits, goals, and criteria.

3.4.6 Conclusion

Water is one of the most used resources in the food industry; demand continues to increase. Processes using water are subject to increasingly stringent regulations for freshwater use or effluent discharge. In addition, the availability of water is becoming a major issue for drought-affected regions. The development of systemic techniques can effectively reduce the overall water demand and also the amount of effluents. This study illustrates the optimization of water use in a typical edible oil processing company. The case study isn't complex but represents an eco-innovative example that will decrease the negative impacts of the food industry on the environment and water resources. The optimization procedure requires specifying limiting data, including the inlet and outlet concentrations of water and the mass transfer of pollutants. The solution provided by the optimization procedure depends on the limiting data because any "non-zero" specification of pollutant concentrations will necessarily be decisive for possible water reuse. This strategy is therefore supposed to be the most economical. Two optimization strategies are studied. The first strategy is based on the definition of an optimization problem with two objectives, including the minimization of water demand and connection number. From the reduction of connection number, we wish to design simplified and less expensive water networks. The second strategy is an extension of the first one by integrating a third objective to assess the additional economic costs linked to the integration of water regeneration units before their reuse.

Both problems are solved with the NSGA-II algorithm configured in the same way. The economic cost assessment includes enough detail to show the flexibility and capacity of the tool to handle the objective functions. Constraint handling is essential to obtain a correct material balance both for water and for the various pollutants. Constraint handling is also essential to ensure that the limit values of concentrations are respected. The interpretation of the two-objective problem is quite simple, given that the data can be represented in a classical 2D Plot. For higher-dimensional data (e.g., tri-objective problem), Parallel Coordinate Plots are used to analyze how dense solutions are distributed in different ranges regarding each objective function. Other techniques may be used to better interpret the results, such as 3D Plot, Pairwise Plot, HeatMap, and Starcordinate. In the case of the tri-objective problem, the interpretation of the result required a manual selection of the solutions. This step can be automated while the program is running. This is possible thanks to a constraint controlling approach based on a penalty-based approach (Wang et al., 2010).

Chapter 4: Conclusion and perspectives

In the food industry, the implementation of sustainable water management is more relevant than ever. The environmental, economic, and legislation issues involve various measures to save water resources as much as possible and minimize wastewater discharge. Furthermore, water resources management becomes an environmentally strategic concern for dealing with climate change at a regional scale. In this context, the food industry must adapt by developing a systemic strategy to reduce water use. The tools developed in this thesis provide a very promising response to this challenge. We can go beyond optimizing a single operation and offer a large-scale design, i.e., company scale.

In the current thesis, the first chapter deals with a comprehensive survey review. A different variation of pinch has been reviewed with a focus on water pinch analyses. Some examples are presented to show their working principle. The review based on four different food sectors shows that applying water pinch can save operational costs from 23% up to 69% with various payback periods from less than one week up to 4 months. In another aspect, applying water pinch to the food sector shows an interesting decrease in water consumption: 27% in the beverage industry up to 65% in the palm oil mills sector. Finally, different challenges regarding the application of the Pinch method in the food sector have been reviewed. one of the most important challenges was selecting the appropriate contaminant indicator for each sector, detailed analysis provides a diagram to show which indicator is most used in each sector. For example, for the dairy sector Microbial count, and the sugar plant COD had the highest priority. Based on the results, some proposals for the next steps are provided.

This thesis work provides two optimization tools based on combining the pinch-based approach and numeric calculation in Python. In addition to their simplicity, the tools have great potential for various applications in the food industry or, more broadly, in any chemical engineering sector. In the second chapter, two articles have been done to present the two optimization tools. The first article proposed an algorithmic approach to minimize water consummation by using a trade-off approach. A multi-contaminant case study from the literature was selected and tested in a designed systematic simulation to prove the applicability of this method. The results and needed time show that this method can be used for small and medium-size case studies and bring good graphical insight by its provided outputs. Based on this article, optimizing a large number of connections may take lots of time and effort. Consequently, a new tool (based on metaheuristic algorithms like NSGA-II) that automatizes all the steps within the current algorithm (faster and more accurate) can be useful to handle the more complicated models proposed for the next steps. It can help also to provide more limitations like cost considerations to the model. The second article proposed a multi-objective mathematical model solved by the NSGA-II algorithm. This development helped to target the optimum faster and with fewer adjustments. Different adjustments have been done to find the best combination of the NSGA-II algorithm. Two case studies (mono and multi-contaminants) were brought from the literature to be tested.

In the third chapter, to show the applicability of this method to the real case studies of the food sector, a real industrial dataset from a French edible oil company was collected and tested. Both manual trade-off and NSGA-II methods were tested with the current data that contain eight operations and two contaminants. Two research works were prepared based on this chapter. The results show the same optimum point by having around 9% of water-saving and 37 k€ cost-saving within the company. Besides the other objective functions, another objective function concerning cost analysis was added to the model. In conclusion, different discussions about the effects of other parameters on the validity of answers, cost analysis, safety issues, etc., have been done.

Work in progress in collaboration with manufacturers aims to extend the application of this tool to other sectors such as the milk, wine, and vegetable sectors. This work aims to develop a common framework in the specification of data collection. The most important is the specification of maximum concentrations, which are difficult to estimate. For example, we propose to combine the existing tools with sensitivity analyses to limit the collection of data only on those parameters which have an apparent influence on the design and performance of the water network.

4.1 Outlook and perspectives

As perspectives for further research, developing an integrated tool including the different variations of a pinch like water and energy and life cycle assessment (LCA) seems interesting.

In this thesis, the main attention is to minimize the total freshwater consumption of industries by respecting the concentration limits. In addition, we have also tried to minimize the number of connections as much as possible to simplify the network. For future research, it’s recommended to add more considerations and details to the tool, i.e., health risk, location, engineering limitation, etc.

In current work, only reuse streams take into account to find the possible water-saving opportunities without using purification equipment. Despite the price of purification equipment, using them is inevitable in some cases. It’s necessary to treat the water between operations by regeneration and recycling units. In this case, it seems necessary to consider regeneration and reuse opportunities and the possibility of installing the purification equipment within the tool. It gives more flexibility to the tool to propose a simpler network with fewer connections but not the cheapest one.

In this work, the cases brought from continuous case studies show that other process types like semi-continues and batch are existing. To have a more comprehensive tool suitable for all types of processes, it’s interesting to upgrade the current tools or develop a model that can handle the batch process.

