# Optimal design of water treatment processes

**Article** *in* Desalination and water treatment · May 2016

DOI: 10.1080/19443994.2016.1173595

# Optimal Design of Water Treatment Processes

M.N.Koleva[a,b], E.M.Polykarpou[b], S.Liu[a], C.A.Styan[b], L.G.Papageorgiou[a,*]

[a]*Centre for Process Systems Engineering, Dept. of Chemical Engineering, UCL, Torrington Place, London, WC1E 7JE, United Kingdom, e-mails: m.koleva@ucl.ac.uk (M.N. Koleva), s.liu@ucl.ac.uk (S. Liu), Tel: +44(0)20 7679 3836; e-mail: l.papageorgiou@ucl.ac.uk (L.G. Papageorgiou), Tel: +44(0)20 7679 2563*

[b]*School of Energy and Resources, UCL Australia, 220 Victoria Square, Adelaide, South Australia, 5000, Australia, e-mails: eria.polykarpou@gmail.com (E.M. Polykarpou), c.styan@ucl.ac.uk (C.A. Styan), Tel: +61 8 8110 9966*

## Abstract

Predicted water shortages assign water treatment a leading role in improving water resources management. One of the main challenges associated with the processes remains early stage design of techno-economically optimised purification. This work addresses the current gap by undertaking a whole-system approach of flowsheet synthesis for the production of water at desired purity at minimum overall cost. The optimisation problem was formulated as a mixed integer non-linear programming (MINLP) model. Two case studies were presented which incorporated the most common commercial technologies and the major pollution indicators, such as chemical oxygen demand (COD), dissolved organic carbon (DOC), total suspended solids (TSS) and total dissolved solids (TDS). The results were analysed and compared to existing guidelines in order to examine the applicability of the proposed approach.

*Keywords:* water purification; process synthesis; techno-economic performance; optimisation; water production cost

## 1. Introduction

Efficient water treatment is recognised as a major solution to the arising burdens on world water resources [1-4]. However, the process still faces challenges such as producing satisfactorily safe and affordable water [5,6]. Examination of the economically viable purification paths at early design stage can address those challenges [7]. Therefore, there is an increasing interest in developing systematic methods for optimising water separation units and their interconnections [8]. The selection of water technologies, process units and their sequence depends on the influent and effluent characteristics, nature of contaminants and treatment cost [9]. Based on those attributes, water treatment can be classified into a number of applications, such as brackish and seawater desalination, and water and wastewater treatment.

Amongst the existing desalination technologies developed in the last decades, thermal (conventional) and membrane (non-conventional) desalination methods take the upper hand in large-scale plants. The conventional methods are represented by multi-stage flash (MSF), multi-effect distillation (MED) and vapour compression (VP), whereas the commercially available membrane technologies include nanofiltration (NF), reverse osmosis (RO) and electrodialysis (ED) [10]. The selection between conventional and non-conventional treatment depends on technical, economic and geographical attributes [11]. Membrane plants, however, exhibit economic and environmental advantages over thermal plants [12]. Pressure and vacuum-driven membrane processes, in particular, are preferred because of their efficiency and no need of fluid phase change [13]. Further, pretreatment technologies are also divided into conventional and non-conventional. The former group is represented by coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF) and granular or multi-media filtration (MMF), and the latter encompasses microfiltration (MF) and ultrafiltration (UF). Over the last decade, membrane pretreatment technologies have advanced significantly and today they accommodate lower footprint, constant permeate quality in cases of algal blooms, higher retention of organics and reduced chemical consumption [14-16]. Recent statistics disclose approximately 32% and 64% of the world desalination plant capacities are operated on the principle of MF/UF for pretreatment, and NF/RO for desalting, respectively [16].

When inorganic and some organic wastes are treated in wastewater during advanced wastewater treatment, and when contaminants from surface or ground water are removed, physico-chemical process units predominate. Such technologies are coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), media and membrane filters, ion exchange and carbon adsorption units [9,17,18]. As the technologies for the major water purification applications coincide, it can, therefore, be possible to develop an approach, followed by a mathematical model, for the synthesis and optimisation of flowsheets taking into account the aforementioned water sources and technologies. From now on the authors would refer to a collective term of all the purification applications solely as water treatment processes.

Numerous works have been published on the design and optimisation of units and processes from water treatment applications. Voutchkov [19] and Lior [4] reviewed overall design of seawater desalination processes. Non-linear program and mixed integer non-linear program models have been proposed for the design and optimisation of MSF, MED, hybrid MED-RO and RO networks by [20-24]. Spiller et al. [25], Avramenko et al. [26], Tchobanoglous et al. [9], Cheremisinoff [18] published guidelines for the design of water and wastewater treatment plants. Roberts and Inniss [27] experimentally determined the link between source water quality and treatment sequence. Franceschi et al. [28] and Rossini et al. [29] investigated the optimal operation of coagulation-flocculation to handle raw water qualities by numerical methods, taking an iterative approach. Mixed Integer Non-Linear Program (MINLP) methods for the synthesis of water and wastewater networks were also considered in some works [30, 31]. Sweetapple et al. [32] suggested a multi-objective optimisation of wastewater treatment plant to minimise the operating cost, greenhouse gas emissions and effluent contaminants concentrations. The economic appraisal of systems as an essential part of optimisation has been discussed in various publications. For instance, Pickering and Wiesner [33] proposed a cost model for low pressure membrane filtration, Wright and Woods [34] developed a capital cost correlation for UF units, whereas Fuqua et al. [35] published a method for the estimation of RO units. Additionally, Lu et al. [36] suggested an MINLP cost model for RO systems in desalination processes with focus on pumping, and membrane cleaning and replacement. Later a model with multiple feed and multiple product to minimise the total annual cost of the system was introduced [37]. A global strategy for the estimation of water production cost in water and wastewater treatment plants was presented by Kumar et al. [38]. Large scale RO network cost minimisation was performed in the work of Jiang et al. [39] and multi-objective MINLP models for annualised cost and energy consumption were presented in the works of Du et al. [40] and Vince et al. [41]. Research has also focused on mathematical modelling for water network synthesis [42, 43] and wastewater, reclamation water and seawater resources management [44, 45]. Yet the optimal synthesis of the entire water treatment processes has not been explored.

The present work addresses the gap by presenting a systematic approach for the design of water treatment processes, with a particular focus on surface water and advanced wastewater treatment, and brackish and seawater desalination. The problem is formulated as a mixed integer non-linear programming (MINLP) model. The rest of the paper is organised as follows: Section 2 outlines the scope of the problem, followed by the presentation of the mathematical model in Section 3. Next, two theoretical case studies, together with results, computational performance and discussion, are presented in Section 4. Finally, the main conclusions are drawn and further work directions are suggested in Section 5.

## 2. Problem statement

The aim of the current work is to develop a methodology for the generation of a combination of technologies and number of passes that result in the most economically favourable flowsheet design. The proposed model involves 4 major contaminants indicators, i.e. chemical oxygen demand (COD), dissolved organic carbon (DOC), total suspended solids (TSS) and total dissolved solids (TDS). The presence of Boron (B), which is classified as part of the TDS group, requires special considerations, consequently, it is considered separately. The technology candidates studied are 9, namely, 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. A model superstructure including all acceptable technology options and connections is presented in Fig. 1. The dashed line boxes represent the blocks of equipment that are associated with the removal of a group of contaminants. For instance, CF, SED, DAF, MMF, MF and UF remove the suspended solids, whereas NF removes the dissolved solids, and RO removes both, dissolved solids and boron. It is assumed that organic matter can be removed by conventional treatment such as CF, smaller pore – size low filtration membranes, such as UF, and larger pore-size high pressure membrane, such as NF. MMF does not exhibit a molecular weight cut-off for organics, and irreversible fouling is observed on RO membranes, hence, not used for that particular application.

(insert Fig.1)

General heuristics that apply to process synthesis advise removal of unstable materials early, separate most abundant components at first and leave the sturdiest operation for last [46]. In this case, suspended solids can be exposed to shear stresses, break up and consequently, clog the equipment which justifies its removal at first. TDS is the most plentiful contaminant and boron is difficult to separate from water, which assigns them a second and third place in the separation sequence, respectively. Filtration processes units decrease in their molecular weight cut-off, or pore size, from left to right in the above figure in order to prevent fouling.

Having defined the separation requirements, the sequence of the technology candidates in the model is pre-fixed. A candidate, however, can be either selected or bypassed. In the majority of cases, coagulation-flocculation requires a clarification process downstream. Two clarification options are provided, SED and DAF, represented by the collective name CLR. If any of those two processes is selected, a clarification process is selected, too. Whenever a clarification process is chosen, the selection of CF is mandatory. On its own, CF can be selected if the separation is efficient enough. In the current work, the filtration processes are allowed to exist in the flowsheet sequentially, although it is possible to restrict the problem to the selection of one low pressure membrane process, i.e. MF or UF, and one high pressure membrane process, i.e. NF and RO. The decision whether a pass from a technology is singled out or not is represented by one binary variable and as many passes as desired can be assigned to a technology.

