

Optimisation Approaches for the Synthesis of Water Treatment Plants

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Abstract

Efficient water treatment design has progressively been growing in importance as the usage of water resources increases with population rise and industrial development. Their availability has been reduced with the more evident effects of climate change. Addressing this challenge necessitates more and efficient purification plants which can be realised by optimal design at conceptual stage. In this work, a mixed integer nonlinear programming (MINLP) model for the synthesis and optimisation of water treatment processes is proposed. Due to its numerous non-linearities and consequently, its non-stability, various linearisation, approximation and reformulation techniques have been implemented. Consequently, two improved formulations are derived, i.e. a partially linearised MINLP (pMINLP) and a mixed integer linear fractional programming (MILFP) models. The applicability of the mathematical formulations are investigated in case studies of seawater desalination and surface water treatment for the production of potable water. Finally, the models performance is analysed and compared against each other.

Keywords: MINLP, reformulation techniques, MILFP, surface water treatment, seawater desalination

1. Introduction

World water baseline scenario for year 2050 reveals approximately 5,500 km³ of freshwater withdrawals will be required to meet the demand of water necessary for manufacturing, electricity production and domestic use. This represents an increase of 55 % from current global demand where 130 % more drinking water will be in demand for households than volumes nowadays (United Nations, 2015).

Water supply to end users is governed by publicly accepted practices which entail sources such as groundwater or surface water to undergo water treatment. Seawater desalination has become an alternative option for the provision of clean water. After purification, the product water is distributed to agriculture, industry and households (shown in Fig. 1).

It can be deduced from Fig. 1 that the connecting role in the water chain belongs to water treatment and desalination. Hence, with the outlook of future water demand, investments on new purification plants have been planned. By 2018, for instance, Middle East and Africa are expected to have an annual growth of water production

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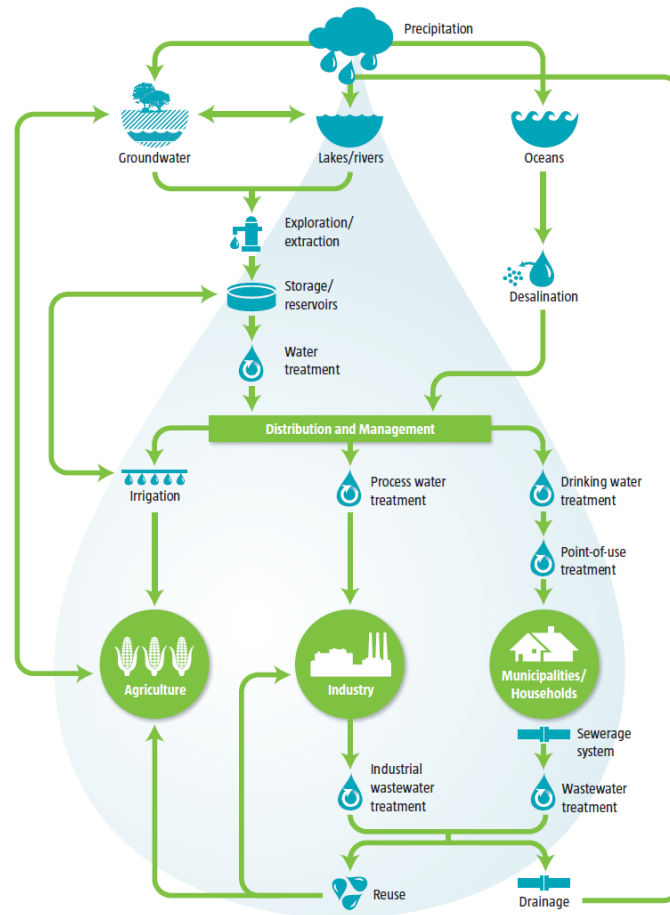


Figure 1: Water path from precipitation to usage; **source:**RobecoSam (2015)

capacity of 13.2 %, followed by Asia with 10.1 % and the Americas with 5.7 % (Fig. 2). Desalination, on the

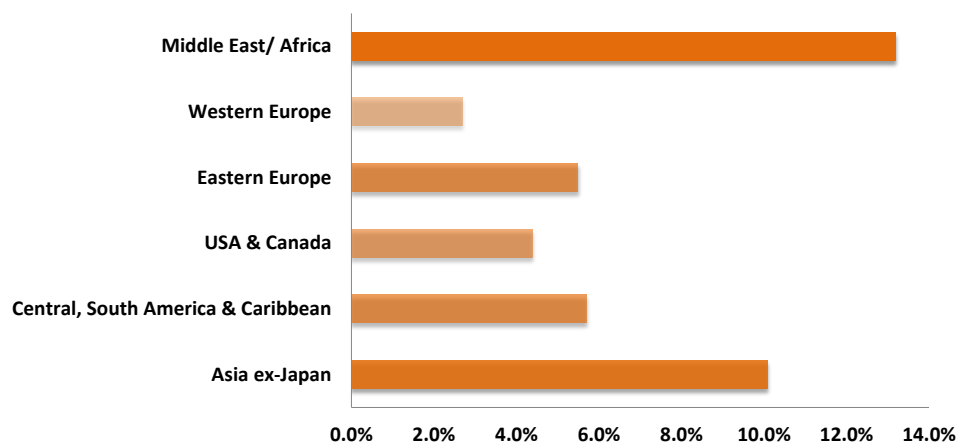


Figure 2: Projected percentage of increase of water utilities by area by 2018; **source:**RobecoSam (2015)

other hand, has gained popularity in less than a century. It has evolved from an idea in 1951 into an industrial

process with large clean water production capabilities today. Fig. 3 depicts the progressively installed desalination plants capacities in selected countries from the discovery of reverse osmosis to 2016. The global desalination

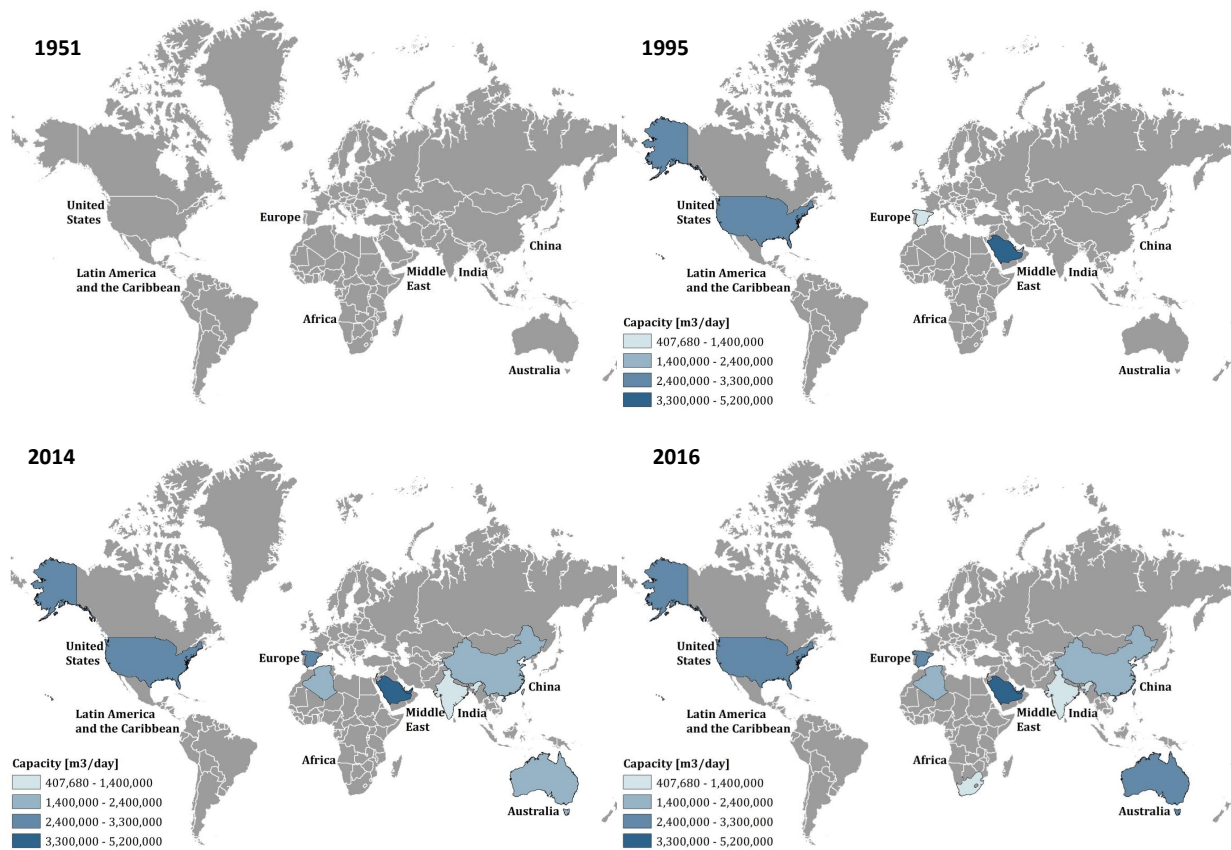


Figure 3: Progress of top 10 countries - leaders in desalination; **source:**Pacific Institute (2013); DesalData (2014); Global Water Intelligence (2016)

capacity by the end of 2016 is projected to be 86.8 million m^3 which is predicted to reach 128 million m^3 by 2018 (International Desalination Association, 2016).

The water challenge has brought questions of how to most efficiently treat water resources to ensure good quality and safety of final products. A number of works published in literature have given answers to those questions. Tchobanoglous et al. (2003) and Cheremisinoff (2002) have outlined guidelines for the design of water and wastewater treatment plants. Voutchkov (2013) and Lior (2013) have provided exhaustive principles of design and cost estimation of seawater desalination plants. Process Systems Engineering, however, and process synthesis, in particular, hold the power of designing flowsheets that will lead not only to water quality up to regulatory standards but also to minimum capital and operating expenditures. Table 1 gives a summary of recent representative contributions in water treatment as stand-alone process and as a component of integrated systems. In some of those works, synthesis and optimisation of wastewater treatment with single and multiple contaminants have been proposed (Tsiakis & Papageorgiou, 2005; Skiborowski et al., 2012; Gabriel et al., 2015; Teles et al.,

Table 1: Recent representative contributions in water treatment synthesis

Categories	Works using deterministic optimisation techniques
Stand-alone process	
Technology	
<i>thermal</i>	Skiborowski et al. (2012); Gabriel et al. (2015); González-Bravo et al. (2015b)
<i>chemical and biochemical</i>	Khor et al. (2012); Sueviriyapan et al. (2016); Koleva et al. (2016)
<i>filters and membranes</i>	Tsiakis & Papageorgiou (2005); Lu et al. (2006, 2012); Sassi & Mujtaba (2012); Khor et al. (2012) Koleva et al. (2016)
Contaminants	
<i>single</i>	Tsiakis & Papageorgiou (2005); Sassi & Mujtaba (2012); Skiborowski et al. (2012) Gabriel et al. (2015)
<i>multi</i>	Teles et al. (2009, 2012); Khor et al. (2012); Koleva et al. (2016)
Application	
<i>seawater</i>	Lu et al. (2006, 2012); Sassi & Mujtaba (2012); Skiborowski et al. (2012); Gabriel et al. (2015) Koleva et al. (2016)
<i>wastewater</i>	Teles et al. (2012); Sueviriyapan et al. (2016)
<i>clean water</i>	Teles et al. (2012); Khor et al. (2012)
Integrated systems	
Energy	Antipova et al. (2013); Wu et al. (2013); González-Bravo et al. (2015a); Gao & You (2015) Guerra et al. (2016); Tovar-Facio et al. (2016)
Supply chain	Liu et al. (2011, 2012); Gao & You (2015); Guerra et al. (2016)
Water-using networks	Bagajewicz (2000); Koppol et al. (2004); Dong et al. (2008) Foo (2009); Jeżowski (2010); Ahmetović & Grossmann (2011) Yang & Grossmann (2013); Ibrić et al. (2014); Grossmann et al. (2014); Alnouri et al. (2014) Khor et al. (2014); Seid & Majozi (2014); da Silva Francisco et al. (2015); Abass & Majozi (2016)

2012; Khor et al., 2012). Deterministic design of water, wastewater and seawater treatment processes formulated as non-linear programming (NLP) or mixed integer non-linear programming (MINLP) models has been studied in various works (Khor et al., 2012; Teles et al., 2012; Sueviriyapan et al., 2016; Koleva et al., 2016). An MINLP model specialised on reverse osmosis (RO) systems and cost estimations such as pumping, membrane cleaning and replacement has been proposed by Lu et al. (2006, 2012). Multi-objective optimisation for minimising operating costs, greenhouse gas emissions and effluent contaminants has been presented by Sweetapple et al. (2014).

Water network systems (WNS) together with wastewater treatment have been the focus of copious articles (Dong et al., 2008; Ahmetović & Grossmann, 2011; Galán & Grossmann, 2011; Rojas-Torres et al., 2013; Ibrić et al., 2014; Yang & Grossmann, 2013). A recent comprehensive review analysed and classified the various contributions made to WNS (Ahmetović et al., 2015). Integrated water resources management studies have taken into account different water and wastewater treatment options formulated as single and multi-objective optimisation problems (Liu et al., 2010, 2011; Liu & Papageorgiou, 2013). Guerra et al. (2016) have presented a

novel method for the design of shale gas supply chain with wastewater management where total dissolved solids are considered.

The intricacy of the design is, normally, due to bilinearities arising from mixing of streams of different qualities, which immensely increases the computational effort to achieve global optimality. Karuppiah & Grossmann (2006) and Castro (2015) have demonstrated the applicability of bilinear relaxations using McCormick envelopes in different problems, including wastewater treatment. Teles et al. (2012) implemented a multiparametric disaggregation technique for water networks design. Castro (2016) proposed a normalised multiparametric disaggregation (MDT) strategy which has been demonstrated to improve the convergence of non-convex problems. The technique has successfully been implemented in wastewater treatment applications (Ting et al., 2016).

This work presents a superstructure optimisation approach for the synthesis of water and water - related treatment processes. The current paper extends the work by Koleva et al. (2016) by introducing essential new alternative paths to its superstructure and hence, illustrating more closely common industrial practices. Three mathematical formulations are developed, an MINLP model ($P0$), a partially linearised MINLP (pMINLP) model ($P1$) and a mixed integer linear fractional programming (MILFP) model ($P2$). The originality of the work lies in: (i) removal efficiencies modelled as continuous variables. Models $P0$ and $P1$ consider removal efficiencies as continuous variables whose values are determined by regression models with independent variables - the operating conditions of the treatment units; (ii) unique superstructure accommodating the technologies used across water, advanced wastewater treatment and desalination; (iii) operating costs breakdowns and capital costs for every candidate technology. The rest of the paper is structured as follows: in Section 2 the superstructure optimisation problem is given together with the assumptions along its development and the problem statement. Next, the mathematical formulations are presented and the solution strategies are discussed in Section 3. The capabilities of the models are then tested on two case studies in Section 4 whose results are discussed and analysed in Section 5. Finally, Section 6 draws conclusions from the obtained results and summarises the major points from this work.