In this work, the main focus was on the food industries. Also, case studies from real food industries have been applied. For the next research works, it’s also interesting to try and test the data from other types of industries like frozen fruits and vegetables, cheese factory, dairy sector, etc.

In this work, it's normal for the more significant problems and multi-contaminant cases to have a set of competing answers. The difference between different answers with high and low total freshwater amounts is related to the number and connections in each answer. The selection criteria are based on water demand and connection number, but the criteria can be mixed with environmental or economic considerations for further research. To consider these new aspects, it is necessary to define new objective functions or constraints management strategies like the penalty-based approach.

References

Ahmad, T., Belwal, T., Li, L., Ramola, S., Aadil, R.M., Abdullah, Xu, Y., Zisheng, L., 2020. Utilization of wastewater from edible oil industry, turning waste into valuable products: A review. Trends Food Sci. Technol. https://doi.org/10.1016/j.tifs.2020.02.017

Ahmed, Y., Yaakob, Z., Akhtar, P., Sopian, K., 2015. Production of biogas and performance evaluation of existing treatment processes in palm oil mill effluent (POME). Renew. Sustain. Energy Rev. 42, 1260–1278. https://doi.org/10.1016/j.rser.2014.10.073

Ahmetović, E., Ibrić, N., Kravanja, Z., Grossmann, I.E., 2015. Water and energy integration: A comprehensive literature review of non-isothermal water network synthesis. Comput. Chem. Eng. 82, 144–171. https://doi.org/10.1016/j.compchemeng.2015.06.011

Akpomiemie, M.O., Smith, R., 2018. Cost-effective strategy for heat exchanger network retrofit. Energy 146, 82–97. https://doi.org/10.1016/J.ENERGY.2017.09.005

Akpomiemie, M.O., Smith, R., 2016. Retrofit of heat exchanger networks with heat transfer enhancement based on an area ratio approach. Appl. Energy 165, 22–35. https://doi.org/10.1016/J.APENERGY.2015.11.056

Akpomiemie, M.O., Smith, R., 2015. Retrofit of heat exchanger networks without topology modifications and additional heat transfer area. Appl. Energy 159, 381–390. https://doi.org/10.1016/J.APENERGY.2015.09.017

Alcamo, J., Döll, P., Henrichs, T., Kaspar, F., Lehner, B., Rösch, T., Siebert, S., 2003. Development and testing of the WaterGAP 2 global model of water use and availability. Hydrol. Sci. J. 48, 317–337. https://doi.org/10.1623/hysj.48.3.317.45290

Almato, M., Espuña, A., Puigjaner, L., 1999. Optimisation of water use in batch process industries. Comput. Chem. Eng. 23, 1427–1437. https://doi.org/10.1016/S0098-1354(99)00302-6

Almató, M., Sanmartí, E., Espun˜a, A., Puigjaner, L., 1997. Rationalizing the water use in the batch process industry. Comput. Chem. Eng. 21, S971–S976. https://doi.org/10.1016/S0098-1354(97)87628-4

Alva-Argáez, A., Kokossis, A.C., Smith, R., 1998. Wastewater minimisation of industrial systems using an integrated approach. Comput. Chem. Eng. 22, S741–S744. https://doi.org/10.1016/S0098-1354(98)00138-0

Alves, J., 1999. Analysis and design of refinery hydrogen distribution systems.

and, B.G., I. E. Grossmann*, ‡, 1998. Optimal Design of Distributed Wastewater Treatment Networks. https://doi.org/10.1021/IE980133H

and, J.J.A., Gavin P. Towler*, ‡, 2002. Analysis of Refinery Hydrogen Distribution

Systems. https://doi.org/10.1021/IE010558V

Arya, D., Bandyopadhyay, S., 2019. Iterative Pinch Analysis to address non-linearity in a stochastic Pinch problem. J. Clean. Prod. 227, 543–553. https://doi.org/10.1016/J.JCLEPRO.2019.04.078

Atkins, M.J., Morrison, A.S., Walmsley, M.R.W., 2010. Carbon Emissions Pinch Analysis (CEPA) for emissions reduction in the New Zealand electricity sector. Appl. Energy 87, 982–987. https://doi.org/10.1016/J.APENERGY.2009.09.002

Bagajewicz, M., 2000. A review of recent design procedures for water networks in refineries and process plants. Comput. Chem. Eng. 24, 2093–2113. https://doi.org/10.1016/S0098-1354(00)00579-2

Bavar, M., Sarrafzadeh, M.-H., Asgharnejad, H., Norouzi-Firouz, H., 2018. Water management methods in food industry: Corn refinery as a case study. J. Food Eng. 238, 78–84. https://doi.org/10.1016/J.JFOODENG.2018.06.018

Blank, J., Deb, K., 2020. Pymoo: Multi-Objective Optimization in Python. IEEE Access 8, 89497–89509. https://doi.org/10.1109/ACCESS.2020.2990567

Boix, M., Montastruc, L., Pibouleau, L., Azzaro-pantel, C., Domenech, S., 2011. A multiobjective optimization framework for multicontaminant industrial water network design. J. Environ. Manage. 92, 1802–1808. https://doi.org/10.1016/j.jenvman.2011.02.016

Buabeng-baidoo, E., Mafukidze, N., Pal, J., 2017. Chemical Engineering Research and Design Study of water reuse opportunities in a large-scale milk processing plant through process integration. Chem. Eng. Res. Des. 121, 81–91. https://doi.org/10.1016/j.cherd.2017.02.031

Buabeng-Baidoo, E., Mafukidze, N., Pal, J., Tiwari, S., Srinivasan, B., Majozi, T., Srinivasan, R., 2017. Study of water reuse opportunities in a large-scale milk processing plant through process integration. Chem. Eng. Res. Des. 121, 81–91. https://doi.org/10.1016/j.cherd.2017.02.031

Casani, S., Knøchel, S., 2002. Application of HACCP to water reuse in the food industry 13, 315–327.

Casani, S., Rouhany, M., Knøchel, S., 2005. A discussion paper on challenges and limitations to water reuse and hygiene in the food industry 39, 1134–1146. https://doi.org/10.1016/j.watres.2004.12.015

Castro, P., Matos, H., … M.F.-C.E., 1999, undefined, n.d. Improvements for mass-exchange networks design. academia.edu.