The selection of the technologies is based on meeting the regulatory requirements for water plant effluent [47,48] and minimising the water net cost, expressed in $\$/m^3$. For modelling purposes, the following simplifications and assumptions were made:

- rejection coefficients and recoveries are the major technological performance criteria;
- modified regression models return a reliable estimation for the rejection coefficients;
- TDS, TSS and boron are the only contaminant indicators in seawater source whereas COD, DOC, TDS and TSS are the contaminants assumed to be present in secondary wastewater effluent;
- the removal of a non-targeted group of contaminants from a particular technology is considered insignificant;
- the selection of initial removal grids and intake screens are not taken into account in design;
- complete recovery of microfiltration and ultrafiltration filters;

- no fouling and flux decrease take place and therefore, the observed phenomena as a result of those do not apply;
- no system pressure losses;
- replacement and cleaning costing for RO is assumed to apply for MF, UF and NF;
- there are 65 days allocated for major maintenance, i.e. plant shut down;
- social, political and geographical dimensions are excluded from the cost model;
- annual water production and operating expenses remain the same throughout the plant's commercial lifespan;
- no government incentives for the construction and commission of the water treatment facilities is considered;

The overall optimisation problem is stated below.

*Given:*

- major constituent contaminants in source water;
- pool of water treatment technologies;
- a number of passes, or sequential units, from a technology;
- source water intake flowrate;
- key parameters of source water contaminants (e.g. initial concentrations) and key parameters for treatment technologies (e.g. recoveries, saturator, pump and motor efficiencies);
- candidate technologies characteristics ranges (e.g. flocculation time and energy input, coagulant concentrations, operating pressures, influent temperature, hydrophobicity, hydrogen ion concentrations, molecular weight cut-offs);
- cost data (e.g. units upfront costs, chemicals and electricity charges, maintenance and replacement rates, carbon tax rate, work pay rate, interest rate and plant life);

*Determine:*

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

*So as to:*

minimise the water production cost which equals the total annualised cost divided by the annual production rate.

# 3. Problem formulation

## 3.1. *Performance criteria*

The main performance criteria for water technologies are based on the purification standards and productivity that have to be achieved. These depend on the extent to which they reject major contaminants under specific set of conditions, and to which the product volumetric flowrate is recovered from the process.

### *3.1.1. Rejection coefficient*

The main performance criteria for water technologies are based on the purification standards and productivity that have to be achieved. These depend on the extent to which they reject major contaminants under specific set of conditions, and to which the product volumetric flowrate is recovered from the process.

For any separation process, contaminant removal efficiency classifies as an essential performance criterion [49] because it guarantees a product meets its design purity specifications.

The removal efficiency of downstream water purification processes can be measured by removal, rejection, retention or deactivation coefficient as a function of the contaminants physicochemical properties ($PP_{tic}$) (Eq.(1)) such as coagulant concentration, headloss, filtration media dimensions, molecular weight, hydrophobicity, feed temperature, pressure and concentration, technology characteristics, etc. [50-52]. It can take values between 0 and 1 as the former refers to no separation from a targeted contaminant and the latter refers to 100% separation achieved.

$$R_{tic} = f(PP_{tic}) = 1 - \frac{c^{P}_{tic}}{c^{F}_{tic}}, \ \ \forall\, t, i \in I_t, c \in C_t \qquad (1)$$

where $c^{P}_{tic}$ and $c^{F}_{tic}$ are the concentrations of contaminant $c$ in permeate and feed, respectively, associated with a technology, $t$, and its pass, $i$. The removal efficiencies following are represented in the form of regression models based on Analysis of Variance (ANOVA) for each of the considered processes.

The coagulation – flocculation treatment stage removes organic matter under the form of chemical oxygen demand (COD) and dissolved organic carbon (DOC), expressed in the constraints below, developed from findings in literature [53,54].

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

$$R_{tic} = 0.046 \cdot CD_{ti} + 2.915 \cdot pH_{ti} - 0.0003 \cdot CD_{ti}^2 - 0.002 \cdot CD_{ti} \cdot pH_{ti} - 0.235 \cdot pH_{ti}^2 - 9.486, \quad \forall\, t \in CF, i \in I_t, c \in DOC \quad (3)$$

where $CD_{ti}$ and $pH_{ti}$ are the coagulant dose and the hydrogen ion concentration for liquid in pass $i$ from technology $t$. In the presence of organic matter, in literature this step is referred to as enhanced coagulation, which for simplification purposes, is going to be called CF in this work.

In the current model it is assumed the rejection of solids occurs at the clarification stage, i.e. sedimentation or dissolved air flotation. This means that rejection coefficients in the conventional candidates will be affected by the performance of the coagulation-flocculation process. Vlaŝki [55] investigated experimentally the removal efficiency of sedimentation and dissolved air flotation depending on the operating characteristics of the typically preceding coagulation-flocculation process. If a clarification technology, CLR, is selected either SED's or DAF's rejection coefficient, $\bar{R}_{sic}$, will be valid (Eq.(4)).

$$R_{tic} = \sum_{s \in TCLR} \bar{R}_{sic} \cdot X_{si}, \quad \forall\, t \in CLR, i \in I_t, c \in TSS \quad (4)$$

where $X_{si}$ is a binary variable denoting the selection of a clarification technology or not.

It has been then reported that sedimentation is strongly influenced by coagulant dose. After performing a regression analysis on the data provided, the following equation has been obtained:

$$\bar{R}_{sic} = 0.22154 + 0.02516 \cdot CD_{ti}, \quad \forall\, s \in SED, t \in CF, i \in I_t, c \in TSS \quad (5)$$

where $CD_{ti}$ is the amount of coagulant used in the coagulation- flocculation process.

DAF, showed dependence not only on the coagulant dose but also on the detention time and velocity gradient, denoted as $tf_{ti}$ and $Gf_{ti}$, respectively, in Eq.(6).

$$\bar{R}_{sic} = 1.85886 - 0.00807 \cdot CD_{ti} - 0.00083 \cdot Gf_{ti} + 2.47 \cdot tf_{ti} - 0.00247 \cdot P_{si}, \quad \forall\, s \in DAF, t \in CF, i \in I_t, c \in TSS \quad (6)$$

where $P_{si}$ is the pressure of the saturator.

A model developed by The Commonwealth Scientific and Industrial Research Organisation (CSIRO) predicted the initial steady-state removal of TSS in multi-stage media filtration (MMF) [56]. The relationship is shown in Eq.(7).

$$R_{tic} = 0.0298 \cdot D_{ti}^{MED} + 0.171 \cdot Ld_{ti} + 0.206 \cdot L_{ti}^{-1} - 0.245, \quad \forall\, t \in MMF, i \in I_t, c \in TSS \quad (7)$$

where $D_{ti}^{MED}$ designates the diametre of the media, $Ld_{ti}$ is the load to the filtration process, $L_{ti}$ is the length of the filter for MMF and pass $i$.

The separation efficiency of TSS from water by MF is shown in Eq.6 derived from experimental work [57].

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

where $Tem_{ti}$ is the temperature of the influent to technology $t$ and pass $i$, and $P_{ti}$ is the pressure of the feed flowrate. Besides TSS, in the work is reported the separation efficiency of MF from COD, expressed in Eq.(9).

$$R_{tic} = 0.189 + 1.09 \cdot P_{ti}, \quad \forall\, t \in MF, i \in I_t, c \in COD \quad (9)$$

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

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

where the equation has been derived from data obtained from pilot plant experimental work. It has been reported that turbidity and total suspended solids are related [58]. Hence, Eq.(10) can give an approximate estimation of the suspended solids removal in water treatment. The removal characteristics of UF embrace the reduction of COD and DOC, shown in Eq.(11) and Eq.(12) [57, 59].

$$R_{tic} = 0.236 - 0.952 \cdot P_{ti}, \quad \forall\, t \in UF, i \in I_t, c \in COD \quad (11)$$

$$R_{tic} = 1.224 - 0.00011 \cdot MWCO_{ti} + 0.79 \cdot P_{ti}, \ \forall\, t \in UF, i \in I_t, c \in DOC \quad (12)$$

where $MWCO_{ti}$ is the molecular weight cut – off in Daltons.

The performance characteristics of nanofiltration membranes are affected by solute properties, solution pH and membrane characteristics such as pore size, hydrophobicity and surface roughness [60]. Hence, the retention of dissolved uncharged organic compounds for NF can be approximated using contaminants hydrophobicity and molecular weight cut - off. The relation has been reported in literature based on laboratory experiments [61].

$$R_{tic} = (0.057 - 0.007 \cdot H_{ti} - 0.00002 \cdot MWCO_{ti})^2, \ \forall\, t \in NF, i \in I_t, c \in TDS \quad (13)$$

where $H_{ti}$ is the common logarithm of the hydrophobicity. Eq.(14) and Eq.(15) show the retention of COD and DOC, respectively, where both coefficients depend on the membrane molecular weight cut – off and pressure [62].

$$R_{tic} = 1.138 - 0.00096 \cdot MWCO_{ti} + 0.087 \cdot P_{ti}, \ \forall\, t \in NF, i \in I_t, c \in COD \quad (14)$$

$$R_{tic} = 1.029 - 0.00037 \cdot MWCO_{ti} + 0.001 \cdot P_{ti}, \ \forall\, t \in NF, i \in I_t, c \in DOC \quad (15)$$

RO rejection coefficient for salt is presented in Eq.(16) as a function of the operating pressure [63].

$$R_{tic} = 0.890 + 0.340 \cdot P_{ti} - 0.003 \cdot P_{ti}^2, \ \forall\, t \in RO1, i \in I_t, c \in TDS \quad (16)$$

The above equation was derived following a study on ROSA software developed by the Dow Chemical Company [64]. The TDS of interest were composed of $K$, $Na$, $Mg$, $Ca$, $Ba$, $Sr$, $CO_3$, $HCO_3$, $NO_3$, $Cl$, $F$, $SO_4$ and $NH_4$.