2. Problem statement

The aim of the current work is to develop a methodology for the generation of a combination of technologies that result in the most economically favourable flowsheet design. The proposed model accounts for contaminants classified into major groups such as total suspended solids (TSS), total dissolved solids (TDS), chemical oxygen demand (COD) and boron (B). Nine technology candidates are considered, i.e. coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), multi-stage media filtration (MMF), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO) for TDS (RO1) and B (RO2) removal. All acceptable connections among those technologies are presented in the model superstructure in Fig. 4. Every technology is associated with the removal of a group or groups of contaminants. It is assumed that CF, SED, DAF, MMF, MF and UF purify water from TSS, NF and RO retain TDS, and COD can be removed by CF, MF, UF and NF. The ability of a technology to remove a particular group of contaminants relies on the available data for separation

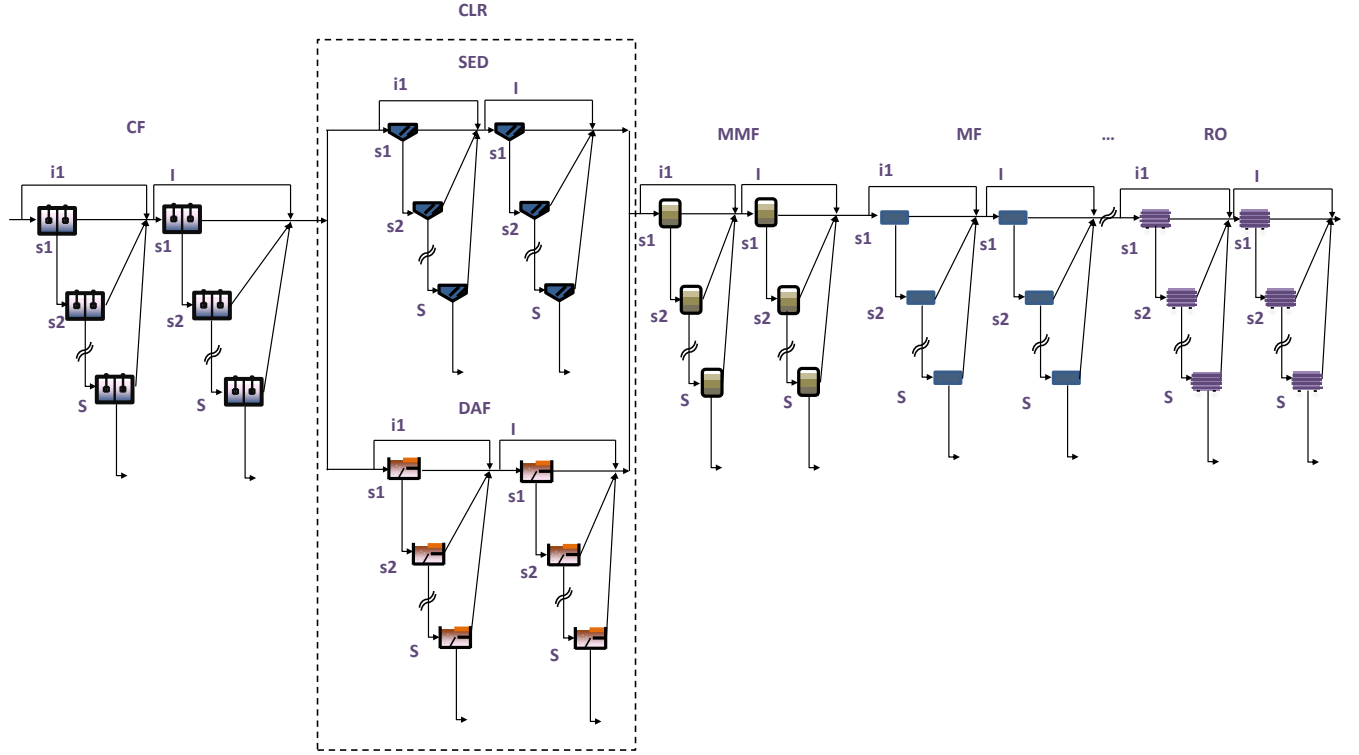


Figure 4: Process superstructure: coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), media filtration (MMF), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF) and reverse osmosis (RO)

efficiencies.

The sequence of the technology candidates in the model is pre-fixed in an order they are most commonly configured in established practices. A candidate, however, can be either selected or bypassed. In conventional treatment, coagulation-flocculation is followed by clarification process. Two clarification options are provided, SED and DAF. They are represented by the collective name CLR which is symbolically depicted with a dotted line in the superstructure. Provided SED or DAF is selected, CLR is selected, too. A selection of a clarification process serves as a prerequisite for the selection of CF. Coagulation-flocculation alone can be selected if the separation is efficient enough. Low pressure membranes (MF and UF) and high pressure membranes (NF and RO) are allowed to exist sequentially in the superstructure. Nevertheless, the problem can be restricted to the selection of either of a membrane from a group.

Every unit can be repeated in a sequential manner, or a *pass*, denoted also by i . A pass is used in order to increase product purity. Every unit can be repeated to treat the concentrate or retentate of a preceding unit. This structure is referred to as *stage* and is denoted by s . A stage is used in order to increase the productivity of the system. Whether a pass and a stage from a technology are singled out is decided by a binary variable. Additionally, a technology can have as many number of passes and stages as economically viable. The unit selection is based on meeting the regulatory requirements depending on the purpose of water usage (The Drinking Water Inspectorate, 2009; U.S. Environmental Protection Agency, 2010). The flowsheet configuration has to be

such as to minimise the water net cost, expressed in $\$/\text{m}^3$. The following assumptions have been made along the mathematical formulation development:

- 95
 - removal efficiencies are the major technological criterion
 - coefficients of determination are satisfactorily high for providing a good fit for removal efficiencies
 - the major contaminant groups depend on water source; the rest are untraceable
 - insignificant removal of a group of contaminants from technologies assigned for removal of other groups
 - initial removal grids, intake screens and post-treatment equipment are not considered
- 100
 - no fouling and flux decrease
 - no system pressure losses
 - cost indices can be grouped for lower pressure membranes (MF and UF) and high pressure membranes (NF and RO)
 - plant shut down for maintenance takes 65 days
- 105
 - annual water production and operating expenses do not fluctuate throughout the commercial lifespan of the plant
 - no government incentives, such as decreased interest rate or no interest rate, apply

The overall optimisation problem can be stated as follows.

Given:

- 110
 - contaminant groups and concentrations in intake
 - industrially available treatment technologies
 - maximum number of passes and stages allowed for a technology
 - intake flowrate
 - recoveries, pump and motor efficiencies for every unit
- 115
 - candidate technologies characteristics ranges ($P0$ and $P1$) or discrete values ($P2$)(e.g. flocculation time and energy input, coagulant concentrations, operating pressures, influent temperature, hydrophobicity, hydrogen ion concentrations, molecular weight cut - offs)
 - cost indices (e.g. units upfront costs, chemicals and electricity charges, equipment replacement rates, labour associated constants, interest rate and plant life)

120 *Determine:*

- process flowsheet including multiple-pass and multiple-stage strategy
- optimal removal efficiencies and operating conditions for the selected units
- contaminants and flowrates profiles
- annual operating and capital costs

125 *So as to:*

minimise the water production cost which is defined as the total annualised cost divided by the annual production rate.

3. Mathematical formulation

The process synthesis problem is formulated as a mixed integer non-linear programming (MINLP) model ($P0$) first. The sources of non-linearities emanate from removal efficiency correlations, mixing constraints, operating costs, economies of scale and fractional objective function. Then, the constraints associated with mixing of streams and economies of scale are reformulated and consequently, a second MINLP (pMINLP) model ($P1$) is presented in Section 3.2. Lastly, the operating conditions participating in regression models and operating costs, and the objective function are linearised completely to obtain a mixed integer linear fractional programming (MILFP) model, or $P2$, (see Section 3.3). Solely the newly added or substituted equations are reported in each section. The majority of the variables are denoted with capital letters while the parameters are designated with small letters. The separation efficiencies of the candidate units are an essential technical aspect subject to optimisation. They are determined by units' operating conditions which are also a decisive factor in the ongoing costs estimation. The key constraints are the removal efficiencies, mass balances, regulatory, logical and economic constraints which are presented in the following sections. A complete list with notations can be found in Appendix A.

3.1. MINLP model

3.1.1. Removal efficiencies

Meeting product specifications is the most important goal of the model which is achieved through the separation performance of the technologies composing a flowsheet. The physicochemical properties of the fluid and the operating conditions of the available technologies (PP_{tis}) impact their separation efficiency and generically, can be stated as follows:

$$R_{tisc} = f(PP_{tis}) = 1 - \frac{C_{tisc}^P}{C_{tisc}^F}, \quad \forall t, i, s \in I_t, c \in CT_t \quad (1)$$

where C_{tisc}^P and C_{tisc}^F are the respective concentrations of contaminant c in permeate and feed, for a technology, t , its pass, i and stage, s . R_{tisc} is the separation efficiency which can take values between 0, meaning no separation is accomplished, and 1, meaning 100 % separation is attained. Thus, the extent of removal can be presented in the form of regression models based on Analysis of Variance (ANOVA), where the removal efficiencies are dependent variables, and the properties and operating conditions are independent variables. The correlations are readily found from laboratory experiments, modified or developed for the purpose of this study.

First, CF is considered where its removal efficiency for COD is determined by Eq. (2) (Sangeetha et al., 2014).

$$R_{tisc} = 0.00058 \cdot CD_{tis} + 0.135 \cdot pH_{tis} - 0.154, \quad \forall t \in CF, i, s \in I_t, c \in COD \quad (2)$$

where CD_{tis} is the amount of coagulant and pH_{tis} is the concentration of hydrogen ions in the water. It is assumed CF has an insignificant effect in the removal of suspended solids, hence, its separation efficiency for this

155 contaminant group is regarded as zero. The chemical dosage, the residence time and mixing in CF, however, effect the removal of TSS in the typically subsequent clarification processes, DAF and SED. Hence, when CLR is selected, CF also has to be selected. Additionally, if CLR is chosen, either SED's or DAF's removal ratio will be valid (Eq. (3)).

$$R_{tisc} = \sum_{q \in TCLR} \bar{R}_{qisc} \cdot X_{qis}, \quad \forall t \in CLR, i, s \in I_t, c \in TSS \quad (3)$$

where X_{qis} is a binary variable for the selection of a clarification technology. It has been reported that sedimentation is strongly influenced by the coagulant dose used in CF (Vlaški, 1998). After performing a regression analysis on the data provided in Vlaški (1998), the following correlation has been obtained:

$$\bar{R}_{qisc} = 0.22154 + 0.02516 \cdot CD_{tis}, \quad \forall q \in SED, t \in CF, i, s \in I_t, c \in TSS \quad (4)$$

where CD_{tis} is the amount of coagulant used in the CF process. Besides coagulant dose, DAF also demonstrated dependence of detention time and velocity gradient in CF's mixing chamber, denoted as Tf_{tis} and Df_{tis} , respectively (Eq. (5)).

$$\begin{aligned} \bar{R}_{qisc} = 1.85886 - 0.00807 \cdot CD_{tis} - 0.00083 \cdot Gf_{tis} + 0.0025 \cdot Tf_{tis} - 2.47 \cdot \bar{P}_{qis}, \\ \forall q \in DAF, t \in CF, i, s \in I_t, c \in TSS \end{aligned} \quad (5)$$

where \bar{P}_{qis} is the pressure of the saturator. The Commonwealth Scientific and Industrial Research Organisation (CSIRO) developed the initial steady-state removal of TSS in media filtration (MMF) (Lin et al., 2006). The relationship is shown in Eq. (6).

$$R_{tisc} = 0.0298 \cdot D_{tis}^{MED} + 0.171 \cdot Ld_{tis} + 0.206 \cdot L_{tis}^{-1} - 0.245, \quad \forall t \in MMF, i, s \in I_t, c \in TSS \quad (6)$$

where D_{tis}^{MED} stands for the diameter of the media, Ld_{tis} is the load to the filtration process, L_{tis}^{-1} is the length of the filter for MMF in pass i and stage s . The separation efficiency of COD from water by MF is shown in Eq. (7), derived from experimental work (Benitez et al., 2006).

$$R_{tisc} = 0.189 + 1.009 \cdot P_{tis}, \quad \forall t \in MF, i, s \in I_t, c \in COD \quad (7)$$

The rejection of TSS by MF is affected by both pressure and temperature, thus:

$$R_{tisc} = 0.126 + 0.001 \cdot Tem_{tis} + 0.97 \cdot P_{tis}, \quad \forall t \in MF, i, s \in I_t, c \in TSS \quad (8)$$

where Tem_{tis} is the temperature of the influent to technology t , pass i and stage s , and P_{tis} is the pressure of the feed flowrate. Cho et al. (2000) studied rejection of natural organic matter in UF membranes. Eq. (9) gives a regression where pressure is the only independent variable.

$$R_{tisc} = 0.236 - 0.952 \cdot P_{tis}, \quad \forall t \in UF, i, s \in I_t, c \in COD \quad (9)$$

For the removal of turbidity by UF, Eq. (10) holds.

$$R_{tisc} = 0.959 - 1.510 \cdot P_{tis}, \quad \forall t \in UF, i, s \in I_t, c \in TSS \quad (10)$$

where the equation has been derived from data obtained from pilot plant experimental work (Benitez et al., 2006).
 160 Artug (2007) pointed out the NF membranes characteristics such as pore size, hydrophobicity and roughness affect their performance. Therefore, the retention for those membranes involves molecular weight cut-off, $MWCO_{tis}$, and hydrophobicity, H_{tis} , shown in Eq. (11) and Eq. (12).

$$R_{tisc} = 1.138 - 0.00096 \cdot MWCO_{tis} - 0.087 \cdot P_{tis}, \quad \forall t \in NF, i, s \in I_t, c \in COD \quad (11)$$

$$R_{tisc} = (0.573 - 0.071 \cdot H_{tis} - 0.0002 \cdot MWCO_{tis})^2, \quad \forall t \in NF, i, s \in I_t, c \in TDS \quad (12)$$

The correlation for TDS has been reported by Boussu et al. (2008) based on laboratory work. RO rejection coefficient for dissolved solids is presented in Eq. (13) as a function of the operating pressure performed on ROSA software (The Dow Chemical Company, 2013) by Chen & Guanghua (2005).

$$R_{tisc} = 0.890 + 0.034 \cdot P_{tis} - 0.003 \cdot P_{tis}^2, \quad \forall t \in RO1, i, s \in I_t, c \in TDS \quad (13)$$

A separate contaminant group is dedicated to boron (B) which is detected in some water sources and its removal is particularly difficult due to its ionic dissolution (Li et al., 2008). Consequently, elevated pH is necessary for its separation profile that can be modelled by Eq. (14).

$$R_{tisc} = 0.408 + 0.046 \cdot pH_{tis} + 0.028 \cdot P_{tis}, \quad \forall t \in RO2, i, s \in I_t, c \in B \quad (14)$$

where pH_{tis} is the alkalinity of the solution to achieve desired separation. The above equation has been developed using ANOVA analysis and data from Mane et al. (2009).

Summary of separation coefficients

The regression equations described above and used in the model are summarised in Table 2.

Table 2: Summary of rejection coefficients correlations in MINLP model

Correlation		Equation
$R_{tisc} = 0.00058 \cdot CD_{tis} + 0.135 \cdot pH_{tis} - 0.154,$	$\forall t \in CF, i, s \in I_t, c \in COD$	(2)
$\bar{R}_{qisc} = 0.22154 + 0.02516 \cdot CD_{tis},$	$\forall q \in SED, t \in CF, i, s \in I_t, c \in TSS$	(4)
$\bar{R}_{qisc} = 1.85886 - 0.00807 \cdot CD_{tis} - 0.00083 \cdot Gf_{tis}$ $+ 0.0025 \cdot Tf_{tis} - 2.47 \cdot \bar{P}_{qis},$	$\forall q \in DAF, t \in CF, i, s \in I_t, c \in TSS$	(5)
$R_{tisc} = 0.0298 \cdot D_{tis}^{MED} + 0.171 \cdot Ld_{tis} + 0.206 \cdot L_{tis}^{-1} - 0.245,$	$\forall t \in MMF, i, s \in I_t, c \in TSS$	(6)
$R_{tisc} = 0.189 + 1.009 \cdot P_{tis},$	$\forall t \in MF, i, s \in I_t, c \in COD$	(7)
$R_{tisc} = 0.126 + 0.001 \cdot Tem_{tis} + 0.97 \cdot P_{tis},$	$\forall t \in MF, i, s \in I_t, c \in TSS$	(8)
$R_{tisc} = 0.236 - 0.952 \cdot P_{tis},$	$\forall t \in UF, i, s \in I_t, c \in COD$	(9)
$R_{tisc} = 0.959 - 1.510 \cdot P_{tis},$	$\forall t \in UF, i, s \in I_t, c \in TSS$	(10)
$R_{tisc} = 1.138 - 0.00096 \cdot MWCO_{tis} - 0.087 \cdot P_{tis},$	$\forall t \in NF, i, s \in I_t, c \in COD$	(11)
$R_{tisc} = (0.57 - 0.07 \cdot H_{tis} - 0.0002 \cdot MWCO_{tis})^2,$	$\forall t \in NF, i, s \in I_t, c \in TDS$	(12)
$R_{tisc} = 0.890 + 0.0340 \cdot P_{tis} - 0.003 \cdot P_{tis}^2,$	$\forall t \in RO1, i, s \in I_t, c \in TDS$	(13)
$R_{tisc} = 0.408 + 0.046 \cdot pH_{tis} + 0.028 \cdot P_{tis},$	$\forall t \in RO2, i, s \in I_t, c \in B$	(14)

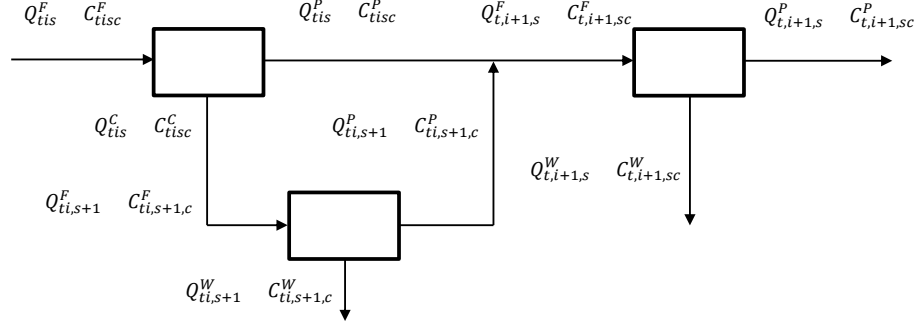


Figure 5: A schematic representation of concentrations and flow streams in a two-pass system with two and one stages

3.1.2. Mass balance constraints

Next, the concentration and mass balances constraints are presented. A simple schematic representation of feed, permeate, concentrate and waste streams is depicted in Fig. 5.