Chin, H.H., Liew, P.Y., Varbanov, P., Klemeš, J.J., 2020. Extension of Pinch Analysis to Targeting and Synthesis of Multi-Contaminant Material Recycle and Reuse Networks. Authorea Prepr. https://doi.org/10.22541/AU.160315137.74142765/V1

Chin, H.H., Varbanov, P.S., Liew, P.Y., Klemeš, J.J., 2021. Pinch-based targeting methodology for multi-contaminant material recycle/reuse. Chem. Eng. Sci. 230, 116129. https://doi.org/10.1016/j.ces.2020.116129

Ching-Huei Huang, Chuei-Tin Chang, * and, Ling, H.-C., Chang, C.-C., 1999. A Mathematical Programming Model for Water Usage and Treatment Network Design. https://doi.org/10.1021/IE990043S

Chungsiriporn, J., Prasertsan, S., Bunyakan, C., 2006. Minimization of water consumption and process optimization of palm oil mills. Clean Technol. Environ. Policy 8, 151–158. https://doi.org/10.1007/s10098-005-0002-y

Compton, M., Willis, S., Rezaie, B., Humes, K., 2018. Food processing industry energy and water consumption in the Paci fi c northwest. Innov. Food Sci. Emerg. Technol. 47, 371–383. https://doi.org/10.1016/j.ifset.2018.04.001

Crilly, D., Zhelev, T., 2008. Emissions targeting and planning: An application of CO2 emissions pinch analysis (CEPA) to the Irish electricity generation sector. Energy 33, 1498–1507. https://doi.org/10.1016/J.ENERGY.2008.05.015

De-León Almaraz, S., Boix, M., Montastruc, L., Azzaro-Pantel, C., Liao, Z., Domenech, S., 2016. Design of a water allocation and energy network for multi-contaminant problems using multi-objective optimization. Process Saf. Environ. Prot. 103, 348–364. https://doi.org/10.1016/j.psep.2016.03.015

Deb, Kalyanmoy, Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic algorithm: NSGA-II. IEEE Trans. Evol. Comput. 6, 182–197. https://doi.org/10.1109/4235.996017

Deb, K., Sindhya, K., Okabe, T., 2007. Self-adaptive simulated binary crossover for real-parameter optimization, in: Proceedings of GECCO 2007: Genetic and Evolutionary Computation Conference. pp. 1187–1194. https://doi.org/10.1145/1276958.1277190

Deng, C., Zhou, Y., Jiang, W., Feng, X., 2017. Optimal design of inter-plant hydrogen network with purification reuse/recycle. Int. J. Hydrogen Energy 42, 19984–20002. https://doi.org/10.1016/J.IJHYDENE.2017.06.199

Dhole, V.R., Ramchandani, N., Tainsh, R.A., Wasilewski, M., 1996. Make your process water pay for itself. Chem. Eng. (New York) 103.

Diamante, J.A.R., Tan, R.R., Foo, D.C.Y., Ng, D.K.S., Aviso, K.B., Bandyopadhyay, S., 2014. Unified pinch approach for targeting of carbon capture and storage (CCS) systems with multiple time periods and regions. J. Clean. Prod. 71, 67–74. https://doi.org/10.1016/J.JCLEPRO.2013.11.027

Ding, Y., Feng, X., Chu, K.H., 2011. Optimization of hydrogen distribution systems with pressure constraints. J. Clean. Prod. 19, 204–211. https://doi.org/10.1016/J.JCLEPRO.2010.09.013

Doyle, S.J., Smith, R., 1997. Targeting Water Reuse with Multiple Contaminants. Process Saf. Environ. Prot. 75, 181–189. https://doi.org/10.1205/095758297529020

El-Halwagi, M.M., Manousiouthakis, V., 1990. Simultaneous synthesis of mass-exchange and regeneration networks. AIChE J. 36, 1209–1219. https://doi.org/10.1002/aic.690360810

Ensinas, A. V., Nebra, S.A., Lozano, M.A., Serra, L.M., 2007. Analysis of process steam demand reduction and electricity generation in sugar and ethanol production from sugarcane. Energy Convers. Manag. 48, 2978–2987. https://doi.org/10.1016/J.ENCONMAN.2007.06.038

Feng, X., Bai, J., Wang, H., Zheng, X., 2008. Grass-roots design of regeneration recycling water networks 32, 1892–1907. https://doi.org/10.1016/j.compchemeng.2007.10.006

Feng, X., Chu, K.H., 2004. Cost Optimization of Industrial Wastewater Reuse Systems. Process Saf. Environ. Prot. 82, 249–255. https://doi.org/10.1205/095758204323066019

Flörke, M., Kynast, E., Bärlund, I., Eisner, S., Wimmer, F., Alcamo, J., 2013. Domestic and industrial water uses of the past 60 years as a mirror of socio-economic development: A global simulation study. Glob. Environ. Chang. 23, 144–156. https://doi.org/10.1016/j.gloenvcha.2012.10.018

Fonseca, C., … L.P.-2006 I. international, 2006, U., 2006. An improved dimension-sweep algorithm for the hypervolume indicator. ieeexplore.ieee.org.

Friedler, F., Varga, J.B., Fehér, E., Fan, L.T., 1996. Combinatorially Accelerated Branch-and-Bound Method for Solving the MIP Model of Process Network Synthesis. Springer, Boston, MA, pp. 609–626. https://doi.org/10.1007/978-1-4613-3437-8_35

Gadalla, M.A., 2015. A new graphical method for Pinch Analysis applications: Heat exchanger network retrofit and energy integration. Energy 81, 159–174. https://doi.org/10.1016/J.ENERGY.2014.12.011

Goldberg, D., 1), K.D.G.A. 1991 (FOGA, 2014, U., 2014. A comparative analysis of selection schemes used in genetic algorithms. books.google.com.

Grobicki, A., 2008. the Future of Water Use in Industry. World Water 5.