Boron (B) removal is identified as one of the main issues in processes where saline water is treated, especially because its concentration in seawater, in particular, is relatively low [65]. Typical water treatment plants with source water containing boron, accommodate an RO pass at an elevated pH, where mainly removal of boron is targeted

[66]. Therefore, its rejection profile is to be considered separately, with an RO unit dedicated to its removal. The regression equation (Eq.(17)) for rejection of boron by a RE4040-SH-module spiral wound RO membrane was derived based on data from literature [67], using ANOVA analysis.

$$R_{tic} = 0.408 + 0.046 \cdot pH_{ti} + 0.03 \cdot P_{ti}, \ \forall\, t \in RO2, i \in I_t, c \in B \tag{17}$$

where $pH_{ti}$ is the alkalinity of the solution to achieve desired separation.

### 3.1.2. *Recovery ratio*

For any process, it is essential to meet the production quantities which depend on the productivity, or recovery, of the system. The recovery ratio is defined as the fraction of product water that has passed through the process unit from the overall feed. As a fraction, it takes values between 0 and 1. Over a technology and pass, it can be expressed by Eq.(18).

$$Y_{ti} = \frac{Q_{ti}^{P}}{Q_{ti}^{F}}, \ \forall\, t, i \in I_t \tag{18}$$

where $Q_{ti}^{P}$ and $Q_{ti}^{F}$ are the permeate and feed flowrates, respectively, associated with a technology $t$ and pass $i$.

The recovery is a function of the salinity of the feed water, system pressure and scaling potential [65]. However, in this work the recoveries for every different technology are assumed to take values recommended in literature and therefore, are modelled as parameters.

## ***3.2. Mass balance constraints***

### 3.2.1. *Concentration constraints*

The set of equations below determines the contaminants concentration profile throughout the separation process. When a technology, $t$, and a pass, $i$, are selected, the binary variable, $W_{ti} = 1$, and the contaminant is reduced, starting from an initial feed concentration, $c_c^{IN}$. Eq.(19) estimates the contaminant concentration after the first selected process pass, i.e. the concentration in the permeate. Every consequent concentration reduction is calculated by Eq.(20). Eq.(21) and Eq.(22) show the interconnection between two potential candidate passes and technologies.

$$c_{tic}^{P} = c_{c}^{IN} \cdot (1 - R_{tic}) \cdot W_{ti} + c_{c}^{IN} \cdot (1 - W_{ti}), \ \forall \, t \in CF, i = 1, c \tag{19}$$

$$c_{tic}^{P} = c_{tic}^{F} \cdot (1 - R_{tic}) \cdot W_{ti} + c_{tic}^{F} \cdot (1 - W_{ti}), \ \forall \, t, i \in \hat{I}_{t}, c \tag{20}$$

$$c_{t,i-1,c}^{P} = c_{tic}^{F}, \ \forall \, t, i \in I_{t}, i > 1, c \tag{21}$$

$$c_{t-1,i,c}^{P} = c_{tjc}^{F}, \ \forall \, t > 1, i = I_{t}^{max}, j = 1, c \tag{22}$$

A similar formulation is implemented in previous works in applications for chromatography processes [68, 69].

A schematic representation of the connections between two candidates is depicted in Fig. 2.

(insert Fig. 2)

### 3.2.2. Flowrate constraints

Similarly, the flowrate constraints are formulated. When a candidate is selected, the permeate is calculated using Eq.(18). Otherwise it takes the value of the feed. Eq.(23) gives the initial mass balances starting from initial flowrate, $Q^{IN}$, and every consequent permeate is estimated from Eq.(24).

$$Q_{ti}^{P} = Q^{IN} \cdot Y_{ti} \cdot W_{ti} + Q^{IN} \cdot (1 - W_{ti}), \ \forall \, t \in CF, i = 1 \tag{23}$$

$$Q_{ti}^{P} = Q_{ti}^{F} \cdot Y_{ti} \cdot W_{ti} + Q_{ti}^{F} \cdot (1 - W_{ti}), \ \forall \, t, i \in \hat{I}_{t} \tag{24}$$

where $Y_{ti}$ is the recovery of a technology $t$ from pass $i$. The clarification technology takes either the recovery value of sedimentation or the recovery value of dissolved air flotation, shown in Eq.(25).

$$Q_{ti}^{P} = Q_{ti}^{F} \cdot \sum_{s \in TCLR} \bar{Y}_{si} \cdot X_{si} + Q_{ti}^{F} \cdot \left(1 - \sum_{s \in TCLR} X_{si}\right), \ \forall \, t \in CLR, i \in \bar{I}_{s} \tag{25}$$

The principles of designing the interconnections, whether a technology is selected or not, are formulated below.

$$Q^{P}_{t,i-1} = Q^{F}_{ti}, \ \forall\, t, i \in I_t, i > 1 \tag{26}$$

$$Q^{P}_{t-1,i} = Q^{F}_{tj}, \ \forall\, t > 1, i = I^{max}_t, j = 1 \tag{27}$$

The effluent is governed by the number of passes for a particular technology. The feed and permeate flowrates are modelled to present single-stage, multiple-pass system over each pass.

The annual production rate of the facility is then modelled by Eq.(28).

$$Q^{AP} = t_h \cdot t_d \cdot PY \cdot Q^{P}_{ti}, \ \forall\, t = T, i = I^{max}_t \tag{28}$$

where $t_h$ and $t_d$ are the respective operating hours per day and days per year. $PY$ is the production yield of the facility, taking the value of a fraction of the total annual production capacity.

### 3.3. Target constraints

The final water purity should satisfy the conditions imposed by the following constraint:

$$c^{P}_{tic} \le M^{conc}_c, \ \forall\, t \in RO2, i = I^{max}_t, c \tag{29}$$

where $M^{conc}_c$ is the maximum allowable concentration of a contaminant. Depending on the process application, the final required concentration can take different values. An additional constraint for the minimum effluent at the final stage is enforced by Eq.(30).

$$Q^{P}_{ti} \ge M^{FLOW}, \ \forall\, t \in RO2, i = I^{max}_t \tag{30}$$

where $M^{FLOW}$ is the minimum allowable effluent flow. This constraint allows us to ensure a minimum plant capacity is met.

### 3.4. Logical constraints

The overall number of the selected passes and technologies should not be greater than a number, $N_{max}$, which is modelled by Eq.(31).

$$\sum_{t}\sum_{i \in I_t} W_{ti} \le N_{max} \tag{31}$$

Eq.(32) is a logical condition that does not allow the selection of any pass if the previous one has not been chosen.

$$W_{t,i+1} \le W_{ti}, \quad \forall\, t, i \in I_t, i+1 \in I_t \tag{32}$$

The clarification processes, sedimentation and dissolved air flotation, have to be chosen together with the chemical treatment, coagulation-flocculation. Hence, Eq.(33) applies:

$$\sum_{i \in I_s} X_{si} \le U \cdot \sum_{i \in I_t} W_{ti}, \quad \forall\, s \in TCLR, t \in CF \tag{33}$$

where $U$ is a big number that takes the maximum number of allowed passes per technology.

Only one of the clarification processes can be chosen at a time, a condition expressed by Eq.(34).

$$\sum_{s \in TCLR} X_{si} \le W_{ti}, \quad \forall\, t \in CLR, i \in I_t \tag{34}$$

The same condition as in Eq.(31) is introduced for the clarification technologies.

$$X_{s,i+1} \le X_{si}, \quad \forall\, t, i \in \bar{I}_s, i+1 \in \bar{I}_s \tag{35}$$

### *3.5. Cost constraints*

Defining water treatment costs at a preliminary stage often proves intricate due to the numerous factors participating in their estimation. Such factors are plant size, source and quality of feed water, site location and accessibility to electricity, distance from final users, qualified labour, energy costs and estimated plant life [70]. All of them come under the operating or capital costs of treatment facilities, as the majority of them are included in the cost estimates demonstrated in the subsequent subsections.