Concentration constraints

The permeate concentrations, C_{tisc}^P , of every unit are calculated in Eq. (15) and Eq. (16). If a unit is selected, its concentration is reduced to C_{tisc}^P . Otherwise, the concentration remains C_{tisc}^F .

$$C_{tisc}^F \cdot (1 - R_{tisc}) - M_c^{BIG} \cdot (1 - E_{tis}) \leq C_{tisc}^P \leq C_{tisc}^F \cdot (1 - R_{tisc}) + M_c^{BIG} \cdot (1 - E_{tis}), \quad \forall t, i, s \in I, c \in CT_t \quad (15)$$

$$C_{tisc}^F - M_c^{BIG} \cdot E_{tis} \leq C_{tisc}^P \leq C_{tisc}^F, \quad \forall t, i, s \in I, c \in CT_t \quad (16)$$

where M_c^{BIG} is a big number with a unique value for every c . M_c^{BIG} should be adjusted for every contaminant because of the difference in concentrations magnitudes. E_{tis} is a binary variable which is activated when a technology t , pass i and stage s are selected. Eq. (15) involves a bilinear product of C_{tisc}^F and R_{tisc} . When a unit is selected, then the retentate concentrations, C_{tisc}^C , would either equate waste concentrations, C_{tisc}^W , or the feed concentrations of the next stage (Eq. (17) - Eq. (19)). The expressions are valid only for the contaminants relevant for a technology.

$$C_{ti,s-1,c}^C = C_{tisc}^F + C_{ti,s-1,c}^W, \quad \forall t, i, s \in I, s > 1, c \in CT_t \quad (17)$$

If a next stage is not selected, the stream goes to waste which can be further diluted or treated, or discharged.

$$C_{ti,s-1,c}^W \leq M_c^{BIG} \cdot (1 - E_{tis}), \quad \forall t, i, s \in I, s > 1, c \in CT_t \quad (18)$$

If a next stage is chosen, the effluent from the previous stage becomes the feed of the next stage.

$$C_{tisc}^F \leq M_c^{BIG} \cdot E_{tis}, \quad \forall t, i, s \in I, s > 1, c \in CT_t \quad (19)$$

In order to ensure no value will be given to the concentrates when a stage is not selected, we enforce the following constraint:

$$C_{tisc}^C \leq M_c^{BIG} \cdot E_{tis}, \quad \forall t, i, s \in I_t, c \in CT_t \quad (20)$$

where M_c^{BIG} is sufficiently large so that it will always be greater than the concentration of the concentrate. Furthermore, we would like to ensure the contaminants that cannot be treated by a technology would have a zero value for their waste concentration:

$$C_{tisc}^C = 0, \quad \forall t, i, s \in I_t, c \notin CT_t \quad (21)$$

Flowrate constraints

Similarly, the flowrate constraints are modelled in Eq. (22) and Eq. (23). When a candidate is selected, the feed Q_{tis}^F is reduced to Q_{tis}^P .

$$y_{tis} \cdot Q_{tis}^F - Q^{IN} \cdot (1 - E_{tis}) \leq Q_{tis}^P \leq y_{tis} \cdot Q_{tis}^F + Q^{IN} \cdot (1 - E_{tis}), \quad \forall t \notin CLR, i, s \in I_t \quad (22)$$

$$Q_{tis}^F - Q^{IN} \cdot E_{tis} \leq Q_{tis}^P \leq Q_{tis}^F, \quad \forall t \in CLR, i, s \in I_t \quad (23)$$

where y_{tis} is the recovery of a technology t , pass i and stage s . Although unit recovery, like removal efficiency, can also be expressed as a function of the system pressure, fluid salinity, etc. (Li et al., 2008), in this work the recoveries are modelled as parameters which take different values for every t . Q^{IN} is the intake flowrate and serves a purpose of an upper bound of the product flow. Q_{tis}^P and Q_{tis}^F are the permeate and feed flowrates, respectively, associated with a technology t , pass i and stage s . As previously mentioned, SED and DAF are represented by CLR, whose flowrate is determined either by the recovery value of SED or the recovery value of DAF (Eq. (24)).

$$Q_{tis}^P = Q_{tis}^F \cdot \sum_{q \in TCLR} (\bar{y}_{qis} \cdot X_{qis}) + Q_{tis}^F \cdot (1 - \sum_{q \in TCLR} X_{qis}), \quad \forall t \in CLR, i, s \in I_t \quad (24)$$

In the cases where there are more than one stage selected, the concentrate flow, Q_{tis}^C from the previous stage equals the feed flow of the next stage (Eq. (25)).

$$Q_{ti,s-1}^C = Q_{tis}^F + Q_{ti,s-1}^W, \quad \forall t, i, s \in I_t, s > 1 \quad (25)$$

Provided a next stage is selected, its feed becomes less or equal than the intake. Otherwise, the feed to the next stage equates 0.

$$Q_{tis}^F \leq Q^{IN} \cdot E_{tis}, \quad \forall t, i, s \in I_t, s > 1 \quad (26)$$

If a next stage is not selected, the value of the concentrate flow will be passed to a waste stream Q_{tis}^W .

$$Q_{ti,s-1}^W \leq Q^{IN} \cdot (1 - E_{tis}), \quad \forall t, i, s \in I_t, s > 1 \quad (27)$$

In order to ensure no flow is passed to the waste stream when a stage is not selected, the following constraint is applied:

$$Q_{tis}^C \leq Q^{IN} \cdot E_{tis}, \quad \forall t, i, s \in I_t \quad (28)$$

When the flows are passed from one pass to another, Eq. (29) holds.

$$\sum_{s \in I_t} Q_{t,i-1,s}^P = Q_{tis|s=1}^F, \quad \forall t, i \in I_t, i > 1 \quad (29)$$

When the flows are passed from one technology to another, Eq. (30) is used.

$$\sum_{s \in I_t} Q_{t-1, is| i=I_t^{max}}^P = Q_{tis| i=1, s=1}^F, \quad \forall t > 1 \quad (30)$$

Balances and interconnections constraints

The mass and concentration balances over a pass and a stage are expressed in Eq. (31) and Eq. (32).

$$C_{tisc}^C \cdot Q_{tis}^C = C_{tisc}^F \cdot Q_{tis}^F - C_{tisc}^P \cdot Q_{tis}^P, \quad \forall t, i, s \in I_t, c \quad (31)$$

$$Q_{tis}^C = Q_{tis}^F - Q_{tis}^P, \quad \forall t, i, s \in I_t \quad (32)$$

The interconnection between two passes is expressed in Eq. (33) and the interconnection between two technologies is expressed in Eq. (34).

$$\sum_{s \in I_t} C_{t,i-1,sc}^P \cdot Q_{t,i-1,s}^P = C_{tisc|s=1}^F \cdot Q_{tis|s=1}^F, \quad \forall t, i \in I_t, i > 1, c \quad (33)$$

$$\sum_{s \in I_t} C_{t-1,isc| i=I_t^{max}}^P \cdot Q_{t-1, is| i=I_t^{max}}^P = C_{tisc| i=1, s=1}^F \cdot Q_{tis| i=1, s=1}^F, \quad \forall t > 1, c \quad (34)$$

The hourly, Q_{out} , and annual, Q^{AP} , production rates of the facility are then expressed by Eq. (35) and Eq. (36), respectively.

$$Q_{out} = \sum_{s \in I_t} Q_{tis}^P, \quad \forall t = T, i = I_t^{max} \quad (35)$$

$$Q^{AP} = t_h \cdot t_d \cdot py \cdot Q_{out} \quad (36)$$

175 where t_h is the number of operating hours per day, t_d is the number of operating days per year and py is the production fraction of the facility relative to its capacity.

3.1.3. Target constraints

The final contaminant concentrations, C_{out_c} , should satisfy the conditions imposed by Eq. (37) and Eq. (38) and do not exceed the maximum allowable concentration, M_c^{CONC} . The final purity requirements alter with the ultimate purpose of the product, i.e. drinking water, process water, water for irrigation.

$$C_{out_c} \cdot Q_{out} = \sum_{s \in I_t} (C_{tisc}^P \cdot Q_{tis}^P), \quad \forall t = T, i = I_t^{max}, c \quad (37)$$

$$C_{out_c} \leq M_c^{CONC}, \quad \forall c \quad (38)$$

A supplementary constraint for minimum effluent amount is enforced by Eq. (39) which would ensure the plant design capacity is met.

$$Q_{out} \geq M^{FLOW} \quad (39)$$

where M^{FLOW} is the minimum allowable effluent flow.

3.1.4. Logical constraints

The overall number of the selected technologies, passes and stages should not be greater than a number, N^{max} , shown in Eq. (40).

$$\sum_t \sum_{i \in I_t} \sum_{s \in I_t} E_{tis} \leq N^{max} \quad (40)$$

Eq. (41) and Eq. (42) are logical conditions that do not allow the selection of any pass or stage provided the previous one has not been chosen.

$$E_{t,i+1,s} \leq E_{tis}, \quad \forall t, i, s \in I_t, i+1 \in I_t \quad (41)$$

$$E_{ti,s+1} \leq E_{tis}, \quad \forall t, i, s \in I_t, s+1 \in I_t \quad (42)$$

Coagulation-flocculation should be selected when sedimentation or dissolved air flotation is selected hence, Eq. (43) applies:

$$E_{qis} \leq E_{tis}, \quad \forall q \in CLR, t \in CF, i = 1, s = 1 \quad (43)$$

Only one of the clarification processes can be chosen at a time, a condition imposed by Eq. (44).

$$\sum_{q \in TCLR} X_{qis} = E_{tis}, \quad \forall t \in CLR, i, s \in I_t \quad (44)$$

The same logical conditions for binary variable X_{qis} are needed.

$$X_{q,i+1,s} \leq X_{qis}, \quad \forall q, i, s \in \bar{I}_q, i+1 \in \bar{I}_q \quad (45)$$

$$X_{qi,s+1} \leq X_{qis}, \quad \forall q, i, s \in \bar{I}_q, s+1 \in \bar{I}_q \quad (46)$$

3.1.5. Cost constraints

Economic appraisal of conceptual design owes its complexity to the various cost components that must be considered. Such components are plant capacity, intake quality and quantity, location, accessibility to electricity and occurring electricity charges, qualified labour, plant life, agreements with banks and local governments (Zhou & Tol, 2004). In the following subsections, many of the factors have been included such as chemical costs for coagulant, pH adjustments and post-treatment, electricity for mixing and pumping, equipment replacement and labour. No carbon taxation is assumed.

Operating costs. Aluminium sulphate (alum) and ferric sulphate are the preferred choice of coagulants where the former is widely used in surface water treatment due to its low cost and the latter is a more common choice in desalination because of its better performance. The annual cost for the chemical requirements is calculated from Eq. (47).

$$CHC_{tis} = cv^{CHC} \cdot t_h \cdot t_d \cdot c^{chem} \cdot CD_{tis} \cdot Q_{tis}^{FL}, \quad \forall t \in CF, i, s \in I_t \quad (47)$$

where cv^{CHC} is a conversion factor, t_d is the number of operating days a year, t_h is the number of operating hours a day, CD_{tis} is the coagulant dose and c^{chem} is the cost of coagulant. Q_{tis}^{FL} is the linearised flowrate of a bilinear term for the multiplication of the feed flowrate and the binary variable E_{tis} . The term is determined by Eqs. (48) and (49).

$$Q_{tis}^{FL} \leq Q^{IN} \cdot E_{tis}, \quad \forall t, i, s \in I_t \quad (48)$$

$$Q_{tis}^F - Q^{IN} \cdot (1 - E_{tis}) \leq Q_{tis}^{FL} \leq Q_{tis}^F + Q^{IN} \cdot (1 - E_{tis}), \quad \forall t, i, s \in I_t \quad (49)$$

The linearised term is used in calculating the electricity cost for the slow mixing in the flocculant tank (Eq. (50)).

$$EMC_{tis} = cv^{EM} \cdot t_d \cdot t_h \cdot \mu \cdot c^E \cdot T_{f_t} \cdot Q_{tis}^{FL} \cdot G_{f_{tis}}^2, \quad \forall t \in CF, i, s \in I_t \quad (50)$$

In Eq. (50), cv^{EM} is conversion factor, μ is the dynamic viscosity of the fluid and c^E is the electricity charge. The ongoing costs for DAF depend mainly on its saturator which is expressed in Eq. (51).

$$SC_{tis} = \frac{cv^{SC} \cdot c^E \cdot \bar{P}_{qis} \cdot Q_{tis}^F \cdot X_{qis}}{\eta^{SAT}}, \quad \forall t \in CLR, q \in DAF, i, s \in I_t \quad (51)$$

where SC_{tis} is the operating cost of the saturator, cv^{SC} is the conversion factor for the equation, η_t^{SAT} is the efficiency of the saturator, \bar{P}_{qis} is the saturator pressure, assumed to be the pressure supplied by the pump and c^E is the electricity cost rate. The most significant contribution to the operating costs stems from electricity, and more specifically, electricity for flowrates distribution and achieving separation pressure. Hence, the feed pumps are the main electricity consumers and their costs, denoted as PC_{tis} , are expressed in the following equation.

$$PC_{tis} = \frac{cv^{PC} \cdot c^E \cdot P_{tis} \cdot Q_{tis}^{FL}}{\eta_t^{FP} \cdot \eta_t^{MT}}, \quad \forall t \notin CLR, i, s \in I_t \quad (52)$$

cv^{PC} is a conversion factor for the pumping cost equation. No pumps are assigned to the clarification processes in order to avoid breaking the flocs formed in CF.

The replacement costs, MRC_{tis} , are estimated for every pass i and stage s . For media filtration, they will depend on the volume of media to be purchased.

$$MRC_{tis} = af^{MRC} \cdot rc_t^M \cdot \frac{\pi \cdot L_{tis} \cdot D_{tis}^{MED2}}{4} \cdot E_{tis} \quad \forall t \in MMF, i, s \in I_t \quad (53)$$

For membrane filtration, the replacement cost is governed by the permeate flowrate:

$$MRC_{tis} = af^{MRC} \cdot t_h \cdot t_d \cdot rc_t^M \cdot y_{tis} \cdot Q_{tis}^{FL} \quad \forall t \in TMM, i, s \in I_t \quad (54)$$

where af^{MRC} is an annualisation factor allowing membrane life of 5 years and rc^M is the membrane replacing cost per cubic metre media purchased (for media filtration) or permeate produced (for membrane filtration). It is assumed that the lifespan of the chambers for CF, SED and DAF lasts as long as the plant's life. The chemical costs for pH adjusting, treatment and post-treatment can also be expressed in terms of the capacity of the plant, hence:

$$ChemC = t_h \cdot t_d \cdot py \cdot r^{ch} \cdot Q_{out} \quad (55)$$

where r^{ch} is the cost for chemicals per volume of produced water.

The labour cost, LC , accounts for another large ongoing expense in a manufacturing facility. It can be estimated based on the production capacity of the plant, as shown in Eq. (56).

$$LC = lc1 \cdot Q_{out} + lc2 \quad (56)$$

190 where $lc1$ and $lc2$ are, respectively, the coefficient and intercept of the linear dependency of daily plant capacity and annual labour cost.