Gunaratnam, M., Alva-Argáez, A., Kokossis, A., Kim, J.K., Smith, H., 2005. Automated design of total water systems. Ind. Eng. Chem. Res. 44, 588–599. https://doi.org/10.1021/ie040092r

Hallale, N., 2002. A new graphical targeting method for water minimisation. Adv. Environ. Res. 6, 377–390. https://doi.org/10.1016/S1093-0191(01)00116-2

Hallale, N., Fraser, D.M., 2000. Capital and total cost targets for mass exchange networks: Part 1: Simple capital cost models. Comput. Chem. Eng. 23, 1661–1679. https://doi.org/10.1016/S0098-1354(99)00316-6

Hallale, N., Fraser, D.M., 1998. Capital cost targets for mass exchange networks A special case: Water minimisation. Chem. Eng. Sci. 53, 293–313. https://doi.org/10.1016/S0009-2509(97)00191-7

Hallale, N., Liu, F., 2001. Refinery hydrogen management for clean fuels production. Adv. Environ. Res. 6, 81–98. https://doi.org/10.1016/S1093-0191(01)00112-5

Hau, J.L., Bakshi, B.R., 2004. Promise and problems of emergy analysis. Ecol. Modell. 178, 215–225. https://doi.org/10.1016/j.ecolmodel.2003.12.016

Helmer, R., Hespanhol, I., 1997. Water pollution control—a guide to the use of water quality management principles [WWW Document]. London, Gt. Britain E FNSpon.

Ho, W.S., Tan, S.T., Hashim, H., Lim, J.S., Lee, C.T., 2015. Waste Management Pinch Analysis (WAMPA) for Carbon Emission Reduction. Energy Procedia 75, 2448–2453. https://doi.org/10.1016/J.EGYPRO.2015.07.213

Hoekstra, A.Y., Chapagain, A.K., 2006. Water footprints of nations: Water use by people as a function of their consumption pattern, in: Integrated Assessment of Water Resources and Global Change. Springer Netherlands, pp. 35–48. https://doi.org/10.1007/978-1-4020-5591-1_3

Ishibuchi, H., Masuda, H., Tanigaki, Y., Nojima, Y., 2015. Modified distance calculation in generational distance and inverted generational distance, in: Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics). Springer Verlag, pp. 110–125. https://doi.org/10.1007/978-3-319-15892-1_8

Jiang, N., Shelley, J.D., Doyle, S., Smith, R., 2014. Heat exchanger network retrofit with a fixed network structure. Appl. Energy 127, 25–33. https://doi.org/10.1016/J.APENERGY.2014.04.028

Jiao, Y., Su, H., Hou, W., 2012a. Improved optimization methods for refinery hydrogen network and their applications. Control Eng. Pract. 20, 1075–1093. https://doi.org/10.1016/J.CONENGPRAC.2012.04.010

Jiao, Y., Su, H., Hou, W., Liao, Z., 2012b. Optimization of refinery hydrogen network based on chance constrained programming. Chem. Eng. Res. Des. 90, 1553–1567. https://doi.org/10.1016/J.CHERD.2012.02.016

Jödicke, G., Fischer, U., Hungerbühler, K., 2001. Wastewater reuse: a new approach to screen for designs with minimal total costs. Comput. Chem. Eng. 25, 203–215. https://doi.org/10.1016/S0098-1354(00)00648-7

Kim, J., Lee, Y., Moon, I., 2008. Optimization of a hydrogen supply chain under demand uncertainty. Int. J. Hydrogen Energy 33, 4715–4729. https://doi.org/10.1016/J.IJHYDENE.2008.06.007

Klemes, Jiri, Friedler, F., Bulatov, I., Varbanov, P., 2010. Sustainibility in the process industry: integration and optimization (Green Manufacturing & Systems Engineering). McGraw-Hill Professional, New York.

Kuo, W.-C.J., Smith, R., 1998. Designing for the Interactions Between Water-Use and Effluent Treatment. Chem. Eng. Res. Des. 76, 287–301. https://doi.org/10.1205/026387698524938

Kuo, W.-C.J., Smith, R., 1997. Effluent treatment system design. Chem. Eng. Sci. 52, 4273–4290. https://doi.org/10.1016/S0009-2509(97)00186-3

Lee, S.C., Sum Ng, D.K., Yee Foo, D.C., Tan, R.R., 2009. Extended pinch targeting techniques for carbon-constrained energy sector planning. Appl. Energy 86, 60–67. https://doi.org/10.1016/J.APENERGY.2008.04.002

Lee, W., Okos, M.R., 2011. Sustainable food processing systems - Path to a zero discharge : reduction of water , waste and energy. Ital. Oral Surg. 1, 1768–1777. https://doi.org/10.1016/j.profoo.2011.09.260

Lee, Z.S., Chin, S.Y., Lim, J.W., Witoon, T., Cheng, C.K., 2019. Treatment technologies of palm oil mill effluent (POME)and olive mill wastewater (OMW): A brief review. Environ. Technol. Innov. https://doi.org/10.1016/j.eti.2019.100377

Lehr, Jay, H., Gass, T.E., Pettyjohn, W., 1980. Domestic water treatment [WWW Document]. McGraw Hill B. Co. New York 33093.

Li, K., Deb, K., Zhang, Q., … S.K.-T. on E., 2014, U., 2014. An evolutionary many-objective optimization algorithm based on dominance and decomposition. ieeexplore.ieee.org.

Li, Y., Guan, J., 2016. A stepwise optimal design of water network. Chinese J. Chem. Eng. 24, 787–794. https://doi.org/10.1016/j.cjche.2016.04.031

Linnhoff, B., Dhole, V.R., 1993. Targeting for CO2 emissions for Total Sites. Chem. Eng. Technol. 16, 252–259. https://doi.org/10.1002/ceat.270160407

Linnhoff, B., Flower, J.R., 1978a. Synthesis of heat exchanger networks: II. Evolutionary generation of networks with various criteria of optimality. AIChE J. 24, 642–654. https://doi.org/10.1002/aic.690240412

Linnhoff, B., Flower, J.R., 1978b. Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks. AIChE J. 24, 633–642. https://doi.org/10.1002/aic.690240411

Linnhoff, B., Hindmarsh, E., 1983. The pinch design method for heat exchanger networks. Chem. Eng. Sci. 38, 745–763. https://doi.org/10.1016/0009-2509(83)80185-7

Louhıchı, G., Bousselmı, L., Ghrabı, A., Khounı, I., 2019. Process optimization via response surface methodology in the physico-chemical treatment of vegetable oil refinery wastewater. Environ. Sci. Pollut. Res. 26, 18993–19011. https://doi.org/10.1007/s11356-018-2657-z

Lu, J., Pua, X., Liu, C., Chang, C., Cheng, K., 2013. ScienceDirect The implementation of HACCP management system in a chocolate ice cream plant. J. Food Drug Anal. 22, 391–398. https://doi.org/10.1016/j.jfda.2013.09.049

M. M. El-Halwagi, *, F. Gabriel, and, Harell, D., 2003. Rigorous Graphical Targeting for Resource Conservation via Material Recycle/Reuse Networks. https://doi.org/10.1021/IE030318A