### *3.5.1. Operating costs*

The operating costs in coagulation are primarily accounted for by chemical consumption. They are determined by the dosage and the price per metric tonne of product. In a case of desalination, ferric chloride is often predominating due to the more satisfactory results obtained downstream. Aluminium sulphate (alum) and ferric sulphate have exhibited more solid outcomes in water and wastewater applications, hence, the preferred types of coagulant. The annual cost for the chemical is calculated from Eq.(36).

$$CHC = \sum_{i \in I_t} cv^{CHC} \cdot CD_{ti} \cdot C_{chem} \cdot t_h \cdot t_d \cdot (Q^{IN}|_{i=1} + Q_{ti}^{F}|_{i>1}) \cdot W_{ti}, \quad \forall\, t \in CF \quad (36)$$

where $cv^{CHC} = 10^{-6}$ is a conversion factor, $t_d$ is the number of operating days a year, $t_h$ is the number of operating hours a day, $CD_{ti}$ is the coagulant dose selected and $C_{chem}$ is the cost of coagulant that alters in accordance with the type of coagulant. The dosage level mostly lies between the range of 0.5 to 100 mg/L of water as specifically it is between 10 to 30 mg/L for alum [18, 71].

The electricity cost for the slow mixing in the flocculant tank, is given by Eq.(37).

$$EMC = \sum_{i \in I_t} cv^{EM} \cdot C^{E} \cdot t_h \cdot t_d \cdot \mu \cdot tf_{ti} \cdot (Q^{IN}|_{i=1} + Q_{ti}^{F}|_{i>1}) \cdot Gf_{ti}^{2} \cdot W_{ti}, \quad \forall\, t \in CF \quad (37)$$

where $cv^{EM} = 16.67 \cdot 10^{-6}$ is conversion factor for the electrical mixing equation. In Eq.(37), μ is the dynamic viscosity of the fluid and $C^{E}$ is the electricity charge, and the power required is calculated for an accumulative number of chambers.

The technical and economic performance of DAF depends mainly on its recirculation ratio and saturator. The former is disregarded in this study and operating cost of the saturator, $SC$, is calculated by:

$$SC = \sum_{i \in I_t} \frac{cv^{SC} \cdot C^{E} \cdot Q_{ti}^{F} \cdot \bar{P}_{si} \cdot X_{si}}{\eta_t^{SAT}}, \quad \forall\, t \in CLR, s \in DAF \quad (38)$$

where $cv^{SC} = 3.6^{-1}$ is the conversion factor for the equation, $\eta_t^{SAT}$ is the efficiency of the saturator, $\bar{P}_{si}$ is the saturator pressure, assumed to be the pressure supplied by the pump and $C^E$ is the electricity cost rate.

The greatest contribution to the operating costs is derived 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 $PC$, are expressed in the following equation.

$$PC = \sum_{t} \sum_{i \in I_t} \frac{cv^{PC} \cdot C^E \cdot (Q^{IN}|_{i=1} + Q_{ti}^{F}|_{i \in M}) \cdot P_{ti} \cdot W_{ti}}{\eta_t^{FP} \cdot \eta_t^{MT}} \tag{39}$$

$cv^{PC} = 3.6^{-1}$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 maintenance $MCC$ and replacement $MRC$ costs are also estimated by the number of passes.

$$MCC = \sum_{t \in TMM} \sum_{i \in I_t} af^{MCC} \cdot MC^O \cdot (D^{FM} + N^{MM} \cdot D^{VM}) \cdot W_{ti} \tag{40}$$

where $af^{MCC}$ is an annualisation factor accounting for 2 times of major cleaning and maintenance in a year, $MC^O$ is the operating cost charge rate during maintenance, $N^{MM}$ is the number of modules in a unit, $D^{FM}$ is the fixed cost for downtime and $D^{VM}$ is the variable cost during maintenance.

$$MRC = \sum_{t \in TMM} \sum_{i \in I_t} af^{MRC} \cdot MC^O \cdot N^{MM} \cdot RC^M \cdot W_{ti} \tag{41}$$

where $af^{MRC}$ is an annualisation factor allowing membrane life of 5 years, i.e. $af^{MRC} = 0.2$ and $RC^M$ is the membrane replacing cost per module.

The labour cost, $LC$, is the second largest expense in a manufacturing facility. Operators working hours requirements can be determined by examining the equipment flowsheet. The method for obtaining the labour cost is first, define the number of operators per shift for a given production rate, which is normally expressed in terms of a function of the number of separation units, as shown in Eq.(42) [72, 73].

$$LC = r^P \cdot t_d \cdot t_s \cdot n_s \cdot \sqrt{lc1 + lc2 \cdot \left(\sum_t \sum_{i \in I_t} W_{ti}\right)^2} \tag{42}$$

where $r^P$ is the pay rate per person, $t_s$ is the number of hours per shift, $lc1 = 6.29$ and $lc2 = 31.7$ are constants associated with the number of operators for all the units. The parameter $n_s$ stands for the number of shifts per day.

For more than four decades, the EPA has used its authority to set cost-effective emission standards that ensure newly constructed sources use the best performing technologies to limit emissions of harmful air pollutants [74]. Owners or operators of facilities where aggregate annual greenhouse gas (GHG) emissions are equal to or more than 25,000 metric tonnes of $CO_{2e}$ must report to EPA under the Clean Air Act. Presently, EPA is not planning on requiring permits for sources that emit less than a 50,000 metric ton threshold until sometime after April 30, 2016 [75]. According to the same literature sources, although there is a continuous encouragement towards fewer emissions, there is no existing limit or taxes if limits are exceeded. With the view that policies of emissions tax will soon come to practice, the plant design can account for carbon taxes. They are calculated from Eq.(44) where the largest component for the emissions is the power consumed.

$$EMS_{ti} = cv^{Ems} \cdot CO_{2_e} \cdot t_h \cdot t_d \cdot P_{ti} \cdot \left(Q^{IN}|_{i=1} + Q^F_{ti}|_{i \in \hat{I}_t}\right) \cdot W_{ti}, \quad \forall\, t, i \in I_t \tag{43}$$

$$EMSC = \sum_t \sum_{i \in I_t} r^{CO_2} \cdot EMS_{ti} \tag{44}$$

where $cv^{Ems} = 3.6^{-1}$ accounts for the conversion factor for the carbon emission equation, $CO_{2_e}$ is the carbon dioxide equivalent and $r^{CO_2}$ is the carbon dioxide tax rate. Compared to pumping, the mixing footprint is relatively negligible, hence, not considered in the above constraints.

### 3.5.2. *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 [76]. In membrane plants especially, the equipment will include membrane elements, pressure vessels and passes. Despite the availability of tools for estimating capital cost, the assumptions in deriving those tools have not been clearly stated. When capital costs are estimated, inflation and other market factors should be taken into account in order to update existing cost models [77].

Adham, S. et al [78], sponsored by the U.S. Environmental Protection Agency (EPA) and AWWA Research Foundation, published correlations for the total construction costs of coagulation – flocculation. The European Commission issued a report on best available techniques in water treatment with construction costs for sedimentation [79]. Wang L.K. et al, [80] reported DAF construction costs for a specified volume. EPA published investment cost equations for production flow ranges [81]. The cost estimation for low-pressure membranes plants, such as MF and UF, was expressed as the cost per unit produced water [82]. In an industrial study for high pressure membranes, a breakdown for the various capital cost components has been shown for different capacities [83]. All the equations can be combined under the common form below.

$$CC_{ti} = infl_t \cdot A_t \cdot (Q_{ti}^{P})^{b_t} \cdot W_{ti}, \quad \forall\, t, i \in I_t \tag{45}$$

where $infl_t$ is inflation factor depending on the year of estimation, $A_t$ and $b_t$ are specific parameters for every technology. In all the cases, the parameter $A_t$ was estimated from the reference capital cost and equipment capacities stated in literature. The capital cost for the clarification technologies is calculated from the expression below.

$$CC_{ti} = \sum_{s \in TCLR} infl_s \cdot A_s \cdot (Q_{ti}^{P})^{b_s} \cdot X_{si}, \quad \forall\, t \in CLR, i \in I_t \tag{46}$$

The capital cost summed and multiplied by the capital recovery factor (CRF) to obtain the total annual capital cost, $ACC$, is given in Eq.(47).

$$ACC = CRF \cdot \sum_{t} \sum_{i \in I_t} CC_{ti} \tag{47}$$

as the CRF is expressed in Eq.(48).

$$CRF = \frac{ir}{1 - \frac{1}{(1+ir)^{yr}}} \quad (48)$$

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

### *3.5.3. Total cost*

The total annual cost, $TC$, is a sum of the chemical $CHC$, mixing $EMC$, saturator $SC$ and pumps $PC$ running costs, membrane cleaning costs $MCC$, membrane replacement costs $MRC$, labour cost $LC$, emissions cost $EMSC$ and the annual capital costs $ACC$ for all the selected technologies.

$$TC = CHC + EMC + SC + PC + MCC + MRC + LC + EMSC + ACC \quad (49)$$

## ***3.6. Objective function***

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

$$WNC = \frac{TC}{Q^{AP}} \quad (50)$$

which is subject to:

- separation efficiency Eq.(2) – Eq.(17)
- mass flow balance Eq.(18) – Eq.(28)
- target purity Eq.(29) and final effluent Eq.(30)
- logical conditions Eq.(31) – Eq.(35)
- operating costs Eq.(36) – Eq.(44)
- capital costs Eq.(45) – Eq.(47)
- total annual cost Eq.(49)

Along with minimising the major capital investment and the annualised operating cost with the objective function, it is aimed to minimise the number of passes for achieving maximum final water purity, and increase the production rate of the facility. The applicability of the proposed method is manifested through two case studies discussed in the next section.