Capital costs. Capital costs for every plant are comprised of four major components, namely, project development, plant equipment and buildings, power supply, and piping and pumps (Blaikie et al., 2013). An estimation of the capital cost, however, can be given by the capacity for water production and thus, the following expression can be used:

$$CC_{tis} = infl_t \cdot A_t \cdot (Q_{tis}^P)^{b_t} \cdot E_{tis}, \quad \forall t \notin CLR, i, s \in I_t \quad (57)$$

where $infl_t$ is inflation factor depending on the year of estimation, A_t and b_t are specific parameters for every technology. The capital cost for the clarification technologies is calculated from Eq. (58).

$$CC_{tis} = \sum_{q \in TCLR} infl_q \cdot A_q \cdot (Q_{tis}^P)^{b_q} \cdot X_{qis}, \quad \forall t \in CLR, i, s \in I_t \quad (58)$$

The capital recovery factory (CRF) is expressed in Eq. (59) (Badiru & Omitaomu, 2007).

$$CRF = \frac{ir}{1 - \frac{1}{(1+ir)^{yr}}} \quad (59)$$

where ir is the bank interest rate and yr is the number of years for investment which often coincides with the plant life.

Total cost. The total annual cost, TC , is a sum of the coagulant CHC_{tis} , chemical conditioning $ChemC$, mixing EMC_{tis} , saturator SC_{tis} , pumping PC_{tis} , replacement MRC_{tis} , labour LC and the annual capital costs for all the

selected technologies.

$$\begin{aligned}
 TC = & \sum_{t \in CF} \sum_{i \in I_t} \sum_{s \in I_t} CHC_{tis} + ChemC + && \text{chemical costs} \\
 & \sum_{t \in CF} \sum_{i \in I_t} \sum_{s \in I_t} EMC_{tis} + \sum_{t \in CLR} \sum_{i \in I_t} \sum_{s \in I_t} SC_{tis} + \sum_{t \notin CLR} \sum_{i \in I_t} \sum_{s \in I_t} PC_{tis} + && \text{power costs} \\
 & \sum_{t \in TMMB} \sum_{i \in I_t} \sum_{s \in I_t} MRC_{tis} + && \text{replacement cost} \quad (60) \\
 & LC + && \text{labour cost} \\
 & \sum_t \sum_{i \in I_t} \sum_{s \in I_t} CRF \cdot CC_{tis} && \text{capital cost}
 \end{aligned}$$

3.1.6. Objective function

195 The objective function for the MINLP model is to minimise the water net cost, WNC , which is the quotient of the total annual cost and the annual plant production rate:

$$\text{minimise } WNC = \frac{TC}{Q^{AP}} \quad (61)$$

which is subject to:

- separation efficiencies Eq. (2) - Eq. (14)
- mass balances Eq. (15) - Eq. (36)
- 200 • targets Eq. (37) - Eq. (39)
- logical conditions Eq. (40) - Eq. (46)
- operating costs Eq. (47) - Eq. (56)
- capital costs Eq. (57) - Eq. (58)
- total annual cost Eq. (60)

205 While minimising the annualised capital investment and running costs, the annual production flowrate is increased and the optimum purity is achieved. Nevertheless, the formulation contains various non-linearities that result in multiple local minima. In pursuit for better model stability, the most abundant non-linearities generated from mass balance constraints are reformulated, together with the capital cost function, which is demonstrated in the next subsection.

210 3.2. *p*MINLP model

The model presented in Section 3.1 can be partially linearised in order to improve convergence. The constraints related to mass balances (Eqs. (31), (33), (34) and (37)) and economies of scale (Eqs. (58) and (59)) are initially reformulated. The relaxation and piecewise approximation procedures are presented in the following sections.

3.2.1. Mass balances linearisations

215 The bilinear terms $C_{tisc}^P \cdot Q_{tis}^P$, $C_{tisc}^F \cdot Q_{tis}^F$, $C_{tisc}^C \cdot Q_{tis}^C$ arising from the multiplication of two continuous variables, i.e. contaminants and flowrates, in Eqs. (31), (33) and (34) were reformulated using multiparametric disaggregation (Teles et al., 2012; Kolodziej et al., 2013; Teles et al., 2013; Castro, 2016) where the flowrate is expressed as a multiparametric sum of active decimal powers determined by binary variables z_{tisckl} and continuous variables \bar{z}_{tisc} , and the concentrations variable is disaggregated into a set of continuous non-negative variables \hat{C}_{tisckl} and \bar{C}_{tisc} . The variables have an additional letter or superscripts corresponding to the stream they belong to, i.e. permeate, feed and concentrate. Thus, the reformulation for permeate, for instance, becomes:

$$CQ_{tisc}^P = \sum_{l=p}^P \sum_{k=0}^9 10^l \cdot k \cdot \hat{C}_{tisckl}^P + \sum_{k=0}^1 10^p \cdot k \cdot \bar{C}_{tisc}^P, \quad \forall t, i, s \in I_t, c \quad (62)$$

where $k = \{0, 1, 2, \dots, 9\}$. The flowrate is represented in Eq. (63) where the second term provides fine tuning and hence, continuity in the domain of the flowrate.

$$Q_{tis}^P = \sum_{l=p}^P \sum_{k=0}^9 10^l \cdot k \cdot z_{p_{tisc}kl} + \sum_{k=0}^1 10^p \cdot k \cdot \bar{z}_{p_{tisc}k}, \quad \forall t, i, s \in I_t, c \quad (63)$$

The newly introduced non-negative continuous variables \hat{C}_{tisckl}^P and \bar{C}_{tisc}^P are bounded by M_c^{BIG} or zeroed depending on the value the binary and pseudo-binary variables will take.

$$\hat{C}_{tisckl}^P \leq M_c^{BIG} \cdot z_{p_{tisc}kl}, \quad \forall t, i, s \in I_t, c, k, l \quad (64)$$

$$\bar{C}_{tisc}^P \leq M_c^{BIG} \cdot \bar{z}_{p_{tisc}k}, \quad \forall t, i, s \in I_t, c, k \leq 1 \quad (65)$$

Eq. (66) and Eq. (67) relate \hat{C}_{tisckl}^P and \bar{C}_{tisc}^P with the variable C_{tisc}^P additional constraints are introduced.

$$\sum_{k=0}^9 \hat{C}_{tisckl}^P = C_{tisc}^P, \quad \forall t, i, s \in I_t, c, l \quad (66)$$

$$\sum_{k=0}^1 \bar{C}_{tisc}^P = C_{tisc}^P, \quad \forall t, i, s \in I_t, c \quad (67)$$

The selection of only one variable over the k set is imposed by Eq. (68) and Eq. (69).

$$\sum_{k=0}^9 z_{p_{tisc}kl} = 1, \quad \forall t, i, s \in I_t, c, l \quad (68)$$

$$\sum_{k=0}^1 \bar{z}_{p_{tisc}k} = 1, \quad \forall t, i, s \in I_t, c \quad (69)$$

The continuous variable $\bar{z}_{p_{tisc}}$ is bounded between 0 and 1. The feed and concentrate have been reformulated using the same method where superscripts F and C are used to designate the respective variables. Replacing the bilinear products, transforms Eq. (31) to the following constraint:

$$CQ_{tisc}^C = CQ_{tisc}^F - CQ_{tisc}^P, \quad \forall t, i, s \in I_t, c \quad (70)$$

Eq. (33) and Eq. (34) acquire the form, shown in Eq. (71) and Eq. (72).

$$\sum_{s \in I_t} CQ_{t,i-1,s}^P = CQ_{tisc|s=1}^F, \quad \forall t, i \in I_t, i > 1, c \quad (71)$$

$$\sum_{s \in I_t} CQ_{t-1,isc|i=I_t^{max}}^P = CQ_{tisc|i=1,s=1}^F, \quad \forall t > 1, c \quad (72)$$

The bilinear terms arising from the multiplication of continuous variables of contaminant levels and flowrates for final effluent in Eq. (37) were reformulated in a similar manner, demonstrated below.

$$CQ_{out_c} = \sum_{l=p}^P \sum_{k=0}^9 10^l \cdot k \cdot \hat{C}_{out_{ckl}} + \sum_{k=0}^1 10^p \cdot k \cdot \bar{C}_{out_{ck}}, \quad \forall c \quad (73)$$

where $\hat{C}_{out_{ckl}}$ and $\bar{C}_{out_{ck}}$ are the auxiliary continuous variables to represent final concentrations. The effluent is expressed as a summation of two terms where z_{ockl} is a binary variable and \bar{z}_{ock} a continuous variable, both to determine the selection of a single digit number k and decimal number raised to power l .

$$Q_{out} = \sum_{l=p}^P \sum_{k=0}^9 10^l \cdot k \cdot z_{ockl} + \sum_{k=0}^1 10^p \cdot k \cdot \bar{z}_{ock}, \quad \forall c \quad (74)$$

$\hat{C}_{out_{ckl}}$ and $\bar{C}_{out_{ck}}$ are bounded by a big number in the following constraints.

$$\hat{C}_{out_{ckl}} \leq M_c^{BIG} \cdot z_{ockl}, \quad \forall c, k, l \quad (75)$$

$$\bar{C}_{out_{ck}} \leq M_c^{BIG} \cdot \bar{z}_{ock}, \quad \forall c, k \leq 1 \quad (76)$$

$\hat{C}_{out_{ckl}}$ and $\bar{C}_{out_{ck}}$ and C_{out_c} are related in Eq. (77) and Eq. (78).

$$\sum_{k=0}^9 \hat{C}_{out_{ckl}} = C_{out_c}, \quad \forall c, l \quad (77)$$

$$\sum_{k=0}^1 \bar{C}_{out_{ck}} = C_{out_c}, \quad \forall c \quad (78)$$

Only the selection of one significant digit for every power is possible:

$$\sum_{k=0}^9 z_{ockl} = 1, \quad \forall c, l \quad (79)$$

$$\sum_{k=0}^1 \bar{z}_{ock} = 1, \quad \forall c \quad (80)$$

The continuous variable \bar{z}_{ock} is between 0 and 1. Because permeate, feed, concentrate and final flowrates are in the same order of magnitude, the power they are raised to is the same. The bilinear products are now substituted in Eq. (37) and it is remodelled to Eq. (81).

$$CQ_{out_c} = \sum_{s \in I_t} CQ_{tisc}^P, \quad \forall t = T, i = I_t^{max}, c \quad (81)$$

3.2.2. Approximation of capital cost constraints

The capital cost is represented by a piecewise linear approximation, defined over the domain of the flowrate. Taking Q^{IN} as an initial point and M^{FLOW} as a final point in this domain, the optimal number of segments and connecting points are obtained with the approach published in Natali & Pinto (2009). The function from Eq. (57) and Eq. (58) is expressed through cco_{tism}^{bp} and q_{tism}^{bbp} , parameters representing segments m of the cost and flowrate, respectively, in Eq. (82).

$$cco_{tism}^{bp} = infl_t \cdot A_t \cdot (q_{tism}^{bbp})^{b_t}, \quad \forall t \notin CLR, i, s \in I_t, m \quad (82)$$

where $infl_t$ is inflation factor depending on the year of estimation, A_t and b_t are specific parameters for every technology. Similar to the formulation in the previous subsection, the cost function of the clarification processes is calculated separately:

$$cco_{qism}^{bp} = infl_q \cdot A_q \cdot (q_{qism}^{bbp})^{b_q}, \quad \forall q \in TCLR, i, s \in \bar{I}_q, m \quad (83)$$

The performed piecewise approximation is shown below where G_{tism} is a continuous variable and Y_{tism}^m is a binary variable.

$$Q_{tis}^P = \sum_m (q_{tism}^{bbp} \cdot G_{tism}), \quad \forall t \notin CLR, i, s \in I_t \quad (84)$$

Eq. (85) connects the flowrate of CLR with the properties of SED and DAF:

$$Q_{tis}^P = \sum_m (q_{qism}^{bbp} \cdot G_{qism}), \quad \forall t \in CLR, q \in TCLR, i, s \in I_t \quad (85)$$

The capital cost $CCol_{tis}$ is related in Eq. (86) and Eq. (87).

$$CCol_{tis} = \sum_m (cco_{tism}^{bp} \cdot G_{tism}), \quad \forall t \notin CLR, i, s \in I_t \quad (86)$$

$$CCol_{qis} = \sum_m (cco_{qism}^{bp} \cdot G_{qism}), \quad \forall q \in TCLR, i, s \in \bar{I}_q \quad (87)$$

Only one segment m for a given technology t , pass i and stage s is allowed (Eq. (88)).

$$\sum_m G_{tism} = 1, \quad \forall t, i, s \in I_t \quad (88)$$

$$G_{tism} \leq Y_{tis, m-1}^m + Y_{tism}^m, \quad \forall t, i, s \in I_t, m < M^{max} - 1 \quad (89)$$

$$\sum_{m < M^{max} - 1} Y_{tism}^m = 1, \quad \forall t, i, s \in I_t \quad (90)$$

Standard piecewise linearisation technique utilising one continuous and one discrete variables instead of SOS2 variables is implemented as SOS variables are not supported by most global non-linear solvers. In order to consider the cost only for the selected units, a bilinear term will appear which has to be linearised. Thus, for non clarification technologies:

$$CC_{tis} \leq U_t^{BIG} \cdot E_{tis}, \quad \forall t \notin CLR, i, s \in I_t \quad (91)$$

$$CCol_{tis} - U_t^{BIG} \cdot E_{tis} \leq CC_{tis} \leq CCol_{tis} + U_t^{BIG} \cdot E_{tis}, \quad \forall t \notin CLR, i, s \in I_t \quad (92)$$

where U_t^{BIG} is a sufficiently big number. The presence or absence of capital cost for CLR rest on the value of the binary variable X_{qis} which can take the value of 1 either for SED or for DAF only.

$$CC_{tis} \leq U_q^{BIG} \cdot X_{qis}, \quad \forall t \in CLR, q \in TCLR, i, s \in I_t \quad (93)$$

$$CCol_{qis} - U_q^{BIG} \cdot (1 - X_{qis}) \leq CC_{tis} \leq CCol_{qis} + U_q^{BIG} \cdot (1 - X_{qis}), \quad \forall t \in CLR, q \in TCLR, i, s \in I_t \quad (94)$$

3.2.3. Objective function

The objective function for the pMINLP model is to minimise the water net cost, WNC , which equals the total annual cost divided by the annual plant production rate:

$$\text{minimise } WNC = \frac{TC}{Q^{AP}}$$

which is subject to:

- separation efficiencies Eq. (2) - Eq. (14)
- mass balances Eq. (15) - Eq. (30), Eqs. (32), Eq. (35), Eq. (36), Eq. (62) - Eq. (72)
- targets Eq. 38, Eq. (39), Eq. (73) - Eq. (81)
- logical conditions Eq. (40) - Eq. (46)
- operating costs Eq. (47) - Eq. (56)
- capital costs Eq. (84) - Eq. (94)
- total annual cost Eq. (60)

An alternative formulation can be obtained if $P1$ is completely linearised.

3.3. MILFP model

The model presented in Section 3.2 can be linearised completely to enhance robustness. Eqs. (2) - (14) contain regressions which are not only linear but also quadratic, logarithmic and reciprocal. Due to the different nature of non-linearities, discretisation of the physicochemical properties and operating conditions is performed. Additionally, the running costs, that also contain operating conditions (Eqs. (47), (50), (51), (52) and (53)), are also reformulated. Finally, a variation of the Dinkelbach's algorithm is implemented as a solution approach to the ratio in the objective function in Eq. (61).

3.3.1. Rejection coefficient discretisations

The separation efficiencies have been discretised to avoid the nonlinearities in Eq. (2) - Eq. (14). A subscript j denotes the levels of discretisations of both, the separation efficiencies and operating conditions, which vary with the technologies. The form the correlations take is summarised in Table 3 where r_{icj} is the separation efficiency

of every technology t and contaminant c and at a discrete level j . Furthermore, the equations differ from the correlations in Section 3.1 with the terms being declared as parameters and denoted with small letters, and the additional index.