Ma, Z., Lei, T., Ji, X., Gao, X., Gao, C., 2015. Submerged membrane bioreactor for vegetable oil wastewater treatment. Chem. Eng. Technol. 38, 101–109. https://doi.org/10.1002/ceat.201400184

Manan, Z.A., Wan Alwi, S.R., Ujang, Z., 2006. Water pinch analysis for an urban system: a case study on the Sultan Ismail Mosque at the Universiti Teknologi Malaysia (UTM). Desalination 194, 52–68. https://doi.org/10.1016/j.desal.2005.11.003

Marchettini, N., Ridolfi, R., Rustici, M., 2007. An environmental analysis for comparing waste management options and strategies. Waste Manag. 27, 562–571. https://doi.org/10.1016/J.WASMAN.2006.04.007

Meneses, Y.E., Stratton, J., Flores, R.A., 2017. Water reconditioning and reuse in the food processing industry: Current situation and challenges. Trends Food Sci. Technol. 61, 72–79. https://doi.org/10.1016/j.tifs.2016.12.008

Mishra, S., Mondal, S., Saha, S., 2016. Fast implementation of steady-state NSGA-II, in: 2016 IEEE Congress on Evolutionary Computation, CEC 2016. Institute of Electrical and Electronics Engineers Inc., pp. 3777–3784. https://doi.org/10.1109/CEC.2016.7744268

Mohammadnejad, S., Bidhendi, G.R.N., Mehrdadi, N., 2011. Water pinch analysis in oil refinery using regeneration reuse and recycling consideration. Desalination 265, 255–265. https://doi.org/10.1016/j.desal.2010.07.059

Molden, D., 2013. Water for food water for life: A comprehensive assessment of water management in agriculture.

Mughees, W., Al-Ahmad, M., 2015a. Application of water pinch technology in minimization of water consumption at a refinery. Comput. Chem. Eng. 73, 34–42. https://doi.org/10.1016/j.compchemeng.2014.11.004

Nemati-Amirkolaii, Romdhana, Lameloise, 2019. Pinch Methods for Efficient Use of Water in Food Industry: A Survey Review. Sustainability 11, 4492. https://doi.org/10.3390/su11164492

Nemerow, Leonard, N., 1978. Industrial water pollution: origins, characteristics, and treatment, Massachusetts: Addison-Wesley Publishing Company.

Ngoie, W.I., Oyekola, O.O., Ikhu-Omoregbe, D., Welz, P.J., 2020. Valorisation of Edible Oil Wastewater Sludge: Bioethanol and Biodiesel Production. Waste and Biomass Valorization 11, 2431–2440. https://doi.org/10.1007/s12649-019-00633-w

Nweke, C.N., Nwabanne, J.T., Igbokwe, P.K., 2014. Kinetics of Batch Anaerobic Digestion of Vegetable Oil Wastewater 1. https://doi.org/10.15764/WPT.2014.02001

Odum, H.T., 1983. Systems ecology; An introduction.

Ohimain, E.I., Izah, S.C., 2017. A review of biogas production from palm oil mill effluents using different configurations of bioreactors. Renew. Sustain. Energy Rev. https://doi.org/10.1016/j.rser.2016.11.221

Olesen, S.G., Polley, G.T., 1997. A Simple Methodology for the Design of Water Networks Handling Single Contaminants. Chem. Eng. Res. Des. 75, 420–426. https://doi.org/10.1205/026387697523886

Ooi, R.E.H., Foo, D.C.Y., Ng, D.K.S., Tan, R.R., 2013. Planning of carbon capture and storage with pinch analysis techniques. Chem. Eng. Res. Des. 91, 2721–2731. https://doi.org/10.1016/J.CHERD.2013.04.007

OOPEC, 1998. COUNCIL DIRECTIVE 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. Off. J. Eur. Communities L 330, 32–54.

Pan, H., Zhang, X., Wu, J., Zhang, Y., Lin, L., Yang, G., Deng, S., Li, L., Yu, X., Qi, H., Peng, H., 2016. Sustainability evaluation of a steel production system in China based on emergy. J. Clean. Prod. 112, 1498–1509. https://doi.org/10.1016/J.JCLEPRO.2015.05.019

Peng, S., Farid, M., Ho, I., Mahdi, K.A., 2008. Water and Wastewater Minimization in Dairy Plants using Water Pinch Technology 3, 43–50.

Peng, S.F., Farid, M., Wilks, T., 2001. Application of water pinch analysis to a dairy plant. Acta Hortic. 566, 199–203. https://doi.org/10.17660/ActaHortic.2001.566.23

Poles, S., Fu, Y., Rigoni, E., 2009. The effect of initial population sampling on the convergence of multi-objective genetic algorithms. Lect. Notes Econ. Math. Syst. 618, 123–133. https://doi.org/10.1007/978-3-540-85646-7_12

Prakash, R., Shenoy, U. V., 2005. Targeting and design of water networks for fixed flowrate and fixed contaminant load operations. Chem. Eng. Sci. 60, 255–268. https://doi.org/10.1016/J.CES.2004.08.005

Ritchie, H., Roser, M., 2017. Water Use and Stress. Our World Data.

Rosegrant, M., Cai, X., Cline, S., 2002. Global water outlook to 2025: averting an impending crisis.

Roychaudhuri, P.S., Bandyopadhyay, S., 2018. Financial Pinch Analysis: Minimum opportunity cost targeting algorithm. J. Environ. Manage. 212, 88–98. https://doi.org/10.1016/j.jenvman.2018.02.005

Roychaudhuri, P.S., Kazantzi, V., Foo, D.C.Y., Tan, R.R., Bandyopadhyay, S., 2017. Selection of energy conservation projects through Financial Pinch Analysis. Energy 138, 602–615. https://doi.org/10.1016/J.ENERGY.2017.07.082

Saranya, P., Ramani, K., Sekaran, G., 2014. Biocatalytic approach on the treatment of edible oil refinery wastewater. RSC Adv. 4, 10680–10692. https://doi.org/10.1039/c3ra43668c

Seckler, David, Amarasinghe, U., David, M., Silva, R. de, Barker, R., 1998. World water demand and supply, 1990 to 2025: Scenarios and issues. Research Report 19. Colombo, Sri Lanka: International Water Management Institute.

Seider, W., Seader, J., Lewin, D., 1999. Process design principles: synthesis, analysis, and evaluation.