## 4. Case studies and computational results

### *4.1. Seawater desalination*

Abundance grants seawater the opportunity to be a major solution to water scarcity. Thus, the first case study in the present work focuses on seawater desalination for the production of potable water.

#### *4.1.1. Given data*

For the case study the influent, $Q^{IN} = 55{,}000\, m^3/h$, as to agree with existing practices. The minimum allowable effluent $M^{FLOW} = 5{,}000\, m^3/h$, resulting in a minimum $120{,}000\, m^3/d$, i.e. medium-to-large size, facility [84]. For the influent and effluent, it is essential to determine the initial contaminants concentration in seawater and the final requirements for drinking water. The American Water Works Association [83] reported typical seawater intake qualities in the range $30{,}000 - 40{,}000\, mg/L$ TDS.

Table 1. Feed water characteristics and final purity requirements

| Contaminant<br>$s$ | Initial concentration<br>$c_c^{IN}\ [\frac{mg}{L}]$ | Final concentration<br>$M_c^{CONC}\ [\frac{mg}{L}]$ |
|---|---|---|
| TDS | 40,000 | 600 |
| TSS | 30 | 1 |
| Boron | 5 | 2.4 |

**Source:** [9, 67, 85]

The selection of the technologies is based on meeting the health regulatory requirements for potable water [47, 48]. The World Health Organization [86] reported drinking water of good quality contains less than ca. 600 mg/L TDS. Although, no explicit limits exist in the Drinking Water Quality Guideline regarding TSS, they can be correlated to turbidity, which should not exceed 1 NTU, and in many cases 0.5 NTU [58]. Thus, the final purity specification used in the model is less than 1 mg/L TSS. The World Health Organization revised the maximum allowable concentration of boron in drinking water from 0.5 mg/L in 2003 to 2.4 mg/L and the latter value is the final purity requirement in the model. The initial and final water characteristics are listed in Table 1.

The operating condition boundaries are determined next. Literature suggests recoveries for MF and UF systems between 85% and 95% which reach 100% depending on the flow configuration [89]. In the current case study, the recoveries of the low pressure membranes are modelled with the assumption of a full flow recovery. Typical system recoveries for NF membranes take values between 75% and 90% whereas they vary from 35% to 50% for RO systems [36, 90]. Based on reported values, recoveries of 80% for NF and 40% for RO are adopted in the model.

In his experimental work, Vlaŝki [55] varied the energy input to the flocculation tank from 10 to 120 $s^{-1}$ and flocculation time from 5 to 35 min to investigate the performance of downstream clarification processes. The chosen boundaries coincide with the values used in the experiments. CSIRO performed experiments where the grade of media were 2.18, 5.18 and 7.55 mm in diametre, the load values attempted were 0.5, 1.0 and 1.5 m/h, and the filters lengths were 0.6, 1.2, 1.8, 2.4 m [56]. The values taken in the case study are rounded down to 2 mm for lower bound and 8 mm for upper bound for diametre. The rest of the boundaries are presented in Table 2.

Table 2. Operating conditions boundaries

| **Operating conditions** | **Range** |
|---|---|
| $CD_{ti}[mg/L]$ | 1 – 30 |
| $Gf_{ti}[s^{-1}]$ | 10 – 120 |
| $tf_{ti}[min]$ | 5 – 35 |
| $D_{ti}[mm]$ | 2.0 – 8.0 |
| $Ld_{ti}[m/h]$ | 0.5 – 1.5 |
| $L_{ti}[m]$ | 0.5 – 2.5 |
| $Tem_{ti}[°C]$ | 20 – 30 |
| $H_{ti}[-]$ | -6.2 – 0.0 |
| $MWCO_{ti}[Da]$ | 300 – 1200 |
| $pH_{ti}[-]$ | 7.5 – 9.5 |

**Source:** [18, 36, 55, 56, 87, 88]

It is assumed that cleaning or replacement takes place simultaneously for all passes, there are no pressure losses from pump to membrane, every pass contains the same number of membrane modules, $N^{MM} = 2000$, cleaning is performed every 6 months, replacement is recommended every 5 years, and the annual operation is 300 days a year (Table 3). The electricity charge, $C^{E}$, has a value of 0.08 \$/kWh to accommodate any future increments from the U.S Energy Information Administration [91] review and to consider literature values [36].

Table 3. Operating costs parameters data

| **Parameter** | **Value** |
|---|---|
| Number of modules, $N^{MM}[-]$ | 2000 |
| Electricity cost, $C^{E}[\$/kWh]$ | 0.08 |
| Operating cost charge rate during maintenance, $MC^{O}[-]$ | 0.2 |
| Membrane replacing cost per module, $RC^{M}[\$]$ | 800 |
| Fixed cost for downtime during maintenance, $DC^{CM}[\$]$ | 200 |
| Ferric coagulant cost, $C_{chem}[\$/tonne]$ | 250 |
| Carbon dioxide equivalent, $CO_{2_e}[kg/kWh]$ | 1.31 |
| Carbon dioxide rate, $r^{CO_2}[\$/kg]$ | 0.023 |
| Seawater viscosity, $\mu[kg/m \cdot s^2]$ | $1.307 \cdot 10^{-3}$ |
| Operating hours a day, $t_h[h/d]$ | 24 |
| Operating days a year, $t_d[d/y]$ | 300 |

**Source:** [36, 92, 93]

To consider updating of the capital costs, the plant location has to be determined. Assuming the facility to be built in the U.S., the inflation for the capital costs from the reference year of citation has been considered. The inflation rates are reported in Table 4 [94]. The term of bank loan was taken as *yr = 30 years*, the interest rate was assumed to be *ir = 6%*, and the plant was considered to produce 95% of its design annual yield based on standard practices [95]. The rest of the design parameters are given in Table 3 and Table 4. Whenever values in literature could not be found, assumptions and approximations were used in accordance with practical cases. Finally, the carbon emissions have been calculated assuming no carbon taxation.

Table 4. Pressure design variables, and efficiency and economic parameters

| **Technology** | **CF** | **CLR** SED/DAF | **MMF** | **MF** | **UF** | **NF** | **RO1** | **RO2** |
|---|---|---|---|---|---|---|---|---|
| $P_{ti}$ 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 |
| $\eta_t^{FP}$ $[-]$ | 0.75 | -/0.75 | 0.80 | 0.80 | 0.75 | 0.80 | 0.75 | 0.75 |
| $\eta_t^{MT}$ $[-]$ | 0.95 | -/0.95 | 0.93 | 0.95 | 0.97 | 0.95 | 0.98 | 0.98 |
| $infl_t$ $[-]$ | 1.143 | 1.288/1.087 | 1.319 | 1.087 | 1.087 | 1.511 | 1.511 | 1.511 |
| $A_t$ $[-]$ | 121701 | 8334/ 4167 | 69547 | 45601 | 45601 | 158177 | 158177 | 158177 |
| $b_t$ $[-]$ | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 |

**Source:** [36, 78 - 83, 87, 88, 94]

### 4.1.2. Results and discussion

The model was solved in GAMS 24.4 [96] on a Dell PC OptiPlex 9010, Intel Core i7 - 3770 CPU at 3.4 GHz and 16 GB RAM. Its computational statistics involve 40 binary variables, 564 continuous variables and 569 constraints. The model was tested on ANTIGONE which returned a solution within 48.8 seconds, with an optimal gap 0. The branch – and – bound solving technique was satisfactory for achieving the optimal solution.

#### 4.1.2.1. Flowsheet configuration

The optimal sequence of process units comprised three ultrafiltration passes that serve as a pretreatment system to the desalting section. Two nanofiltration and one reverse osmosis passes were chosen, the former for the TDS removal and the second one for the boron removal (Fig. 3).

(include Fig.3)

#### 4.1.2.2. Operating conditions

Table 5 summarises the operating conditions returned by ANTIGONE. The predominant results lie in the lower bounds of the variables, showing the constraints are active. On the other hand, lower power translates into lower costs. It is also worth mentioning that some of the technological characteristics, such as molecular weight cut -off, hydrophobicity and pH, do not influence the operating costs directly. This might result in observing differences in the final purities, when there is a nanofiltration and reverse osmosis selected, while the water net cost will remain the same with various non-linear solvers or few runs with one solver. The reason for this observation lies in the exclusion of chemicals costs for altering the alkalinity of the feed and also, in the assumption of no fouling occurring, where cleaning cycles and replacement can be predicted by the pore size of the membranes.

Table 5. Operating conditions for seawater case study

| **Operating conditions** | **Range** |
|---|---|
| $P_{UF}[MPa]$ | 0.1 |
| $P_{UF}[MPa]$ | 0.1 |
| $P_{NF}[MPa]$ | 0.5 |
| $P_{RO2}[MPa]$ | 5.0 |
| $H_{NF}[-]$ | -2.7 |
| $MWCO_{NF}[Da]$ | 300 |
| $pH_{NF}[-]$ | 8.0 |

#### 4.1.2.3.Cost

The largest contributor to the operating costs was the electricity, followed by the labour cost, representing 21% of the operating costs. The cleaning and replacement costs were relatively insignificant due to the fixation of the number of membrane modules, no cleaning chemicals costing and assumption of activities repetitiveness.