Table 3: Summary of rejection coefficients correlations in MILFP model

Correlation		Equation
$r_{tcj} = 0.00058 \cdot cd_{tj} + 0.135 \cdot ph_{tj} - 0.154,$	$\forall t \in CF, c \in COD, j \in J_t$	(95)
$rq_{tqcj} = 0.22154 + 0.02516 \cdot cd_{tj t=CF},$	$\forall t \in CLR, q \in SED, c \in TSS, j \in J_t$	(96)
$rq_{tqcj} = 1.85886 - 0.00807 \cdot cd_{tj t=CF} - 0.00083 \cdot gf_{tj t=CF} +$ $0.0025 \cdot tf_{tj t=CF} - 2.47 \cdot \bar{p}_{qj},$	$\forall t \in CLR, q \in DAF, c \in TSS, j \in J_t$	(97)
$r_{tcj} = 0.0298 \cdot d_{tj}^{MED} + 0.171 \cdot ld_{tj} + 0.206 \cdot l_{tj}^{-1} - 0.245,$	$\forall t \in MMF, c \in TSS, j \in J_t$	(98)
$r_{tcj} = 0.189 + 1.009 \cdot p_{tj},$	$\forall t \in MF, c \in COD, j \in J_t$	(99)
$r_{tcj} = 0.126 + 0.001 \cdot tem_{tj} + 0.97 \cdot p_{tj},$	$\forall t \in MF, c \in TSS, j \in J_t$	(100)
$r_{tcj} = 0.236 - 0.952 \cdot p_{tj},$	$\forall t \in UF, c \in COD, j \in J_t$	(101)
$r_{tcj} = 0.959 - 1.510 \cdot p_{tj},$	$\forall t \in UF, c \in TSS, j \in J_t$	(102)
$r_{tcj} = 1.138 - 0.00096 \cdot mwco_{tj} - 0.087 \cdot p_{tj},$	$\forall t \in NF, c \in COD, j \in J_t$	(103)
$r_{tcj} = (0.57 - 0.07 \cdot h_{tj} - 0.0002 \cdot mwco_{tj})^2,$	$\forall t \in NF, c \in TDS, j \in J_t$	(104)
$r_{tcj} = 0.890 + 0.0340 \cdot p_{tj} - 0.003 \cdot p_{tj}^2,$	$\forall t \in RO1, c \in TDS, j \in J_t$	(105)
$r_{tcj} = 0.408 + 0.046 \cdot ph_{tj} + 0.028 \cdot p_{tj},$	$\forall t \in RO2, c \in B, j \in J_t$	(106)

The selection of the rejection coefficient is expressed through a binary variable, W_{tisj} , which designates if a combinatorial option from the given operating conditions is selected or not.

$$R_{tisc} = \sum_{j \in J_t} r_{tcj} \cdot W_{tisj}, \quad \forall t \notin CLR, i, s \in I_t, c \in CT_i \quad (107)$$

Then, the discrete levels selected, should equal the binary variable E_{tis} , shown in Eq. (108).

$$\sum_{j \in J_t} W_{tisj} = E_{tis}, \quad \forall t \notin CLR, i, s \in I_t \quad (108)$$

For the clarification technologies, $W_{Q_{tqisj}}$ triggers the selection (Eq. (109) and Eq. (110)).

$$R_{tisc} = \sum_{q \in TCLR} \sum_{j \in J_t} rq_{tqcj} \cdot W_{Q_{tqisj}}, \quad \forall t \in CLR, i, s \in I_t, c \in CT_i \quad (109)$$

where rq_{tqcj} is the separation efficiency of a clarification technology SED or DAF.

$$\sum_{q \in TCLR} \sum_{j \in J_t} W_{Q_{tqisj}} = E_{tis}, \quad \forall t \in CLR, i, s \in I_t \quad (110)$$

3.3.2. Further linearisations of mass balance constraints

Concentration constraints

Section 3.2 demonstrated the reformulation of some of the material balances involved. The bilinear product of the concentrations and removal efficiencies is addressed by substituting Eq. (15) with the constraint below:

$$C_{tisc}^F - CR_{tisc}^F - M_c^{BIG} \cdot (1 - E_{tis}) \leq C_{tisc}^P \leq C_{tisc}^F - CR_{tisc}^F + M_c^{BIG} \cdot (1 - E_{tis}), \quad \forall t, i, s \in I_t, c \in CT_i \quad (111)$$

where CR_{tisc}^F replaces the aforementioned bilinear product using multiparametric disaggregation technique described previously.

$$CR_{tisc}^F = \sum_{z=lp}^P \sum_{k=0}^9 10^{lp} \cdot k \cdot \hat{C}r_{tiscz}^F + \sum_{k=0}^1 10^{lp} \cdot k \cdot \bar{C}r_{tisc}^F, \quad \forall t, i, s \in I_t, c \quad (112)$$

where $\hat{C}r_{tiscz}$ and $\bar{C}r_{tisc}$ are a set of continuous non-negative variables the concentrations variable is disaggregated into. The separation efficiency is expressed as a multi-parametric sum of active decimal powers determined by binary variables zr_{tiscz} and continuous variables $\bar{z}r_{tisc}$.

$$R_{tisc} = \sum_{z=lp}^P \sum_{k=0}^9 10^{lp} \cdot k \cdot zr_{tiscz} + \sum_{k=0}^1 10^{lp} \cdot k \cdot \bar{z}r_{tisc}, \quad \forall t, i, s \in I_t, c \quad (113)$$

$$\hat{C}r_{tiscz}^F \leq M_c^{BIG} \cdot zr_{tiscz}, \quad \forall t, i, s \in I_t, c, k, z \quad (114)$$

$$\bar{C}r_{tisc}^R \leq M_c^{BIG} \cdot \bar{z}r_{tisc}, \quad \forall t, i, s \in I_t, c, k \leq 1 \quad (115)$$

The connection of $\hat{C}r_{tiscz}$ and $\bar{C}r_{tisc}$ with C_{tisc}^F is given in Eq. (116) and Eq. (117).

$$\sum_{k=0}^9 \hat{C}r_{tiscz}^F = C_{tisc}^F, \quad \forall t, i, s \in I_t, c, z \quad (116)$$

$$\sum_{k=0}^1 \bar{C}r_{tisc}^F = C_{tisc}^F, \quad \forall t, i, s \in I_t, c \quad (117)$$

$$\sum_{k=0}^9 zr_{tiscz} = 1, \quad \forall t, i, s \in I_t, c, z \quad (118)$$

Only one significant digit can exist for every technology t , pass i , stage s , contaminant c :

$$\sum_{k=0}^1 \bar{z}r_{tisc} = 1, \quad \forall t, i, s \in I_t, c \quad (119)$$

The separation efficiency ranges between 0 and 1 and therefore, the power lp is chosen accordingly.

Flowrate constraints

As the recovery for clarification technologies becomes a variable (Eq. (120)), the product for the feed flowrate and the recovery has to be linearised.

$$\bar{Y}_{tis} = \sum_{q \in TCLR} (\bar{y}_{qis} \cdot X_{qis}) \quad \forall t \in CLR, i, s \in I_t \quad (120)$$

It is known that the recovery can take either one or another value which does not necessitate a complicated representation such as the multiparametric disaggregation. Therefore, a simple approximation where the recovery is discretised is sufficient.

$$QY_{tis}^F = \sum_r (\bar{Q}_{tisr}^F \cdot \hat{Y}_{tisr}) \quad \forall t \in CLR, i, s \in I_t \quad (121)$$

where QY_{tis}^F represents the bilinear product of flowrate and recovery and \bar{Q}_{tisr}^F is an auxiliary continuous variable.

$$\bar{Y}_{tis} = \sum_r (\hat{Y}_{tisr} \cdot zy_{tisr}) \quad \forall t \in CLR, i, s \in I_t \quad (122)$$

where zy_{tisr} is a binary variable.

$$\sum_r (zy_{tisr}) = 1 \quad \forall t \in CLR, i, s \in I_t \quad (123)$$

$$\bar{Q}_{tisr}^F \leq Q^{IN} \cdot zy_{tisr} \quad \forall t \in CLR, i, s \in I_t \quad (124)$$

$$\sum_r (\bar{Q}_{tisr}^F \cdot zy_{tisr}) = Q_{tis}^F \quad \forall t \in CLR, i, s \in I_t \quad (125)$$

Thus, the equivalent equations representing the permeate flowrate for CLR are:

$$QY_{tis}^F - Q^{IN} \cdot (1 - E_{tis}) \leq Q_{tis}^P \leq QY_{tis}^F + Q^{IN} \cdot (1 - E_{tis}), \quad \forall t \in CLR, i, s \in I_t \quad (126)$$

$$Q_{tis}^F - Q^{IN} \cdot E_{tis} \leq Q_{tis}^P \leq Q_{tis}^F, \quad \forall t \in CLR, i, s \in I_t \quad (127)$$

255 3.3.3. Linearisations of operating cost constraints

After having discretised operating conditions, the decision of which level to pick has to be addressed in the ongoing costs, which depend on flow, already linearised capacity or production rate, operating conditions and a binary variable. Eq. (47) will then alter to Eq. (128).

$$CHC_{tis} = cv^{CHC} \cdot t_h \cdot t_d \cdot c^{chem} \cdot QCD_{tis}, \quad \forall t \in CF, i, s \in I_t \quad (128)$$

where QCD_{tis} is the product of flow and selected operating condition when the cost is active. Thus, the additional constraint for the chemical dosage and flowrate is given in Eq. (129).

$$QCD_{tis} \leq cd_{tj} \cdot Q_{tis}^{FL} + M^{CD} \cdot (1 - W_{tisj}), \quad \forall t \in CF, i, s \in I_t, j \in J_t \quad (129)$$

where M^{CD} is a big number for the chemical dosage. Minimising the dosage will presumably lead to lower cost, thus, the constraint provided is sufficient. Electrical costs for mixing are modified accordingly in the equation below where QtG_{tis} is the linearised product of flowrate, retention time and energy input.

$$EMC_{tis} = cv^{EM} \cdot t_d \cdot t_h \cdot \mu \cdot c^E \cdot QtG_{tis}, \quad \forall t \in CF, i, s \in I_t \quad (130)$$

Two constraints are necessary for representing QtG_{tis} because its resulting cost is a trade-off among the participating variables.

$$QtG_{tis} \leq tf_{tj} \cdot gf_{tj}^2 \cdot Q_{tis}^{FL} + M^{TG} \cdot (1 - W_{tisj}), \quad \forall t \in CF, i, s \in I_t, j \in J_t \quad (131)$$

$$QtG_{tis} \geq tf_{tj} \cdot gf_{tj}^2 \cdot Q_{tis}^{FL} - M^{TG} \cdot (1 - W_{tisj}), \quad \forall t \in CF, i, s \in I_t, j \in J_t \quad (132)$$

where M^{TG} is a big number for energy input and time. In the saturator and pumping costs, the product of the pressure and flowrate appear (Eq. (51) and Eq. (52)) which is also substituted by a single continuous variable, QPF_{tis} , shown in Eq. (133) and Eq. (134).

$$SC_{tis} = \frac{cv^{SC} \cdot c^E \cdot QPF_{tis}}{\eta^{SAT}}, \quad \forall t \in CLR, i, s \in I_t \quad (133)$$

$$PC_{tis} = \frac{cv^{PC} \cdot c^E \cdot QPF_{tis}}{\eta_t^{FP} \cdot \eta_t^{MT}}, \quad \forall t \notin CLR, i, s \in I_t \quad (134)$$

QPF_{tis} is derived from p_{tj} , Q_{tis}^{FL} and W_{tisj} in Eq. (135) and Eq. (136).

$$QPF_{tis} \leq p_{tj} \cdot Q_{tis}^{FL} + M^P \cdot (1 - W_{tisj}), \quad \forall t, i, s \in I_t, j \in J_t \quad (135)$$

$$QPF_{tis} \geq p_{tj} \cdot Q_{tis}^{FL} - M^P \cdot (1 - W_{tisj}), \quad \forall t, i, s \in I_t, j \in J_t \quad (136)$$

where M^P is a big number for the pressure. It should be pointed out that the pressure values for DAF are the ones CLR adopts. The replacement cost of media for MMF involves only operating characteristics of the filter from which one is singled out in the formulation below.

$$MRC_{tis} = \sum_{j \in J_t} a_f^{MRC} \cdot rc_t^M \cdot \frac{\pi \cdot l_{tj} \cdot d_{tj}^{MED2}}{4} \cdot W_{tisj} \quad \forall t \in MMF, i, s \in I_t \quad (137)$$

3.3.4. Objective function

The objective function for the MILFP model is to minimise the water net cost, WNC , which equals the total annual cost divided by the annual plant production rate:

$$\text{minimise } WNC = \frac{TC}{Q^{AP}}$$

As the objective function is a fraction of two variables, a reformulation is applied for its linearisation. It has been demonstrated that the Dinkelbach's algorithm (Dinkelbach, 1967) finds optimal solution for both, MILFP maximisation and minimisation problems (You et al., 2009; Yue & You, 2013; Liu et al., 2014). A variation of the algorithm is used in this work to reformulate the objective function and accommodate the MILFP as follows:

$$\text{minimise } TC - \alpha \cdot Q^{AP}, \quad (138)$$

where α is a parameter. The objective function is subject to:

- separation efficiencies Eq. (107) - Eq. (110)
- mass balances Eq. (16) - Eq. (23), Eq. (25) - Eq. (30), Eqs. (32), Eq. (35), Eq. (36), Eq. (62) - Eq. (72), Eq. (111) - Eq. (127)
- targets Eq. (38), Eq. (39), Eq. (73) - Eq. (81)
- logical conditions Eq. (40) - Eq. (46)

- operating costs Eq. (48), Eq. (49), Eq. (54) - Eq. (56), Eq. (128) - Eq. (137)
- capital costs Eq. (84) - Eq. (94)
- total annual cost Eq. (60)

The algorithm is implemented in two loops whose steps are outlined below and shown in Fig. 6.

1. Initialise the parameter α ;
2. Relax binary variables related to multi-parametric disaggregation , i.e. $z_{f_{tisckl}}$, $z_{p_{tisckl}}$, $z_{c_{tisckl}}$, $z_{o_{ckl}}$ and $z_{r_{tisczk}}$;
3. Solve the MILP model where the values of the total cost, TC , and the annual production flow, Q^{AP} , returned are designated as TC^* and Q^{AP*} ;
4. When $|TC^* - \alpha \cdot Q^{AP*}| \leq \epsilon$, terminate and return the optimal solution $WNC = TC^* / Q^{AP*}$; otherwise update $\alpha = TC^* / Q^{AP*}$ and return to 3;
5. Fix E_{tis} for pass 1 and stage 1 of selected E_{tis} from step 4;
6. Unrelax $z_{f_{tisckl}}$, $z_{p_{tisckl}}$, $z_{c_{tisckl}}$, $z_{o_{ckl}}$ and $z_{r_{tisczk}}$;
7. Solve the MILP model where the values of the total cost, TC , and the annual production flow, Q^{AP} , returned are designated as TC^* and Q^{AP*} ;
8. When $|TC^* - \alpha \cdot Q^{AP*}| \leq \epsilon$, terminate and return the optimal solution $WNC = TC^* / Q^{AP*}$; otherwise update $\alpha = TC^* / Q^{AP*}$ and return to 7.

The approximations and linearisations contribute to the heavy size of the model and therefore, increase in the computational performance. Therefore, Dinkelbach's algorithm has been applied two consecutive times, once with relaxed binary variables derived from reformulations and a second time when the binary variables are not relaxed. It has been deducted this strategy reduces the computational time immensely.

3.4. Models summary

The objective functions and constraints valid for models $P0$, $P1$ and $P2$ are summarised and listed in Table 4.

Unlike in models $P0$ and $P1$, in model $P2$, a hierarchical solution approach is applied by solving the Dinkelbach's algorithm twice in a sequential manner - once with relaxed binary variables which appear in the multiparametric disaggregation technique. The results from both, $P1$ and $P2$ are post-processed with $P0$ immediately after $P1$ and $P2$ in order to (i) obtain exact and not approximated solution and (ii) be able to compare the solutions with the ones obtained from $P0$. Scaling the variables and equations for the models has been performed accordingly.

4. Illustrative examples

To illustrate the capability of the three proposed approaches, they have been applied to two theoretical examples with data from industrial practices. The first case study looks at seawater desalination while the latter examines surface water treatment; both to produce drinking water.

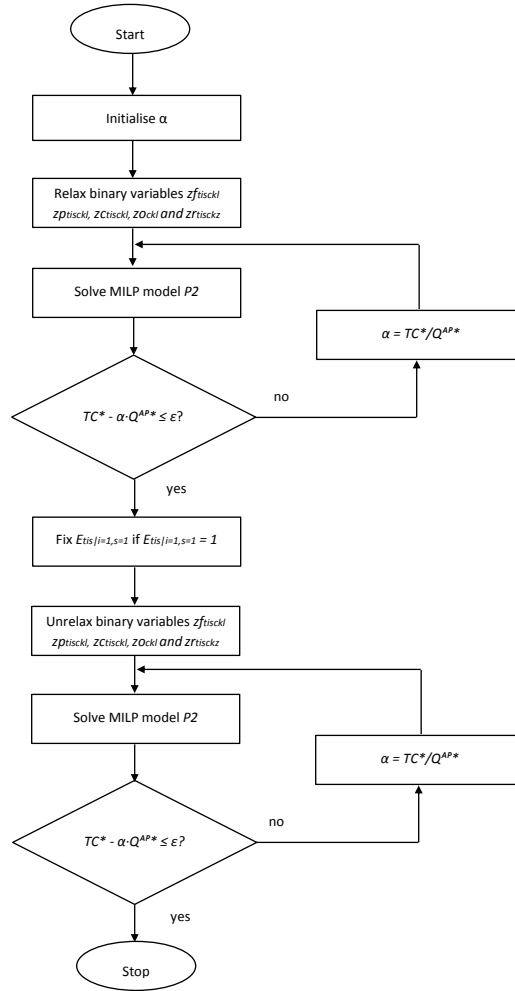


Figure 6: Algorithm for solving MILFP model $P2$

4.1. Seawater desalination example

Countries with arid land and prolonged droughts have included in their water supply planning sources such as seawater. Consequently, a number of seawater desalination projects have already been realised and many are contracted to be completed in the near future. With an outlook of the foreseen trends, the first example focuses its attention on seawater desalination plants design.