Skouteris, G., Ouki, S., Foo, D., Saroj, D., Altini, M., Melidis, P., Cowley, B., Ells, G., Palmer, S., O'Dell, S., 2018. Water footprint and water pinch analysis techniques for sustainable water management in the brick-manufacturing industry. J. Clean. Prod. 172, 786–794. https://doi.org/10.1016/J.JCLEPRO.2017.10.213

Suárez, A., Fidalgo, T., Riera, F.A., 2014. Recovery of dairy industry wastewaters by reverse osmosis . Production of boiler water 133, 204–211.

https://doi.org/10.1016/j.seppur.2014.06.041

Suárez, A., Riera, F.A., 2015. Journal of Industrial and Engineering Chemistry Production of high-quality water by reverse osmosis of milk dairy condensates. J. Ind. Eng. Chem. 21, 1340–1349. https://doi.org/10.1016/j.jiec.2014.06.004

Takama, N., Kuriyama, T., Shiroko, K., Umeda, T., 1980. Optimal water allocation in a petroleum refinery. Comput. Chem. Eng. 4, 251–258. https://doi.org/10.1016/0098-1354(80)85005-8

Tan, R.R., Aviso, K.B., Foo, D.C.Y., 2018. Carbon emissions pinch analysis of economic systems. J. Clean. Prod. 182, 863–871. https://doi.org/10.1016/j.jclepro.2018.02.082

Tan, R.R., Foo, D.C.Y., 2007. Pinch analysis approach to carbon-constrained energy sector planning. Energy 32, 1422–1429. https://doi.org/10.1016/J.ENERGY.2006.09.018

Tan, Y.L., Manan, Z.A., Foo, D.C.Y., 2007. Retrofit of Water Network with Regeneration Using Water Pinch Analysis. Process Saf. Environ. Prot. 85, 305–317. https://doi.org/10.1205/PSEP06040

Thevendiraraj, S., Klemeš, J., Paz, D., Aso, G., Cardenas, G.J., 2003a. Water and wastewater minimisation study of a citrus plant. Resour. Conserv. Recycl. 37, 227–250. https://doi.org/10.1016/S0921-3449(02)00102-7

Tokos, H., Novak Pintarič, Z., 2009a. Synthesis of batch water network for a brewery plant. J. Clean. Prod. 17, 1465–1479. https://doi.org/10.1016/j.jclepro.2009.06.009

Van Veldhuizen, D.A., 1999. AIR FORCE INSTITUTE OF TECHNOLOGY Wright-Patterson Air Force Base, Ohio DTIC QUALITY INSPECTED 4.

Wang, M., Dai, G., Hu, H., 2010. Improved NSGA-II algorithm for Optimization of Constrained Functions, in: 2010 International Conference on Machine Vision and Human-Machine Interface, MVHI 2010. pp. 673–675. https://doi.org/10.1109/MVHI.2010.209

Wang, Smith, 1995. Waste-Water Minimization with Flow-Rate Constraints. Chem. Eng. Res. Des. 73, 889–904.

Wang, Smith, 1994. Design of distributed effluent treatment systems. Chem. Eng. Sci. 49, 3127–3145. https://doi.org/10.1016/0009-2509(94)E0126-B

Wang, Y., Pan, M., Bulatov, I., Smith, R., Kim, J.-K., 2012. Application of intensified heat transfer for the retrofit of heat exchanger network. Appl. Energy 89, 45–59. https://doi.org/10.1016/J.APENERGY.2011.03.019

Wang, Y.P., Smith, R., 1994. Wastewater minimisation. Chem. Eng. Sci. 49, 981–1006. https://doi.org/10.1016/0009-2509(94)80006-5

World Development Report 2008, 2007. , World Development Report 2008. The World Bank. https://doi.org/10.1596/978-0-8213-6807-7

Wujie, Zhufei, X., 2011. The Influence of Water Quality on Food Quality and the

Treatment of Water for Food Processing 10, 2671–2676. https://doi.org/10.1016/j.proenv.2011.09.415

Yu, N., Xing, D., Li, W., Yang, Y., Li, Z., Li, Y., Ren, N., 2017. Electricity and methane production from soybean edible oil refinery wastewater using microbial electrochemical systems. Int. J. Hydrogen Energy 42, 96–102. https://doi.org/10.1016/j.ijhydene.2016.11.116

Žbontar Zver, L., Glavič, P., 2005. Water minimization in process industries: Case study in beet sugar plant. Resour. Conserv. Recycl. 43, 133–145. https://doi.org/10.1016/j.resconrec.2004.04.014

Zhang, H., Guan, X., Ding, Y., Liu, C., 2018. Emergy analysis of Organic Rankine Cycle (ORC) for waste heat power generation. J. Clean. Prod. 183, 1207–1215. https://doi.org/10.1016/J.JCLEPRO.2018.02.170

Zhang, H., Rangaiah, G.P., 2013. One-step approach for heat exchanger network retrofitting using integrated differential evolution. Comput. Chem. Eng. 50, 92–104. https://doi.org/10.1016/J.COMPCHEMENG.2012.10.018

Zhelev, T.K., 2005. On the integrated management of industrial resources incorporating finances. J. Clean. Prod. 13, 469–474. https://doi.org/10.1016/J.JCLEPRO.2003.09.004

Zhelev, T.K., 2002. Wastewater Treatment Management Using Combined Water-Oxygen-Thermal Pinch Analysis. Comput. Aided Chem. Eng. 10, 391–396. https://doi.org/10.1016/S1570-7946(02)80093-1

Zhelev, T.K., Bhaw, N., 2000. Combined water-oxygen pinch analysis for better wastewater treatment management. Waste Manag. 20, 665–670. https://doi.org/10.1016/S0956-053X(00)00050-7

Zhelev, T.K., Ntlhakana, J.L., 1999. Energy-environment closed-loop through Oxygen Pinch. Comput. Chem. Eng. 23, S79–S83. https://doi.org/10.1016/S0098-1354(99)80021-0

Zhelev, T.K., Ridolfi, R., 2006a. Energy recovery and environmental concerns addressed through emergy–pinch analysis. Energy 31, 2486–2498. https://doi.org/10.1016/J.ENERGY.2005.10.021

Zhou, L., Liao, Z., Wang, J., Jiang, B., Yang, Y., Hui, D., 2013. Optimal design of sustainable hydrogen networks. Int. J. Hydrogen Energy 38, 2937–2950. https://doi.org/10.1016/J.IJHYDENE.2012.12.084

Appendix1: Manual Trade-Off Tool Simulation - Iterations Results

Here are the intermediate results of each simulation iteration for the manual trade-off tool proposed in chapter 2 (second publication). First Table shows the Flowrates and detailed mass balances. The second Table shows the connection matrix R or reuse streams between processes by their associated flow rates. Within the following Tables, for the mass load and inlet/outlet concentration two amounts are presented: one in the braces {} and another out of braces. The amount in the braces is related to the upper boundaries and the amount outside of the braces is related to the optimized values that find by the algorithm in this step by respecting these boundaries. For the Mass load, the amount in the braces defines the lower bound that shows the Minimum transfer of pollution that is necessary. For the inlet and outlet concentration, the amount in the braces defines the upper bound of the Maximum allowed concentration.