In 2012 IWA published a book dedicating a chapter on seawater desalination where the water net cost lay between US\$0.5/m$^3$ and US\$3.0/m$^3$, depending on the capacity of the facility [97]. The optimal solution returned by ANTIGONE was

US\$1.044/m$^3$ with a daily production 337,920 m$^3$/d and consequently, the result fell into the suggested limits. In addition the report by UNESCO from 2008 gives unit costs of the desalination plants in Perth (150,000 m$^3$/d) and Sydney (250,000 m$^3$/d) with total product costs US\$0.83/m$^3$ and US\$1.64/m$^3$, respectively. It should be noted that the transportation costs for those plants is less than US\$0.06/m$^3$, meaning the water net cost will not be significantly influenced if they are added to it.

Next, sensitivity analysis was performed for the number of passes per technology, maximum number of passes, influent contaminants fluctuation, and interest rates and plant life.

#### 4.1.2.4. Sensitivity analysis of passes

In the base case study above, four passes for every technology were allowed. It was then investigated how the results change with the number of passes. It is expected that global solvers do not experience any changes down to two passes as this is the maximum number of passes per technology returned in the optimum solution. For $i = 1$, however, ANTIGONE returned water net cost US\$2.105/ m$^3$ with flowsheet configuration shown in Fig. 4.

(insert Fig.4)

Followed tightening of the total allowable number of passes in the flowsheet. In the case study out of 10, the global solvers return 6 passes, meaning the solution would not change if $N_{max} > 6$. When $N_{max} = 5$, the water net cost returned was US\$1.982/m$^3$ with a configuration *MF - 2xNF - RO1 - RO2* (Fig. 5).

(insert Fig.5)

Selecting more passes of the same technology leads to economically more favourable flowsheets. In the studied case, the difference in price is due to the coagulant cost for the CF unit and its capital cost. The flowsheet in Fig. 5 differs from the optimal solution, presented in the previous subsections, by the RO pass for TDS removal. Pumping cost is, thus, the major contributor to the difference in price between the two.

#### 4.1.2.5. Sensitivity analysis of TDS and TSS

Seawater desalination plants are exposed to daily and seasonal contaminants variations. Hence, it is necessary to explore how the flowsheet can alter or what the fluctuation in final purity of the initially selected flowsheet will be. The TDS concentration was varied from 20,000 mg/L to 40,000 mg/L with a step change 5,000 mg/L. No changes occurred in the flowsheet configuration and water cost, meaning the system is overdesigned with respect to total dissolved solids and it is capable to handle feed variations and still meet model restriction criteria. Another reason is already the mentioned technological characteristics which do not affect the final cost, meaning fluctuations in TDS would not change the flowsheet significantly unless additional constraints are introduced or NF is no longer able to remove the contaminant group down to the required purity. Although fluctuations in dissolved solids is likely, it is more likely that the seawater is exposed to turbidity variations due to weather conditions, recycled water streams that were directed to the sea, etc. Thus, the change of suspended solids feed concentrations was studied by varying it from 20 mg/L to 80 mg/L. Not only did the final TSS concentration altered but also the choice of technologies in the relevant section and the final product cost (Fig. 6). The water cost increases with TSS because of the need for higher number of passes or more efficient and expensive technology choices. As Eq.(8) and Eq.(10) suggest, for separation of higher TSS concentration, more units and with higher pressure will be selected. Therefore, the increase in price stems from the electricity cost for pumping.

(insert Fig.6)

#### 4.1.2.6. Sensitivity analysis of carbon emissions

The designed facility would annually emit greenhouse gases at the rate 634,040 tonnes/year, 49% less than the desalination plant in Sydney, for instance, while exceeding its production by 33% [92]. Other sources have demonstrated that the range of kilogram emissions per volume of water produced can vary from 2.03 kg/m$^3$ in Spain to 7.80 kg/m$^3$ in Australia [98]. The emissions produced for the designed conceptual flowsheet did not exceed 6.25 kg/m$^3$. Current regulatory practices will impose official annual reporting to EPA. To reflect future intentions of environmental regulatory bodies, an option of carbon taxation of US\$0.023/$CO_2$/kg was studied in the model. The option affected the flowsheet configuration by substituting one of the pretreatment ultrafiltration passes with a microfiltration. Thus, the emissions and their respective taxation would decrease while the water quality would be still met. The water net cost rose to US\$1.195/m$^3$, approximately 14% difference in comparison to the WNC from the base case.

#### 4.1.2.7. Sensitivity analysis of interest rate and plant life

Local authorities in the US provide financing through low-interest loans and such initiatives are a common practice for boosting water treatment facilities commissioning

[99]. Hence, it is worth examining the water cost modifications at different interest rates and designing for shorter and longer plant lifetimes.

(insert Fig.7)

From Fig.7 it is observed that the lower cost range will lie in the low interest rate - short plant lifetime and high interest rate - longer plant lifetime area. The minimum water cost is US\$0.846/m$^3$ at 1% interest and 40 years project scope. Under these conditions the water net cost undergoes nearly 23% reduction as a result of the decrease in annual capital cost. Currently, the design integrates one of the worst case scenarios where no governmental incentives are available. From this follows the higher unit cost.

### *4.2. Tertiary wastewater treatment*

Water reclamation and advanced water treatment have recently faced significant enhancement due to membrane improvement. Thus, the second case study focuses on tertiary wastewater treatment for the production of potable water.

#### *4.2.1. Given data*

It is assumed that wastewater, with the characteristics listed in Table 6, enters the purification system.

Table 6. Feed water characteristics and final purity requirements

| Contaminant<br>$s$ | Initial concentration<br>$c_c^{IN}$ $[\frac{mg}{L}]$ | Final concentration<br>$M_c^{CONC}$ $[\frac{mg}{L}]$ |
|---|---|---|
| COD | 70 | 5 |
| DOC | 8 | 2 |
| TDS | 15,000 | 600 |
| TSS | 200 | 1 |
| Boron | 2.4 | 2.4 |

**Source:** [9, 18, 100 - 104]

The main characteristics of wastewater impose taking into account the organic matter, such as COD and DOC, in the case study. The initial secondary effluent concentrations were decided based on similar values in literature [101 - 103]. No standards have been mentioned for the maximum contaminant level (MCL) by the World Health Organisation. However, a number of sources declare < 5mg/L for COD and roughly < 2 mg/L for DOC drinking water quality at neutral pH [103, 104]. Boron is an issue specifically for seawaters, therefore, in this case study, it was assumed its influent concentration equals to the required concentration of boron in drinking water. As the total dissolved solids concentration is significantly lower, the reverse osmosis systems will work with higher recoveries. For the case study, a value of 0.6 was assumed.

According to the application, aluminium sulphate (alum) coagulant is used. Its dosage is reported to be in the standard range of 10 to 30 mg/L for treatment of suspended solids [18]. Organics necessitate a higher dose, hence, up to 50 mg/L dose was allowed as performed in experiments [105]. The price of alum can be found at approximately US$150/tonne [106]. Additionally, viscosity value of 1.002 kg/m·s at ambient temperature was taken.

The rest of the data overlaps with the given data from Section 4.1.1.

### *4.2.2. Results and discussion*

For the second case study with 715 constraints and 730 continuous variables, it took ANTIGONE 204.18 seconds to return a solution, with an optimality gap 0.

#### 4.2.2.1. Flowsheet configuration

The advanced wastewater treatment flowsheet consisted of one coagulation-flocculation process unit, followed by a sedimentation step. Two nanofiltration units were allocated for the removal of the organic matter and the total dissolved solids. This flowsheet configuration is common for water and advanced wastewater treatment. A schematic of the optimal flowsheet is given in Fig. 8.

(insert Fig.8)

#### 4.2.2.2. Operating conditions

The operating conditions from the advanced wastewater treatment case study are reported in Table 7. Unlike in the previous case study, here, some of the operating conditions have inactive boundaries, such as coagulant dosage. Consequently, the computational time increased.

Table 7. Operating conditions for advanced wastewater case study

| **Operating conditions** | **Range** |
|---|---|
| $CD_{CF}[mg/L]$ | 30.7 |
| $pH_{CF}[-]$ | 7.24 |
| $tf_{CF}[min]$ | 5 |
| $Gf_{CF}[s^{-1}]$ | 10 |
| $P_{NF,i}[MPa]$ | 0.5 |

#### 4.2.2.3.Cost

Al-Hamdi [107] compared desalination and wastewater treatment where the unit costs reported only for advanced wastewater treatment are in the range US$0.31/m$^3$ - US$ 0.6/m$^3$. The values agree with other literature sources [9, 108] that report average values ca. US$ 0.5/m$^3$ as the cost can drop down to around US$ 0.14/m$^3$ [109] for large – scale plants. Compared to the aforementioned water net values, the obtained optimal solution lies in the low boundary of the given ranges, i.e. US$0.22/m$^3$, for a designed facility with capacity 802,560 m$^3$/d.