- **Intake and production capacities.** The water intake $Q^{IN} = 55,000 \text{ m}^3/\text{h}$ for a system with minimum allowable effluent $M^{FLOW} = 5,000 \text{ m}^3/\text{h}$ which, for instance, corresponds to the production capacity of Carboneras SWRO plant in Spain. Additional production capacities of membrane desalination plants not only in Spain but in Algeria, US, China and India predominantly vary between $4,000 \text{ m}^3/\text{h}$ and $10,000 \text{ m}^3/\text{h}$ (Abengoa Water, 2016). One of the largest membrane seawater desalination projects is situated in Ras Alkhair (Saudi Arabia) where it provides circa $41,667 \text{ m}^3/\text{h}$ (Better World Solutions, 2016). Seawater

Table 4: Summary of constraints and objective functions for MINLP, pMINLP and MILFP models

Constraints	MINLP model ($P0$)	pMINLP model ($P1$)	MILFP model ($P2$)
separation efficiencies	Eq. (2) - Eq. (14)	Eq. (2) - Eq. (14)	Eq. (107) - Eq. (110)
mass flow balance	Eq. (15) - Eq. (36)	Eq. (15) - Eq. (30), Eqs. (32), Eq. (35), Eq. (36), Eq. (62) - Eq. (72)	Eq. (16) - Eq. (23), Eq. (25) - Eq. (30), Eq. (35), Eq. (36), Eq. (62) - Eq. (72), Eq. (111) - Eq. (127)
target purity	Eq. (37) - Eq. (39)	Eq. 38, Eq. (39), Eq. (73) - Eq. (81)	Eq. (38), Eq. (39), Eq. (73) - Eq. (81)
logical conditions	Eq. (40) - Eq. (46)	Eq. (40) - Eq. (46)	Eq. (40) - Eq. (46)
operating costs	Eq. (47) - Eq. (56)	Eq. (47) - Eq. (56)	Eq. (48), Eq. (49), Eq. (54) - Eq. (56), Eq. (128) - Eq. (137)
capital costs	Eq. (57) - Eq. (58)	Eq. (84) - Eq. (94)	Eq. (84) - Eq. (94)
total annual cost	Eq. (60)	Eq. (60)	Eq. (60)
objective function	Eq. (61)	Eq. (61)	Eq. (138)

intakes, on the other hand, must be more than twice as much as the desired production rate in order to overcome the low yield of the membrane plants. For example, Adelaide Desalination Plant's (Australia) intake capacity approximates 28,400 m³/h with production capacity of roughly 12,500 m³/h and Qingdao Desalination Plant's (China) intake capacity surpasses 10,000 m³/h with an output of 4,167 m³/h (Acciona Agua, 2016; Clemente, 2013).

- **Intake and product quality.** The quality of the seawater ranges from 30,000 mg/L to 40,000 mg/L TDS depending on the location of the sea or ocean (American Water Works Association, 2007). The TSS and boron have typical values of 30 mg/L and 5 mg/L, respectively (Tchobanoglous et al., 2003; Mane et al., 2009), which are the values used for the initial concentrations of contaminants in the source water. The final contaminants concentrations for drinking water must not exceed 600 mg/L, 1 mg/L and 2.4 mg/L for TDS, TSS and boron according to regulatory standards (The Drinking Water Inspectorate, 2009; U.S. Environmental Protection Agency, 2010; World Health Organization, 2011).

- **Performance parameters.** Conventional technologies using chemicals exhibit a removal mechanism where it can be assumed that essentially they operate at almost full recovery. Hence, CF, SED and DAF's recoveries are set at 99 %. The recoveries of the filters can reach 100 %, however, it is more likely they lie between 85 % and 95 % (US Interior Reclamation Department, 2013), therefore, a value of 95 % is used. The high pressure membranes manifest lower percentage recoveries and based on reported values in literature (Lu et al., 2006; Mickley et al., 2006), 80 % is effective for NF and 45 % for RO. A satisfactorily performing coagulant in seawater and hence, often the choice is ferric coagulant which costs roughly \$250/tonne. The dosage range used in the model is 1 mg/L-20 mg/L. The labour cost coefficients $lc1 = 148.9$ and $lc2 = 69,289$ are derived from a set of data from Contra Costa Water District et al. (2007). In the same source, chemical costs involved in filtration, desalination and post-treatment as a function of the filtered product have been reported which have been aggregated in the current work to $r^{ch} = 0.0326$ \$/m³. The costs have been converted to SI units and the inflation has been accounted for. Additional performance

Table 5: Seawater desalination: pressure design variables, efficiencies and economic parameters

Technology	CF	CLR	MMF	MF	UF	NF	RO1	RO2
		SED / DAF						
γ_{iis} range [-]	1	0.99/0.99	0.95	0.95	0.95	0.80	0.45	0.45
P_{iis} range [MPa]	0.1 - 0.2	- / 0.4 - 0.7	0.1 - 0.2	0.1 - 0.2	0.1 - 0.3	0.5 - 1.6	5.0 - 6.0	5.0 - 6.0
η_t^{FP} [-]	0.75	- / 0.75	0.80	0.80	0.75	0.80	0.75	0.75
η_t^{MT} [-]	0.95	- / 0.95	0.93	0.95	0.97	0.95	0.98	0.98
rc_t^M [\$/m ³]	-	- / -	12,359	0.00396	0.00396	0.0528	0.0528	0.0528
$infl_t$ [-]	1.143	1.288/1.087	1.319	1.087	1.087	1.511	1.511	1.511
A_t [-]	121,701	8,334 / 4,167	69,547	45,601	45,601	158,177	158,177	158,177
b_t [-]	0.6	0.6 / 0.6	0.6	0.6	0.6	0.6	0.6	0.6

Source: Lu et al. (2006); Bastaki (2004); Hassan et al. (1999); Adham et al. (2006); European Commission (2003); Wang et al. (2010); Whitman et al. (2002); University of New Hampshire (2016); Mallevialle et al. (1996); Contra Costa Water District et al. (2007); FilterWater (2016); US Inflation Calculator (2016)

and costing parameters for models can be found in Table 5 and the remaining of the data are reported elsewhere (Koleva et al., 2016). It must be noted that in Table 5, the replacement cost, rc_t^M , for MMF and the membrane technologies differs significantly as the former is the cost per cubic metres media while the latter is the cost per filtrate produced. The discretised data for model *P2* is located in the Supplementary Material.

- **Passes and stages.** Considering that the recovery of the CF and CLR is practically complete, and furthermore, following the pattern of industrial practices where vessels are attached in series only, in this work, the number of passes (chambers in series) equals to 3 and the number of stages - to 1. Filters, in particular membrane systems can take up configurations of various numbers of passes and stages where London's Desalination Plant, for example, has a 4-pass, 4-stage RO system. In this example, we allow 3 passes and 3 stages for every filtration technology.

4.2. Surface water treatment example

Despite disruptive climatic changes and aquifer depletion, drinking water treatment plants (DWTP) with surface water intake are the main and socially accepted method for obtaining potable water. Consequently, the pick for the second case study in the current paper.

- **Intake and production capacities.** The water intake $Q^{IN} = 10,000$ m³/h for a system with minimum allowable effluent $M^{FLOW} = 2,000$ m³/h which, for instance, falls in the middle of the production capacities of the DWTPs in Dogubayazit, Turkey (1,458.3 m³/h) and El Conquero, Spain (3,750 m³/h). Drinking water treatment plants generally exhibit a higher yield with maximum abstraction twice as much as the production capacity. At Ballyfarnan DWTP for instance, the intake is 135 m³/h whereas the production rate capacity is estimated as 75 m³/h. Similarly, Rockingham DWTP abstracts 500 m³/h at most to produce maximum 250 m³/h (Doris, 2015; Doris et al., 2015). At the world's largest Water Purification Plant in

Table 6: Surface water treatment: pressure design variables, efficiencies and economic parameters

Technology	CF	CLR	MMF	MF	UF	NF	RO1	RO2
		SED / DAF						
γ_{iis} range [-]	0.99	0.99/ 0.99	0.95	0.95	0.95	0.80	0.6	0.6
P_{iis} range [MPa]	0.1 - 0.2	- / 0.4 - 0.7	0.1 - 0.2	0.1 - 0.2	0.1 - 0.3	0.5 - 1.6	3.0 - 5.0	3.0 - 5.0
η_t^{FP} [-]	0.75	- / 0.75	0.80	0.80	0.75	0.80	0.75	0.75
η_t^{MT} [-]	0.95	- / 0.95	0.93	0.95	0.97	0.95	0.98	0.98
rc_t^M [-]	-	- / -	12,359	0.00396	0.00396	0.0132	0.0132	0.0132
$infl_t$ [-]	1.143	1.288/1.087	1.319	1.087	1.087	1.511	1.511	1.511
A_t [-]	121,701	8,334 / 4,167	69,547	45,601	45,601	158,177	158,177	158,177
b_t [-]	0.6	0.6 / 0.6	0.6	0.6	0.6	0.6	0.6	0.6

Source: Lu et al. (2006); Bastaki (2004); Hassan et al. (1999); Adham et al. (2006); European Commission (2003); Wang et al. (2010); Whitman et al. (2002); University of New Hampshire (2016); Mallevialle et al. (1996); US Inflation Calculator (2016); Contra Costa Water District et al. (2007); FilterWater (2016); Nunes & Peinemann (2006)

Chicago, Illinois - the James W. Jardine 41,666,666 m³/h are treated on average (Center for Mechanical Simulation Technology, 2011). Typical DWTP sizes enclose production capacities from 1,000 m³/h to 15,000 m³/h (Abengoa Water, 2016).

• **Intake and product quality.** Unlike in seawater, boron is not present in abundance. In surface water, however, the organic content of the water is taken into account. Hence, the quality of the source water is: 200 mg/L TSS, 800 mg/L TDS and 30 mg/L COD (Tchobanoglous et al., 2003; Cheremisinoff, 2002; Chowdhury et al., 2013). The final contaminants concentrations for drinking water must not exceed 600 mg/L, 1 mg/L and 5 mg/L for TDS, TSS and COD according to regulatory standards (The Drinking Water Inspectorate, 2009; U.S. Environmental Protection Agency, 2010; World Health Organization, 2011).

• **Performance parameters.** In surface water treatment, the preferred choice for coagulant is aluminium sulphate (alum) due to its cheaper price of approximately \$150/tonne (Global B2B Marketplace, 2015). Its dosage also differs by increasing to 10 mg/L - 30 mg/L. CF cannot take a full recovery because of its separating performance for COD. Thus, a value of 0.99 is assumed. Additionally, viscosity value of 1.000 kg/m·s at ambient temperature is taken. Reverse osmosis has a higher recovery (see Table 6) due to the lower salt content in the water. The rest of the data overlaps with the given data from Section 4.1.

• **Passes and stages.** The same number of allowed passes and stages is adopted from the example in Section 4.1.

Multiparametric disaggregation with $p = \{2, 3, 4\}$ for concentrations and flowrates, and with $lp = \{-3, -2, -1, 0\}$ for concentrations and separation efficiencies have lead to reaching optimality gaps 0% for $P1$ and $P2$ and no further refinement was necessary. The conclusion applied to both case studies.

5. Computational results

The developed MINLP and pMINLP models have been tested on various solvers while the MILFP model has been implemented using CPLEX 12.6.3 in GAMS 24.7.1 on a PC with Intel Core *i7* – 3770 CPU 3.40GHz, RAM 16GB. The relative optimal gap has been set to 0 % for models *P0* and *P1*. A 90 % gap has been used for each MILP model, in both loops of the Dinkelbach algorithm, which does not compromise the optimality of the final solution, unless larger than 100 % gap is used (Liu et al., 2014). Additionally, for solving the MINLP and pMINLP models, besides lower and upper bounds on the operating conditions, physicochemical properties, flowrates and concentrations, initialisation points have also been provided.

5.1. Seawater desalination results

First, the performance of the proposed models with respect to their computational statistics and objective function is investigated. Then, the flowsheet configurations, and cost breakdown analysis and comparison are performed relative to each model and common industrial practices.

5.1.1. Computational statistics

Several deterministic non-linear solvers have been used for models *P0* and *P1*. A time limit of 10,000 s has been set for all of them. From Table 7, it can be observed that ANTIGONE returns a solution within 120 s for *P0* and 1,499 s for *P1*. Despite the computational advantage of *P0*, the solver terminates at 58 % relative gap thus, not being able to solve the model to global optimality. On the contrary, the best possible solution for *P1* is US\$ 0.7346/m³ which coincides with the best feasible solution returned. As shown in Table 7, ANTIGONE demonstrates overall better results with significantly lower CPU times than BARON. Although BARON finds the best optimal solution for the MINLP model, its solution deteriorates for the pMINLP model. The former solution is found at CPU time 632 s corresponding to a 0.004 % gap which did not improve by the end of the resource limit time. However, a complete convergence does not occur within the assigned resource limit. The pMINLP model terminates at a gap of 50 % and an objective function of US\$1.0588/m³ is returned. SCIP, DICOPT and SBB do not provide any feasible integer solution for any of the two non-linear models within the time limit. The post-processing of the results is a necessary step to obtain a corrected result of the linearisations and approximations made in *P1* and *P2*. For the pMINLP model, post-processing is performed with the same solver that is implemented in the optimisation runs, whereas for the MILFP model, ANTIGONE was used.

The models statistics of the seawater desalination case study are also given in Table 7. It can further be concluded from the table that all the implemented reformulations in *P2* have lead to almost 24 times larger model size than *P0*. Although the number of equations and variables increase with the models, it can be observed the solution improves with ANTIGONE. Compared to *P1*, *P0* returns results one order of magnitude as fast, at the expense of a worse solution. The post-processed results for *P1* and *P2* prove a better solution exists which is 11 % better than the solution in *P0*. Furthermore, the implemented approximations have translated in a tight difference, i.e. 0.4 % from the real solutions. From the table it becomes ostensible that model *P2* has the upper

Table 7: Computational statistics and comparative results of seawater desalination example

	MINLP model	pMINLP model	MILFP model
Discrete variables	96	18,780	27,243
Continuous variables	1,237	23,239	31,295
Equations	1,673	28,217	39,992
Solvers	Objective function [US\$/m ³] (CPU time)		
Antigone	0.8363 (120s)	0.7346* (1,499s)	-
Baron	0.7346 (10,000s)	1.0588* (10,000s)	-
Cplex	-	-	0.7346* (388s)

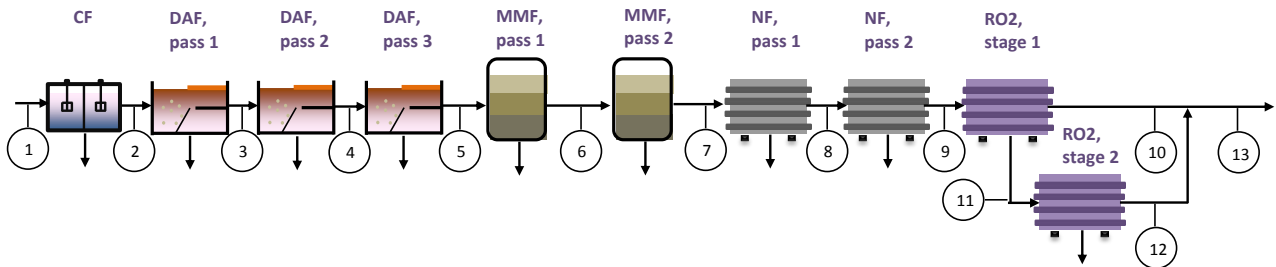
* after post-processing results with MINLP

hand in the trade-off between computational times and objective function, with respect to the rest of the models. The reported solution for MILFP at optimal gap 90 % translated to 3 iterations for the first loop and 4 iterations for the second one.

The flowsheet configurations and cost comparisons in the following sections are presented based on the solutions reported by ANTIGONE of $P0$ and $P1$, and the post-processed results of $P1$ and $P2$.