1. First Iteration:

Process	Freshwater m3/h	Contaminant	mass load kg/h	Cin ppm	Cout ppm
Process 1	50.00				
		A	0.75 {0.75}	0 {0}	15 {15}
		B	20.00 {20.00}	0 {0}	400 {400}
		C	1.75 {1.75}	0 {0}	35 {35}
Process 2	33.18				
		A	3.98 {3.40}	0 {20}	120 {120}
		B	414.80 {414.80}	0 {300}	12500 {12500}
		C	5.97 {4.59}	0 {45}	180 {180}
Process 3	54.82				
		A	12.06 {5.60}	0 {120}	220 {220}
		B	2.47 {1.40}	0 {20}	45 {45}
		C	520.80 {520.80}	0 {200}	9500 {9500}
Process 4	8.00				
		A	0.16 {0.16}	0 {0}	20 {20}
		B	0.48 {0.48}	0 {0}	60 {60}
		C	0.16 {0.16}	0 {0}	20 {20}
Process 5	7.60				
		A	1.14 {0.80}	0 {50}	150 {150}
		B	60.80 {60.80}	0 {400}	8000 {8000}
		C	0.91 {0.48}	0 {60}	120 {120}
Tot	153.61	-	-	-	-

	Process 1	Process 2	Process 3	Process 4	Process 5
Process 1	0.00	0.00	0.00	0.00	0.00
Process 2	0.00	0.00	0.00	0.00	0.00
Process 3	0.00	0.00	0.00	0.00	0.00
Process 4	0.00	0.00	0.00	0.00	0.00
Process 5	0.00	0.00	0.00	0.00	0.00

2. Second Iteration:

Process	Freshwater m3/h	Contaminant	mass load kg/h	Cin ppm	Cout ppm
Process 1	50.00				
		A	0.75 {0.75}	0 {0}	15 {15}
		B	20.00 {20.00}	0 {0}	400 {400}
		C	1.75 {1.75}	0 {0}	35 {35}
Process 2	1717.00				
		A	208.59 {3.40}	9 {20}	120 {120}
		B	22873.33 {414.80}	378 {300} !	12500 {12500}
		C	4.59 {4.59}	178 {45} !	180 {180}
Process 3	25890.67				
		A	5728.15 {5.60}	1 {120}	220 {220}
		B	1.40 {1.40}	45 {20} !	45 {45}
		C	248069.45 {520.80}	21 {200}	9500 {9500}
Process 4	8.00				
		A	0.16 {0.16}	0 {0}	20 {20}
		B	0.48 {0.48}	0 {0}	60 {60}
		C	0.16 {0.16}	0 {0}	20 {20}
Process 5	621.00				
		A	94.95 {0.80}	6 {50}	150 {150}
		B	5119.96 {60.80}	254 {400}	8000 {8000}
		C	0.48 {0.48}	119 {60} !	120 {120}
Tot	28286.67	-	-	-	-

	Process 1	Process 2	Process 3	Process 4	Process 5
Process 1	0.00	34.00	56.00	0.00	8.00
Process 2	0.00	34.00	56.00	0.00	8.00
Process 3	0.00	34.00	56.00	0.00	8.00
Process 4	0.00	34.00	56.00	0.00	8.00
Process 5	0.00	34.00	56.00	0.00	8.00

3. Third Iteration:

Process	Freshwater m3/h	Contaminant	mass load kg/h	Cin ppm	Cout ppm
Process 1	50.00				
		A	0.75 {0.75}	0 {0}	15 {15}
		B	20.00 {20.00}	0 {0}	400 {400}
		C	1.75 {1.75}	0 {0}	35 {35}
Process 2	0.00				
		A	5.95 {3.40}	62 {20} !	120 {120}
		B	987.36 {414.80}	2820 {300} !	12500 {12500}
		C	12.41 {4.59}	58 {45} !	180 {180}
Process 3	49.78				
		A	22.15 {5.60}	11 {120}	220 {220}
		B	1.40 {1.40}	32 {20} !	45 {45}
		C	1003.77 {520.80}	11 {200}	9500 {9500}
Process 4	8.00				
		A	0.16 {0.16}	0 {0}	20 {20}
		B	0.48 {0.48}	0 {0}	60 {60}
		C	0.16 {0.16}	0 {0}	20 {20}
Process 5	0.00				
		A	2.12 {0.80}	18 {50}	150 {150}
		B	124.32 {60.80}	230 {400}	8000 {8000}
		C	1.48 {0.48}	28 {60}	120 {120}
Tot	107.78	-	-	-	-

	Process 1	Process 2	Process 3	Process 4	Process 5
Process 1	0.00	34.00	0.00	0.00	8.00
Process 2	0.00	0.00	0.00	0.00	0.00
Process 3	0.00	0.00	0.00	0.00	0.00
Process 4	0.00	34.00	56.00	0.00	8.00
Process 5	0.00	34.00	0.00	0.00	0.00

4. Fourth Iteration:

Process	Freshwater m3/h	Contaminant	mass load kg/h	Cin ppm	Cout ppm
Process 1	50.00				
		A	0.75 {0.75}	0 {0}	15 {15}
		B	20.00 {20.00}	0 {0}	400 {400}
		C	1.75 {1.75}	0 {0}	35 {35}
Process 2	0.00				
		A	6.97 {3.40}	18 {20}	120 {120}
		B	834.36 {414.80}	230 {300}	12500 {12500}
		C	10.37 {4.59}	28 {45}	180 {180}
Process 3	37.11				
		A	11.76 {5.60}	7 {120}	220 {220}
		B	1.40 {1.40}	20 {20}	45 {45}
		C	523.20 {520.80}	7 {200}	9500 {9500}
Process 4	8.00				
		A	0.16 {0.16}	0 {0}	20 {20}
		B	0.48 {0.48}	0 {0}	60 {60}
		C	0.16 {0.16}	0 {0}	20 {20}
Process 5	0.00				
		A	2.12 {0.80}	18 {50}	150 {150}
		B	124.32 {60.80}	230 {400}	8000 {8000}
		C	1.48 {0.48}	28 {60}	120 {120}
Tot	95.11	-	-	-	-