#### 4.2.2.4.Comparison between seawater and advanced wastewater case studies

Lastly, a comparison between the two case studies was conducted based on technologies selection and costs breakdown. Nowadays pretreatment systems can operate without sedimentation or dissolved air flotation. Sedimentation basins are capable of producing seawater with approximately less than 1 mg/L. This, however, depends on the source of water. If TSS > 100 mg/L, SED is recommended to be installed [110]. DAF is more energy intensive than SED and when the total suspended solids are high, the process is economically unfavourable. On the other hand, the processes are efficient for intense removal of TSS without the concerns about equipment fouling. With the assumption of no need for removing boron, the reverse osmosis becomes redundant. The choice of equipment pre-determines the operating costs of the systems.

(insert Fig.9)

In Fig. 9 the breakdown costs per volume for both applications are presented. Seawater desalination demonstrates approximately ten times higher electricity cost because of the pumping requirements in overcoming osmotic pressure of saline water. When the TSS is high, coagulants that treat the water are significantly less expensive while their dosage rises less than double at maximum. Therefore, CF becomes economically advantageous but accounts for the extra chemical cost. The labour cost per volume of water is significantly higher in seawater desalination due to the extra pass and lower production rate. The capital costs of the two case studies fall in the same order of magnitude, as the two flowsheets have six and four process units, respectively. Future refinements of the mathematical model can lead to a more accurate representation of the physico-chemical system of water treatment.

## 5. Conclusions

In this work a systematic approach for the design and optimisation of water treatment processes was proposed. The problem was formulated as a mixed integer non-linear program model. The objective function minimises the water production cost manipulated by the techno-economic performance of the technologies selected. Two case studies were presented with two applications, on seawater desalination and advanced wastewater treatment. The computational results demonstrated an alignment with existing water engineering technical and economic practices which proved the applicability of the proposed approach and model. Current limitations of the model involve data retrieval and assumptions for its development. Therefore, further work will be able to refine the obtained results, enlarge the technological scope of the project, and enable the model to mimic more accurately the design of water treatment processes.

## Acknowledgements

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

## List of Symbols

*Indices*

$c -$ contaminants

$i, j -$ passes

$s -$ parallel technologies for CLR

*Sets*

$\bar{I}_s -$ a set of passes of parallel technologies, $s$, for CLR

$\hat{I}_s -$ a set of all the passes $i$ of technology $t$, except for the first pass of technology CF

$C_t -$ a set of contaminants processed by technology $t$

$I_t -$ a set of passes of technology t with a final pass, $I_t^{max}$

$TCLR -$ clarification processes

$TMM -$ membrane processes

*Parameters*

$\bar{Y}_{si} -$ recovery factor of technology $s$ and pass $i$, $[-]$

μ $-$ viscosity of water source, $[kg/m \cdot s]$

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

$af^{MCC} -$ constant accounting for annualisation for equipment cleaning and maintenance

$af^{MRC} -$ constant accounting for annualisation for equipment replacement

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

$C^E -$ electricity charge, $[\$/kWh]$

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

$C_{chem} -$ coagulant price, $[\$/tonne]$

$CO_{2_e} -$ carbon dioxide equivalent, $[kg/kWh]$

$CRF -$ capital recovery factor, $[-]$

$cv^{CHC} -$ a conversion constant for the chemical costs, $[-]$

$cv^{Ems} -$ a conversion constant for the emissions taxes, $[-]$

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

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

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

$D^{FM} -$ fixed cost for downtime, $[\$]$

$D^{VM} -$ variable cost for downtime, $[\$]$

$infl_t -$ inflation rate, $[-]$

$ir -$ interest rate, $[-]$

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

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

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

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

$MC^O -$ operating cost charge rate during maintenance, $[-]$

$N^{MM} -$ number of membrane modules, $[-]$

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

$n_s -$ number of shifts per day, $[-]$

$PY -$ annual production yield, $[-]$

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

$r^{CO_2} -$ carbon dioxide price, $[\$/kg]$

$r^P -$ pay rate per hour, $[\$/h]$

$RC^M -$ replacement cost per module, $[\$]$

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

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

$U -$ big number equal to the cardinality of the number of allowed passes, $[-]$

$Y_{ti} -$ recovery factor of technology $t$ and pass $i$, $[-]$

$yr -$ years of investment, $[-]$

$\eta_t^{FP} -$ pump efficiency, $[-]$

$\eta_t^{MT} -$ motor efficiency, $[-]$

$\eta^{SAT} -$ saturator efficiency, $[-]$

*Binary variables*

$W_{ti} -$ binary variable equal to 1 if technology $t$ and pass $i$ is selected, otherwise equal to 0, $[-]$

$X_{si}$ binary variable equal to 1 if technology $s$ and pass $i$ is selected, otherwise equal to 0, $[-]$

*Continuous variables*

$\bar{P}_{si} -$ operating pressure of unit s and pass $i$, $[MPa]$

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

$ACC -$ total annualised capital cost, $[\$/yr]$

$c_{tic}^{F} -$ feed concentration of contaminant c to technology $t$ and pass $i$, $[mg/L]$

$c_{tic}^{P} -$ permeate concentration of contaminant $c$ from technology $t$ and pass $i$, $[mg/L]$

$CC_{ti} -$ capital cost for unit belonging to technology $t$ and pass $i$, [\$]

$CD_{ti} -$ coagulant dose, $[mg/L]$

$CHC -$ chemical cost for technology $t$ and pass $i$, $[\$/yr]$

$D_{ti}^{MED} -$ media diametre of multi-stage media filtration, $[m]$

$EM_{ti} -$ mixing cost for technology $t$ and pass $i$, $[\$/yr]$

$EMS_{ti} -$ annual carbon emissions for technology $t$ and pass $i$, $[kg/yr]$

$EMSC -$ emission charges for $t$ and pass $i$, $[\$/yr]$

$Gf_{ti}$ − flocculation energy input, $[s^{-1}]$

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

$LC$ − labour cost, $[\$/yr]$

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

$MCC$ − cleaning and maintenance cost for technology $t$ and pass $i$, $[\$/yr]$

$MRC$ − replacement cost for technology $t$ and pass $i$, $[\$/yr]$

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

$P_{ti}$ − operating pressure of unit $t$ and pass $i$, $[MPa]$

$PC$ − pumping cost for technology $t$ and pass $i$, $[\$/yr]$

$pH_{ti}$ − hydrogen ion concentration in feed to technology $t$ and pass $i$, $[-]$

$PP_{tic}$ − physicochemical properties of flow and operating conditions of technology $t$ in pass $i$

$Q^{AP}$ − annual production rate, $[m^3/yr]$

$Q_{ti}^{F}$ − feed flowrate to a technology $t$ and pass $i$, $[m^3/h]$

$Q_{ti}^{P}$ − permeate from technology $t$ and pass $i$, $[m^3/h]$

$R_{tic}$ − rejection coefficient of a contaminant c in technology $t$ and pass $i$, $[-]$

$SC$ − operating cost for running the saturator in technology $t$ and pass $i$, $[\$/yr]$

$TC$ − total annualised cost, $[\$/yr]$

$Tem_{ti}$ − operating temperature for technology $t$ and pass $i$, $[°C]$

$tf_{ti}$ − flocculation time, $[min]$

$WNC$ − water net cost, $[\$/m^3]$

$H_{ti}$ – natural logarithm of component hydrophobicity influencing rejection in technology $t$ and pass $i$, $[-]$

## References

[1] United Nations. Managing water under uncertainty and risk: The United Nations world water development report 4, 2012, pp. 1 – 909.

[2] British Petroleum, BP Enegry Outlook 2030, 2013. URL http://www.bp.com/content/dam/bp/pdf/statisticalreview/BP_World_Energy_Outlook_booklet_2013.pdf. Accessed 17/12/2013.

[3] R. Chandrappa, S. Gupta and U.C. Kulshrestha, editors. Coping with Climate Change: Principles and Asian Context. Springer, Heidelberg, 1st edition, 2011, pp. 113 - 114.

[4] N. Lior. Advances in water desalination, Wiley, New Jersey, US, 2013.

[5] T. Hinkebein. Water and sustainable development: Opportunities for the chemical sciences: A workshop report to the chemical sciences roundtable. desalination: Limitations and challenges, 2004. Accessed 19/12/2013.

[6] National Centre of Excellence in Desalination Australia. Australian Desalination Research Roadmap. Murdoch University, Rockingham, Western Australia 6168, 2011. pp.1 - 114.

[7] S.D. Barnicki and J.J. Siirola, editors. Formal Engineering Design. Systematic Chemical Process Synthesis. Cambridge University Press, UK, 1st edition, 2005. pp.362 - 366.

[8] N. Nishida, G. Stephanopoulos and A.W. Westerberg. A review of process synthesis. AIChE J., 27 (2004) 321–351.

[9] G. Tchobanoglous, F. Burton and H. Stensel. Wastewater Engineering, Treatment and Reuse. McGraw-Hill, New York, 4th edition, 2003. pp.1035 - 1211.

[10] A. Afify. Prioritizing desalination strategies using multi-criteria decision analysis. Desalination, 250 (2010) 928 – 935.