5.1.2. Flowsheet configurations

The flowsheet configurations for the proposed models are depicted in Fig. 7 and Fig. 8. The conceptual design for the MINLP model contains one CF, three DAF chambers in series, two passes MMF, two passes NF and one-pass, two-stage RO system. The choice for conventional technologies in pre-treatment with a sequence of coagulation-flocculation and dissolved air flotation is one of the typical possible combinations in practice. Globally, DAF and UF have an installed capacity of 19 % while MMF's installed capacity accounts for 49 % (DesalData, 2014). The second stage in the reverse osmosis configuration contributes to the higher overall recovery of the flowsheet, i.e. 39 %, which is slightly lower than in existing desalination plants. The total number of units is 10, which is the maximum allowed number of units, i.e. the constraint is active. The final purity of the product is 1.000 mg/L TSS, 600 mg/L TDS and 0.799 mg/L boron thus, meeting drinking water requirements. The full concentrations and flowrates profiles of the flowsheet in Fig. 7 are shown in Table 8.

Figure 7: Optimal flowsheet configuration for $P0$ model for seawater desalination case study

Since the same objective function was observed for $P1$ and $P2$, their technology selection is also the same,

Table 8: Concentration and flowrate profiles for *P0* model for seawater desalination case study

Stream	Concentrations			Flowrates
	TSS [mg/L]	TDS [g/L]	B [mg/L]	[m ³ /h]
1	30.00	40.00	5.00	55,000
2	30.00	40.00	5.00	55,000
3	21.21	40.40	5.05	54,450
4	12.34	40.81	5.10	53,906
5	3.37	41.22	5.15	53,366
6	1.14	43.39	5.42	50,698
7	0.45	45.68	5.71	48,163
8	0.56	4.12	7.14	38,531
9	0.69	0.42	8.92	30,824
10	1.55	0.93	0.78	13,871
11	-	-	15.58	16,953
12	-	-	0.83	7,629
13	1.00	0.60	0.79	21,500

hence, presented in a common figure. In Fig. 8, the flowsheet consists of three UF passes, two NF passes and one - pass, three - stage RO system. Although, solely 1 % of desalination worldwide is performed by NF, it has been gaining more interest recently due to lower operating costs and higher yield (DesalData, 2014). Therefore, the flowsheet has kept the selection of TDS removal system from *P0*. The selection of a three - stage configuration for the RO system has been a preferred choice in order to increase the productivity of the plant and therefore, decrease the cost. With this configuration, the plant is capable of producing 25,158 m³/h, i.e. circa 46 % total recovery, which means 7 % improvement compared to the recovery for the flowsheet in Fig. 7. The water quality of the effluent is 0.40 mg/L TSS, 600 mg/L TDS and 0.29 mg/L boron for *P1* and 0.40 mg/L TSS, 600 mg/L TDS and 0.61 mg/L boron for *P2*. The discrepancy in the boron concentrations come from the different pH selected for stage 2 of the reverse osmosis. The pH is not reflected in the operating cost therefore, it affects only the rejection. In Table 9 all the concentrations and flowrates of the flowsheet in Fig. 8 are listed.

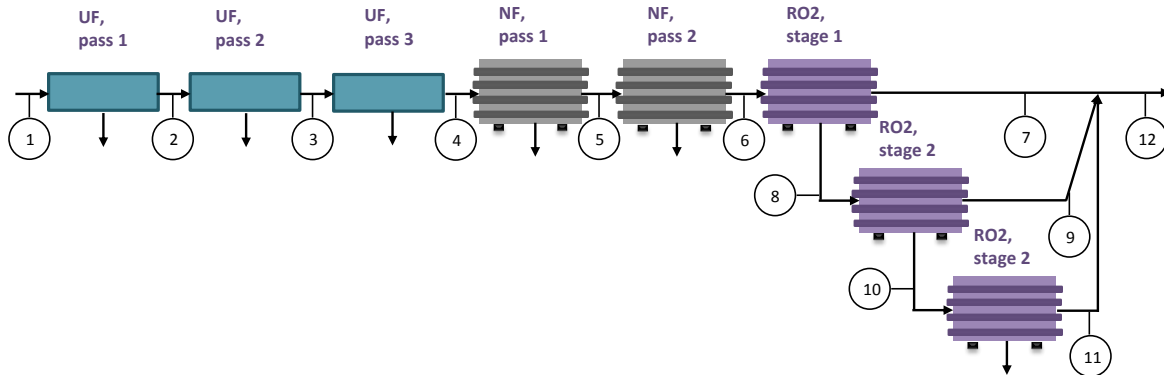


Figure 8: Optimal flowsheet configuration for *P1* and *P2* models for seawater desalination case study

Table 9: Concentration and flowrate profiles for *P1* and *P2* models for seawater desalination case study

Stream	pMINLP model				MILFP model			
	Concentrations			Flowrates [m ³ /h]	Concentrations			Flowrates [m ³ /h]
	TSS [mg/L]	TDS [g/L]	B [mg/L]		TSS [mg/L]	TDS [g/L]	B [mg/L]	
1	30.00	40.00	5.00	55,000	30.00	40.00	5.00	55,000
2	5.76	42.07	5.26	52,250	5.76	42.07	5.26	52,250
3	1.11	44.27	5.54	49,638	1.11	44.27	5.54	49,638
4	0.21	46.65	5.83	47,156	0.21	46.65	5.83	47,156
5	0.27	4.20	7.28	37,725	0.27	4.20	7.28	37,725
6	0.33	0.50	9.11	30,180	0.33	0.50	9.11	30,180
7	0.74	1.12	0.18	13,580	0.74	1.11	0.18	13,580
8	-	-	16.42	16,599	-	-	16.42	16,599
9	-	-	0.32	7,470	-	-	1.44	7,470
10	-	-	29.68	9,129	-	-	28.68	9,129
11	-	-	0.57	4,108	-	-	0.55	4,108
12	0.40	0.60	0.29	25,158	0.40	0.60	0.61	25,158

5.1.3. Costing comparisons

The cost breakdown differences in the MINLP model, and the pMINLP and MILFP models are disclosed in Fig. 9 where every cost component is represented as a percentage of the cost per water volume produced. Included in the cost breakdown are the annual labour, power, capital, replacement, chemical for treatment and conditioning, and post-treatment chemical costs. The lower number of units in models *P1* and *P2* contribute to capital cost representing 30 % of the total cost compared to a capital cost share of 35 % for *P0*. Typical ranges of capital costs are between 30 % and 40 % of the total cost for seawater desalination facilities. The elevated percentage of power cost for *P1* and *P2* with respect to *P0* is due to the higher number of RO units selected, which overall contribute to a lower water net cost. Approximately 13 % of running costs is for maintenance and consumables which is also observed for all of the presented models and is comparable to the lower range of operating and maintenance costs in existing practices (Voutchkov, 2013).

5.1.4. Comparisons with existing plants

According to the International Water Association (IWA), seawater desalination water net cost lies between US\$0.5/m³ and US\$3.0/m³ (Lazarova et al., 2012). Furthermore, this range coincides with the range reported by Voutchkov (2013). The optimal solution returned by ANTIGONE and CPLEX is US\$0.7346/m³ and consequently, the result falls into the suggested limits. Kurnell and Victorian desalination plants in New South Wales and Victoria, for instance, produce at maximum 500,000 m³/d and 550,000 m³/d at respective costs US\$1.75/m³ and US\$1.78/m³ (UNESCO Centre for Membrane Science and Technology, 2008). In comparison, the production rate of the best optimal solution obtained from pMINLP and MINLP models is around 600,000 m³/d with 60 % lower cost.

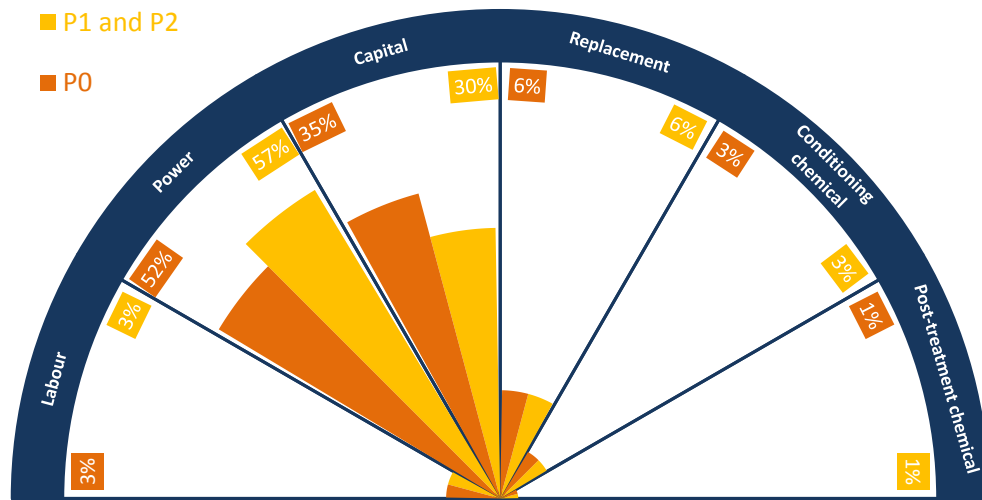


Figure 9: Cost breakdown comparison among proposed models for seawater desalination case study

5.2. Surface water treatment results

5.2.1. Computational statistics

460 The models statistics and comparative results of the surface water treatment case study are shown in Table 10.

Table 10: Computational statistics and comparative results of surface water treatment example

	MINLP model	pMINLP model	MILFP model
Discrete variables	87	16,305	23,568
Continuous variables	1,117	20,230	26,640
Equations	1,652	24,695	34,790
Solvers	Objective function [US\$/m³] (CPU time)		
Antigone	0.5346 (160s)	0.1888* (466s)	-
Baron	No solution (10,000s)	0.1888* (3,946s)	-
Cplex	-	-	0.1888* (138s)

* after post-processing results with MINLP

As in case study 1, a similar trend of ANTIGONE's performance over $P0$ and $P1$ is observed for case study 2. The solver returns a solution three times faster but with a worse result of US\$ 0.5346/m³ and a termination relative gap of 72 %. For $P1$ that gap approaches 0 and therefore, the best possible solution is US\$ 0.1888/m³. 465 Unlike ANTIGONE, BARON fails to return a solution for $P0$. It can be observed, however, both ANTIGONE and BARON perform equally well and obtain the same results for $P1$. Yet, ANTIGONE outperforms BARON with CPU times 90 % lower. SCIP, DICOPT and SBB do not provide any feasible integer solution for any of the two non-linear models within the time limit.

Models $P1$ and $P2$ returned the same solution of US\$0.1870/m³ which has been corrected by post-processing

those results to US\$0.1888/ m^3 , meaning only approximately 0.5 % has been the underestimation in the objective function. On the other hand, the improvement from the MINLP model is more than twofold. The best trade-off between CPU times and obtained solution is seen in the MILFP model which is an order of magnitude faster than model $P1$. The reported solution for MILFP at optimal gap 90 % translated to 4 iterations in the first loop and 3 iterations in the second loop. Overall, the results from the surface water treatment case study follow the same trends as the results from seawater desalination case study.

The flowsheet configurations and cost comparisons are presented based on the solutions reported by ANTIGONE of $P0$ and $P1$, and the post-processed results of $P1$ and $P2$.

5.2.2. Flowsheet configurations

The locally optimal solution for $P0$ translates into a technology configuration (Fig. 10) of two CF chambers in series, one pass MMF, three MF passes, two UF passes and a one-pass, two-stage RO system. The design is capable of an hourly production rate of 12,104 m^3/h . The final concentrations of COD, TSS and TDS are, respectively, 4.08 mg/L, 1.00 mg/L and 275 mg/L thus, meeting drinking water requirements. Additionally, the maximum allowable number of technologies is reached. In practice, drinking water treatment plants have less complicated flowsheet design than the one illustrated in the figure. Table 11 displays the concentrations and flowrates profiles of the flowsheet in Fig. 10.

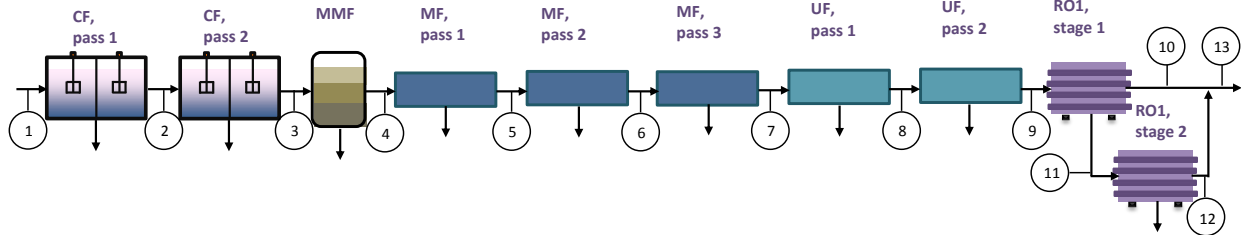


Figure 10: Optimal flowsheet configuration for $P0$ model for surface water treatment case study

The flowsheet configuration of $P1$ and $P2$, like in the seawater desalination case study, is the same and shown in Fig. 11. The sequence of technologies is with three UF passes and one NF pass. This flowsheet is capable of producing 13,71 m^3/h and potable water with COD, TSS and TDS specifications 4.05 mg/L, 0.885 mg/L and 600 mg/L for $P1$ and 5.0 mg/L, 0.885 mg/L and 600 mg/L for $P2$ (see Table 12). The discrepancy in the COD concentrations arises from the different values for molecular weight cut-off of nanofiltration, in $P1$ $MWCO = 300$ Da and in $P2$ $MWCO = 372$ Da. Molecular weight cut-off, like pH, is also not expressed in the operating costs, hence, differences are plausible.

5.2.3. Costing comparisons

The costs breakdown and comparisons for $P0$, and $P1$ and $P2$ are manifested in Fig. 12. Unlike for seawater desalination, surface water treatment capital costs in general take a more considerable fraction from the total

Table 11: Concentration and flowrate profiles for *P0* model for surface water treatment case study

Stream	Concentrations			Flowrates
	COD [mg/L]	TSS [mg/L]	TDS [g/L]	[m ³ /h]
1	30.00	100.00	4.00	20,000
2	21.21	99.99	4.04	19,800
3	12.34	99.99	4.08	19,602
4	12.98	52.98	4.30	18,622
5	9.21	39.92	4.52	17,691
6	6.54	30.16	4.76	16,806
7	4.65	22.79	5.01	15,966
8	3.99	4.38	5.27	15,168
9	3.43	0.84	5.55	14,409
10	5.72	1.40	0.19	8,646
11	-	-	13.59	5,764
12	-	-	0.48	3,458
13	4.08	1.00	0.27	12,104

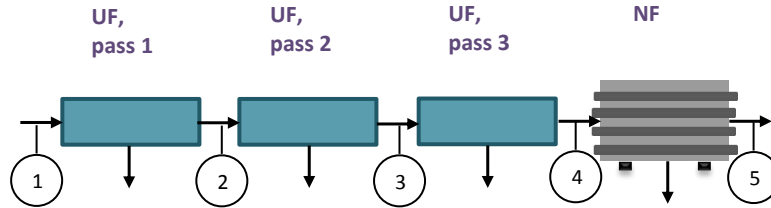


Figure 11: Optimal flowsheet configuration for *P1* and *P2* models for surface water treatment case study

costs. Opposed to capital costs, power expenses percentage is lower. The commonly involved lower and upper percentages for power costs in industry are 10 % and 22 % and it can be deduced both of the values in the figure fall in the interval. Mixing and pumping account for 37 % in *P0* and pumping represents 16% of the total cost in *P1* and *P2*, which falls in the reported range. In practice, low salinity plants exhibit capital cost fraction between 0.4 and 0.6 (Voutchkov, 2013). All of the models have a capital cost percentage in the middle of the range. Ongoing costs to total cost ratio is higher (8 % - 22 %) in water treatment plants due to the chemicals usage for removal of COD and TSS. The increase of conditioning chemical from *P0* to *P1* and *P2* can be explained with the lower unit number and higher effluent, therefore, greater amount of chemicals used.