	Process 1	Process 2	Process 3	Process 4	Process 5
Process 1	0.00	34.00	0.00	0.00	8.00
Process 2	0.00	0.00	0.00	0.00	0.00
Process 3	0.00	0.00	0.00	0.00	0.00
Process 4	0.00	34.00	18.00	0.00	8.00
Process 5	0.00	0.00	0.00	0.00	0.00

5. Fifth Iteration:

Process	Freshwater m3/h	Contaminant	mass load kg/h	Cin ppm	Cout ppm
Process 1	50.00				
		A	0.75 {0.75}	0 {0}	15 {15}
		B	20.00 {20.00}	0 {0}	400 {400}
		C	1.75 {1.75}	0 {0}	35 {35}
Process 2	1.70				
		A	3.56 {3.40}	15 {20}	120 {120}
		B	414.80 {414.80}	300 {300}	12500 {12500}
		C	5.11 {4.59}	30 {45}	180 {180}
Process 3	52.23				
		A	12.02 {5.60}	1 {120}	220 {220}
		B	1.43 {1.40}	19 {20}	45 {45}
		C	520.80 {520.80}	2 {200}	9500 {9500}
Process 4	8.00				
		A	0.16 {0.16}	0 {0}	20 {20}
		B	0.48 {0.48}	0 {0}	60 {60}
		C	0.16 {0.16}	0 {0}	20 {20}
Process 5	0.00				
		A	1.08 {0.80}	15 {50}	150 {150}
		B	60.80 {60.80}	400 {400}	8000 {8000}
		C	0.68 {0.48}	35 {60}	120 {120}
Tot	111.93	-	-	-	-

	Process 1	Process 2	Process 3	Process 4	Process 5
Process 1	0.00	24.30	2.60	0.00	8.00
Process 2	0.00	0.00	0.00	0.00	0.00
Process 3	0.00	0.00	0.00	0.00	0.00
Process 4	0.00	8.00	0.00	0.00	0.00
Process 5	0.00	0.00	0.00	0.00	0.00

ÉCOLE DOCTORALE
Agriculture, alimentation, biologie, environnement, santé (ABIES)

Titre : Optimisation des réseaux d'eau industriels. Développement d'outils de conception générique et application à un site industriel.

Mots clés : Efficience de l'eau industrielle, réutilisation de l'eau, optimisation multi-objectifs, recherche opérationnelle, industrie agroalimentaire, huiles alimentaires

Résumé : L'application d'une gestion durable de l'eau est vitale pour tous les secteurs industriels, en particulier l'industrie alimentaire qui est l'un des secteurs les plus consommateurs d'eau. Elle peut être gérée par l'optimisation de la réutilisation, de la régénération et du recyclage de l'eau afin d'optimiser les coûts de production et de réduire les effets sur l'environnement. L'utilisation de certaines méthodes classiques d'intégration de masse peut aider à réduire la consommation d'eau et les rejets d'eaux usées. La mise en œuvre de ces méthodes dans le secteur alimentaire se heurte à différents obstacles, tels que le manque d'informations sur les volumes détaillés d'eau et d'eaux usées dans les différentes opérations et les données relatives aux indicateurs de polluants. L'analyse du pincement massique qui est une variante du pincement énergétique, est une approche globale et systématique qui vise à minimiser la consommation d'eau et la production d'eaux usées. Cette méthode classique est normalement adaptée aux réseaux d'eau avec un seul contaminant.
En réalité, la plupart des systèmes industriels sont complexes et multi-contaminants, notamment dans le secteur alimentaire. La méthode classique n'est pas en mesure de traiter ce type de problème. L'utilisation d'outils d'optimisation numérique en s'inspirant de la logique du pincement de l'eau est une approche appropriée pour traiter les problèmes réels et complexes. Deux outils numériques basés sur la logique d'analyse du pincement de l'eau sont développés. Le premier outil est basée sur une approche d'optimisation manuelle assistée par des algorithmes numériques. Le deuxième outil est basé sur une optimisation multi-objectifs avec contraintes. Ces deux outils sont conçus pour prendre en charge des réseaux d'eau industriels réels, complexes et qui contiennent plusieurs contaminants. Les approches conçues permettent d'identifier le minimum d'eau et proposer une conception optimale du réseau d'eau.
Une application des deux outils a été réalisée pour une entreprise de raffinage des huiles alimentaires.

Title: Optimization of industrial water networks. Development of generic design tools and application in a real industrial site.

Keywords: Industrial water efficiency, water reuse, multi-objective optimization, operational research, food industry, edible oil

Abstract: The application of sustainable water management is vital for all industrial sectors, especially the food industry, one of the most water-consuming sectors. It can be managed by optimizing water reuse, regeneration, and recycling to optimize the production costs and reduce the environmental impacts. Using classical mass integration methods can help to reduce water consumption and wastewater production. Implementing these methods in the food sector faces various challenges, such as the lack of water and wastewater volume in different operations and the data related to pollutant indicators. As a variation of energy pinch, water pinch analysis is a comprehensive and systematic approach that tries to minimize water consummation and wastewater production. This classic method is suitable for mono-contaminant systems.
However, most industrial systems are complex and involve multiple contaminants, especially in the food sector. The classic methods are not able to deal with these kinds of problems. Using numerical optimization tools by inspiring water pinch logic is a suitable approach to handling real and complex water networks.
Two numerical tools based on the logic of water pinch analysis are developed. The first tool is based on a manual optimization approach assisted by numerical algorithms. The second tool is based on constrained multi-objective optimization. These two tools are developed to handle real and complex industrial water systems that contain multiple contaminants. The designed approaches lead to target the minimum freshwater by using the maximum possibility of reuse. A French edible oil company has been selected as the real industrial application of the developed tools.

Maison du doctorat de l'Université Paris-Saclay
2ème étage aile ouest, Ecole normale supérieure Paris-Saclay
4 avenue des Sciences,
91190 Gif sur Yvette, France