5.2.4. Comparisons with existing plants

The production cost of drinking water from surface water is situated at the lower end of brackish water treatment processes costs. Ben Aim (2013) reported costs between US\$0.2/m³ and US\$0.3/m³ whereas Voutchkov (2013) gave a range of US\$0.2/m³ - US\$0.4/m³. For the minimisation problem we are considering, the water net cost of the improved formulations is US\$0.188/m³. The results are in proximity of the lower end of the reported

Table 12: Concentration and flowrate profiles for *P1* and *P2* models for surface water treatment case study

Stream	pMINLP model				MILFP model			
	Concentrations			Flowrates [m ³ /h]	Concentrations			Flowrates [m ³ /h]
	COD [mg/L]	TSS [mg/L]	TDS [g/L]		COD [mg/L]	TSS [mg/L]	TDS [g/L]	
1	30.00	100.00	4.00	20,000	30.00	100.00	4.00	20,000
2	25.78	19.20	4.21	19,000	25.78	19.20	4.21	19,000
3	22.15	3.69	4.43	18,050	22.15	3.69	4.43	18,050
4	19.04	0.71	4.67	17,148	19.04	0.71	4.67	17,148
5	4.05	0.89	0.60	13,718	5.00	0.89	0.60	13,718

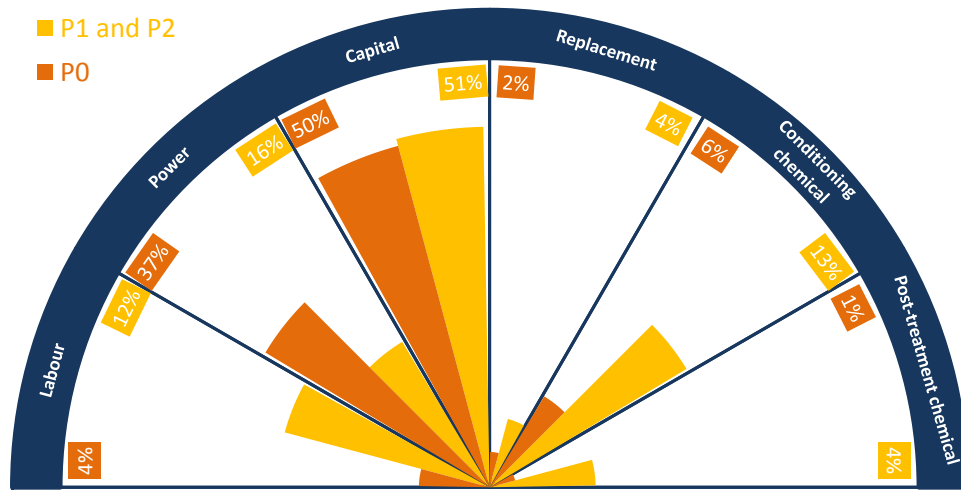


Figure 12: Cost breakdown comparison among proposed models for surface water treatment case study

ranges and thus, show conformity with existing practices.

6. Concluding remarks

In this work, optimisation-based frameworks for the synthesis of water treatment processes have been proposed. First, the MINLP model has been developed to minimise water net cost. The large number of non-linearities compromised the stability of the model by using various commercial MINLP solvers, which either obtained local optimum or even failed to return a feasible solution. To overcome the difficulties, key bilinear terms and non-linear functions have then been reformulated, and the pMINLP model has been introduced. Finally, the MILFP model has been proposed, which includes further discretisations of continuous domains together with a two-step iterative solution procedure based on Dinkelbach's algorithm. The applicability of the models has been demonstrated through two case studies: (i) seawater desalination and (ii) surface water treatment, both for the production of drinking water. The solutions obtained are in a good agreement with existing industrial practices. Comparing the results among the proposed approaches, it can be concluded the proposed MILFP model performs most efficiently

in obtaining the best solution with shorter computational times.

Acknowledgements

The authors would like to acknowledge the financial support of BHP Billiton.

Appendix A. Notations

525 Nomenclature

Indices

c contaminants

i passes

j discretisation points

530 l positions in multiparametric disaggregation

m positions in piecewise approximation with a final position M^{max}

q parallel technologies for CLR

r positions in piecewise reformulation

s stages

535 t technologies

z positions in multiparametric disaggregation

Sets

\bar{I}_q a set of passes and stages of parallel technologies, q , for CLR

CF set of coagulation technologies with operating conditions within a given range

540 CLR clarification processes representative

CT_t a set of contaminants processed by technology t

I_t a set of passes and stages of technology t with a final pass, I_t^{max}

J_t a set of discrete levels for operating conditions of technology t

MF set of microfiltration technologies with operating conditions within a given range

545 MMF set of multi-media filtration technologies with operating conditions within a given range

NF set of nanofiltration technologies with operating conditions within a given range

$RO1$ set of reverse osmosis technologies with operating conditions within a given range to remove dissolved solids

$RO2$ set of coagulation technologies with operating conditions within a given range to remove boron

550 $TCLR$ clarification processes SED and DAF

TMM membrane processes

$TMMB$ filtration processes

UF set of ultrafiltration technologies with operating conditions within a given range processes

Parameters

555 \bar{p}_{qj} operating pressure at discrete level j for technology q , [MPa]

\bar{y}_{qis} recovery factor of technology q , pass i and stage s , $[-]$

$\hat{Y}_{t isr}$ clarification technologies' recovery at discrete level r , $[-]$

μ viscosity of water source, $[\text{kg}/\text{m} \cdot \text{s}]$

A_q parameter associated with the capital cost of technology q , $[-]$

560 A_t parameter associated with the capital cost of technology t , $[-]$

α_f^{MRC} constant accounting for annualisation for equipment replacement

b_q parameter associated with the capital cost of technology q , $[-]$

b_t parameter associated with the capital cost of technology t , $[-]$

c^{chem} coagulant price, $[\$/\text{t}]$

565 c^E electricity charge, $[\$/\text{kWh}]$

c_c^{IN} initial feed concentration of contaminant c , $[\text{mg}/\text{L}]$

cco_{tism}^{bp} capital cost at point m for unit belonging to technology t , pass i and stage s in piecewise linearisation, $[\$]$

cd_{tj} coagulant dose at discrete level j for technology t , $[\text{mg}/\text{L}]$

570 CRF capital recovery factor, $[-]$

cv^{CHC} a conversion factor for the coagulant costs, $[-]$

cv^{EM} a conversion factor for the electrical mixing costs, $[-]$

cv^{PC} a conversion factor for the pumping costs, $[-]$

cv^{SC} a conversion factor for the saturator costs, $[-]$

575 d_{tj}^{MED} media diameter of multi-stage media filtration at discrete level j for technology t , $[m]$

gf_{tj} flocculation energy input at discrete level j for technology t , $[s^{-1}]$

$infl_q$ inflation rate for clarification technologies, $[-]$

$infl_t$ inflation rate, $[-]$

ir interest rate, $[-]$

580 l_{tj} length of the filter in multi-stage media filtration at discrete level j for technology t , $[m]$

$lc1$ constant associated with labour cost, $[-]$

$lc2$ constant associated with labour cost, $[-]$

ld_{tj} load to the multi-stage media filtration at discrete level j for technology t , $[m/s]$

M_c^{BIG} big number for contaminant c , $[mg/L]$

585 M^{CD} big number for coagulant cost, $[\$/h]$

M_c^{CONC} maximum allowable concentration of a contaminant c , $[mg/L]$

M^{FLOW} minimum allowable final effluent from technology t , $[m^3/h]$

M^P big number for pumping pressure, $[MPa]$

M^{TG} big number for energy input and time, $[-]$

590 $mwco_{tj}$ molecular weight cut-off at discrete level j for technology t , $[Da]$

N^{max} maximum allowable number of passes, $[-]$

p_{tj} operating pressure at discrete level j for technology t , $[MPa]$

ph_{tj} hydrogen ion concentration at discrete level j for technology t , $[-]$

py annual production yield, $[-]$

595 Q^{IN} initial feed flowrate, $[m^3/h]$

q_{tism}^{pbp} product flowrate at point m for unit belonging to technology t , pass i and stage s in piecewise linearisation, $[\$]$

r^{ch} cost of treatment and post-treatment chemicals per volume of produced water, [\$/m³]

r_{tcj} rejection coefficient of a contaminant c at discrete level j for technology t , [—]

600 rc_t^M equipment replacement price for technology t per produced permeate, [\$/m³]

rq_{tqcj} clarification technologies' rejection coefficients of a contaminant c at discrete level j , [—]

t_d number of operating days a year, [d/y]

t_h number of operating hours a day, [h/d]

tem_{tj} operating temperature at discrete level j for technology t , [°C]

605 tf_{tj} flocculation time at discrete level j for technology t , [min]

U_t^{BIG} big number for capital costs, [\$]

y_{tis} recovery factor of technology t , pass i and stage s , [—]

yr years of investment, [—]

η_t^{FP} pump efficiency, [—]

610 η_t^{MT} motor efficiency, [—]

η^{SAT} saturator efficiency, [—]

π the ratio of a circle's circumference to its diameter, [—]

h_{tj} natural logarithm of component hydrophobicity at discrete level j for technology t , [—]

Binary variables

615 E_{tis} binary variable equal to 1 if technology t , pass i and stage s is selected, otherwise equal to 0, [—]

W_{tisj} binary variable equal to 1 if level j of technology t , pass i and stage s is selected, otherwise equal to 0, [—]

W_{qtqisj} binary variable equal to 1 if level j of technology q , pass i and stage s is selected, otherwise equal to 0, [—]

620 X_{qis} binary variable equal to 1 if technology q , pass i and stage s is selected, otherwise equal to 0, [—]

Y_{tism}^m binary variable equal to 1 if position m of technology t , pass i and stage s is selected, otherwise equal to 0, [—]

zc_{tisckl} binary variable equal to 1 if for technology t , pass i and stage s a number k and for power l is selected for concentrate, otherwise equal to 0, [—]

625 $z_{f_{tiskl}}$ binary variable equal to 1 if for technology t , pass i and stage s a number k and for power l is selected for feed, otherwise equal to 0, $[-]$

$z_{o_{ckl}}$ binary variable equal to 1 if a number k for power l is selected in effluent, otherwise equal to 0, $[-]$

$z_{p_{tiskl}}$ binary variable equal to 1 if for technology t , pass i and stage s a number k and for power l is selected for permeate, otherwise equal to 0, $[-]$

630 $z_{r_{tiskz}}$ binary variable equal to 1 if for technology t , pass i and stage s a number k and for power l is selected for separation efficiency and concentration disaggregation, otherwise equal to 0, $[-]$

$z_{y_{tistr}}$ binary variable equal for the reformulation of flowrate and recovery for clarification technologies, otherwise equal to 0, $[-]$

Continuous variables

635 $\bar{C}out_{ck}$ auxiliary variable for effluent concentration for digit k , $[mg/L]$

$\bar{C}R_{tisk}^F$ auxiliary variable for feed concentration for technology t , pass i , stage s and digit k , $[mg/L]$

\bar{C}_{tisk}^C auxiliary variable for concentrate concentration for technology t , pass i , stage s and digit k , $[mg/L]$

\bar{C}_{tisk}^F auxiliary variable for feed concentration for technology t , pass i , stage s and digit k , $[mg/L]$

\bar{C}_{tisk}^P auxiliary variable for permeate concentration for technology t , pass i , stage s and digit k , $[mg/L]$

640 \bar{P}_{qis} operating pressure of unit q , pass i and stage s , $[MPa]$

\bar{Q}_{tistr}^F auxiliary variable for feed flow for technology t , pass i , stage s , $[m^3/h]$

\bar{R}_{qisc} clarification technologies' rejection coefficients of a contaminant c in technology s and pass i , $[-]$

\bar{Y}_{tis} recovery factor for CLR in MILFP model, $[-]$

$\bar{z}_{c_{tisk}}$ continuous variable for disaggregation, $[-]$

645 $\bar{z}_{f_{tisk}}$ continuous variable for disaggregation, $[-]$

$\bar{z}_{o_{ck}}$ continuous variable for disaggregation, $[-]$

$\bar{z}_{p_{tisk}}$ continuous variable for disaggregation $[-]$

$\bar{z}_{r_{tisk}}$ continuous variable for disaggregation, $[-]$

$\hat{C}out_{ckl}$ auxiliary variable for effluent concentration for digit k and point l , $[mg/L]$

650 $\hat{C}R_{tiskz}^F$ auxiliary variable for feed concentration for technology t , pass i , stage s , digit k and point z , $[mg/L]$

\hat{C}_{tiskl}^C auxiliary variable for concentrate concentration for technology t , pass i , stage s , digit k and point l , [mg/L]

\hat{C}_{tiskl}^F auxiliary variable for feed concentration for technology t , pass i , stage s , digit k and point l , [mg/L]

\hat{C}_{tiskl}^P auxiliary variable for permeate concentration for technology t , pass i , stage s , digit k and point l , [mg/L]

655 C_{tisc}^C concentrate concentration of contaminant c from technology t , pass i and stage s , [mg/L]

C_{tisc}^F feed concentration of contaminant c to technology t , pass i and stage s , [mg/L]

C_{tisc}^P permeate concentration of contaminant c from technology t , pass i and stage s , [mg/L]

C_{tisc}^W concentration to waste of contaminant c from technology t , pass i and stage s , [mg/L]

CC_{tis} capital cost for unit belonging to technology t , pass i and stage s , [\$]

660 $CCol_{tis}$ capital cost for unit belonging to technology t , pass i and stage s in piecewise linearisation, [\$]

CD_{tis} coagulant dose of technology t , pass i and stage s , [mg/L]

CHC_{tis} coagulant cost for technology t , pass i and stage s , [\$/y]

$ChemC$ chemical cost for pH adjustment and post-treatment, [\$/y]

$Cout_c$ final purity for contaminant c , [mg/L]

665 CQ_{tisc}^C continuous variable representing multiplication of concentrate concentration and flowrate to a technology t , pass i and stage s , [g/h]

CQ_{tisc}^F continuous variable representing multiplication of feed concentration and flowrate to a technology t , pass i and stage s , [g/h]

670 CQ_{tisc}^P continuous variable representing multiplication of permeate concentration and flowrate from a technology t , pass i and stage s , [g/h]

$CQout_c$ continuous variable representing multiplication of concentrate concentration and flowrate to a technology t , pass i and stage s , [g/h]

CR_{tisc}^F continuous variable representing multiplication of separation efficiency and concentration to a technology t , pass i and stage s , [mg/L]

675 D_{tis}^{MED} media diameter of multi-stage media filtration, [m]

EMC_{tis} mixing cost for technology t , pass i and stage s , [\$/y]

G_{tism} continuous variable in piecewise approximation, [—]

Gf_{tis} flocculation energy input of technology t , pass i and stage s , [s^{-1}]

L_{tis} length of the filter in multi-stage media filtration, [m]

680 LC labour cost, [\$/y]

Ld_{tis} load to the multi-stage media filtration, [m/s]

MRC_{tis} replacement cost for technology t , pass i and stage s , [\$/y]

$MWCO_{tis}$ molecular weight cut-off for a membrane in technology t , pass i and stage s , [Da]

P_{tis} operating pressure of unit t , pass i and stage s , [MPa]

685 PC_{tis} pumping cost for technology t , pass i and stage s , [\$/y]

pH_{tis} hydrogen ion concentration in feed to technology t , pass i and stage s , [-]

PP_{tis} physicochemical properties of flow and operating conditions of technology t in pass i and stage s , [-]

Q^{AP} annual production rate, [m^3/y]

Q_{tis}^C concentrate flowrate from technology t , pass i and stage s , [m^3/h]

690 Q_{tis}^{FL} linearised feed flowrate and binary variable, [m^3/h]

Q_{tis}^F feed flowrate to a technology t , pass i and stage s , [m^3/h]

Q_{tis}^P permeate flowrate from technology t , pass i and stage s , [m^3/h]

Q_{tis}^W flowrate to waste from technology t , pass i and stage s , [m^3/h]

695 QCD_{tis} auxiliary variable to represent the multiplication of flowrate and coagulant dosage for a technology t , pass i and stage s , [g/h]

Q_{out} hourly capacity of the plant, [m^3/h]

QPf_{tis} auxiliary variable to represent the multiplication of flowrate and pressure for a technology t , pass i and stage s , [m^3MPa/h]

700 QtG_{tis} auxiliary variable to represent the multiplication of flowrate, flocculation energy input and time for a technology t , pass i and stage s , [m^3/h]

QY_{tis}^F continuous variable representing multiplication of feed flowrate and recovery to a technology t , pass i and stage s , [m^3/h]

R_{isc} rejection coefficient of a contaminant c in technology t , pass i and stage s , [-]

SC_{tis} operating cost for running the saturator in technology t , pass i and stage s , [\$/y]

TC total annualised cost, [\$/yr]

Tem_{tis} operating temperature for technology t , pass i and stage s , [°C]

Tf_{tis} flocculation time of technology t , pass i and stage s , [min]

WNC water net cost, [\$/m³]

H_{tis} natural logarithm of component hydrophobicity of technology t , pass i and stage s , [—]

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