[11] F. Vince, F. Marechal, E. Aoustin and P. Breant. Multi-objective optimisation of RO desalination plants. Desalination, 222 (2007) 96 – 118.

[12] K.M. Sassi and I.M. Mujtaba. Simulation and optimization of full scale reverse osmosis desalination plant. 20th European Symposium on Computer Aided Process Engineering, 28 (2010) 895 – 900.

[13] W.H. Chan and S.C. Tsao. Fabrication of nanofiltration membranes with tunable separation characteristics using methods of uniform design and regression analysis. Chemometr. and Intell. Lab. Syst., 65 (2003) 241–256.

[14] M. Wilf and M.K. Schierach. Improved performance and cost reduction of RO seawater systems using UF pretreatment. Desalination, 135 (2001) 61–68.

[15] M. Wilf, L. Awerbuch, C. Bartels, Mickley M., G. Pearce and N. Voutchkov. Guidebook to Membrane Desalination Technology. Balaban Desalination Publications, L’Aquila 2007. pp.524.

[16] L.O. Villacorte. Algal Blooms and Membrane Based Desalination Technology. PhD thesis, Delft University of Technology, The Netherlands, January 2014.

[17] C. Forster. Wastewater Treatment and Technology. Thomas Telford Publishing, London, UK, 3rd edition, 2003. pp. 1 - 90.

[18] N.P. Cheremisinoff. Handbook of Water and Wastewater Treatment Technologies. Butterworth-Heinemann, USA, 2002. pp. 1 - 631.

[19] N. Voutchkov. Desalination Engineering: Planning and Design. McGraw Hill, USA, 2012.

[20] S. Mussati, P. Aguirre and N.J. Scenna. Optimal MSF plant design. Desalination, 138 (2001) 341 – 347.

[21] P. Druetta, P. Aguirre and S. Mussati. Optimization of multi-effect evaporation desalination plants. Desalination, 311 (2013) 1–15.

[22] M. Skiborowski, A. Mhamdi, K. Kraemer and W. Marquardt. Model-based structural optimization of seawater desalination plants. Desalination, 292 (2012) 30 – 44.

[23] K.M. Sassi and I.M. Mujtaba. Optimal operation of RO system with daily variation of freshwater demand and seawater temperature. Comput. Chem. Eng., 59 (2013) 101 – 110.

[24] E. Ruiz-Saavedra, A. Ruiz-García and A. Ramos-Martín. A design method of the RO system in reverse osmosis brackish water desalination plants (calculations and simulations). Desal. Wat. Treat., 55 (2014) 2562 – 2572.

[25] M. Spiller, J.H.G. Vreeburg, I. Leusbrock and G. Zeeman. Flexible design in water and wastewater engineering definitions, literature and decision guide. J. Environ. Manage., 149 (2015) 271 – 281.

[26] Y. Avramenko, A. Kraslawski and N. Menshutina. Decision supporting system for design of wastewater treatment. Comput. Aided Chem. Eng., 18 (2004) 337 – 342.

[27] C.M. Roberts and E.C. Inniss. Implementing treatment sequences to promote reduction of dbps in small drinking water systems. Water Resources Management, 28 (2014) 1631–1643.

[28] M. Franceschi, A. Girou, A.M. Carro-Diaz, M.T. Maurette and E. Puech-Costes. Optimisation of the coagulation - flocculation process of raw water by optimal design method. Wat. Res., 36 (2002) 3561 – 3572.

[29] M. Rossini, M.G. Garrido, and M. Galluzzo. Optimization of the coagulation flocculation treatment: influence of rapid mix parameters. Wat. Res., 33 (1999) 1817 – 1826.

[30] B. Galán and I.E. Grossmann. Optimal design of real world industrial wastewater treatment networks. Comput. Aided Chem. Eng., 29 (2011) 1251 – 1255.

[31] N. Ibri´c, E. Ahmetovíc, and Z. Kravanja. Synthesis of water, wastewater treatment, and heat-exchanger networks. In: Varbanov P.S. Klemeŝ, J.J. and P.Y. Liew, editors, 24th European Symposium on Computer Aided Process Engineering, Comput. Aided Chem. Eng., 33 (2014) 1843 – 1848.

[32] C. Sweetapple, G. Fu and D. Butler. Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions. Water Research, 55 (2014)

52 – 62.

[33] K.D. Pickering and M.R.Wiesner. Cost model for low - pressure membrane filtration. J. Environ. Eng., 119 (1993) 772–797.

[34] D.G. Wright and D.R. Woods. Evaluation of capital cost data. Part 7: Liquid waste disposal with emphasis on physical treatment. Can. J. Chem. Eng., 71 (1993) 575 – 590.

[35] T. Fuqua, R. Ortiz, P. Bowen and R. Creighton. Membrane treatment and the use of the Floridan aquifer in South Florida. Technical report, American Water Works Association, U.S., 1991. pp. 63 - 78.

[36] Y. Lu, Y. Hu, D. Xu and L. Wu. Optimum design of reverse osmosis seawater desalination system considering membrane cleaning and replacing. J. Membr. Sci., 282 (2006) 7–13.

[37] Y. Lu, A. Liao and Y. Hu. The design of reverse osmosis systems with multiple-feed and multiple-product. Desalination, 307 (2012) 42 – 50.

[38] S. Kumar, A. Groth and L. Vlacic. Cost evaluation of water and wastewater treatment plants using water price index. Water Resources Management, 29 (2015) 3343–3356.

[39] A. Jiang, J. Wang, L.T. Biegler, W. Cheng, C. Xing and Z. Jiang. Operational cost optimization of a full-scale SWRO system under multi-parameter variable conditions. Desalination, 355 (2015) 124 – 140.

[40] Y. Du, L. Xie, J. Liu, Y. Wang, Y. Xu and S. Wang. Multi-objective optimization of reverse osmosis networks by lexicographic optimization and augmented epsilon constraint method. Desalination, 333 (2014) 66 – 81.

[41] F. Vince, F. Marechal, E. Aoustin, and P. Brant. Multi-objective optimization of RO desalination plants. Desalination, 222 (2008) 96 – 118.

[42] H. Tokos and Z. N. Pintarich. Development of a MINLP model for the optimization of a large industrial water system. Optimization and Engineering, 13 (2009) 625 – 662.

[43] C.S. Khor, B. Chachuat, and N. Shah. A superstructure optimization approach for water network synthesis with membrane separation - based regenerators. Computers and Chemical Engineering, 14 (2012) 265 – 272.

[44] S. Liu, F. Konstantopoulou, P. Gikas and L.G. Papageorgiou. A mixed integer optimisation for integrated water resources. Comput. Chem. Eng., 35 (2011) 858–875.

[45] S. Liu, L.G. Papageorgiou, and P. Gikas. Integrated management of non-conventional water resources in Anhydrous islands. Water Resources Management, 26 (2012) 359–375.

[46] R.W. Rousseau, editor. Handbook of separation process technology. John Wiley & Sons, Inc., US, 1987.

[47] The Drinking Water Inspectorate. Drinking Water Safety. Guidance to Health and Water Professionals, 2009. URL http://dwi.defra.gov.uk/stakeholders/information-letters/2009/09_2009annex.pdf. Accessed 06/05/2015.

[48] U.S. Environmental Protection Agency. Development Document for Effluent Limitations Guidelines and Standards for the Centralized Waste Treatment Industry - Final. U.S. Environmental Protection Agency,Washington DC, U.S., 2010. pp.1 - 44.

[49] S. Judd and B. Jefferson, editors. Membranes for Industrial Wastewater Recovery and Re-use. Chapter 2: Membrane Technology. Elsevier, UK, 1st edition, 2003. pp. 362 - 366.

[50] M.M. Benjamin and D.F. Lawler. Water Quality Engineering: Physical/ Chemical Treatment Processes. Wiley, New Jersey, 1st edition, 2013.

[51] K. Scott and R. Hughes, editors. Industrial Separation Technology. Blackie Academic and Professional, UK, 1st edition, 1996. pp.75 - 76.

[52] P. Xu, J.E. Drewes, C. Bellona, G. Amy, T. Kim, M. Adam and T. Heberer. Rejection of emerging organic micropollutants in nanofiltration - reverse osmosis membrane applications. Wat. Environ. Res., 77 (2005) 40 – 48.

[53] V. Sangeetha, V. Sivakumar, A. Sudha and KS. P. Devi, Optimization of process parameters for COD removal by Coagulation Treatment using Box – Behnken design.

Int. J. Eng. Technol., 6 (2014) 1053 – 1058.

[54] K. Park, Y.T. Seo, G.D. Whang and W.Lee. Optimizing enhanced coagulation for DOC removal with ultrafiltration membrane separation using response surface methods and particle trajectory analysis. Wat. Sci. Technol., 42 (2000) 187 – 192

[55] A. Vlaŝki. Microcystis aeruginosa Removal by Dissolved Air Flotation (DAF). Options for Enhanced Process Operation and Kinetic Modelling. PhD thesis, UNESCO-IHE Institute of Water Education, The Netherlands, 1998.

[56] E. Lin, D. Page, P. Pavelic, P. Dillon, S. McClure and J. Hutson. Evaluation of roughing filtration for pre-treatment of stormwater prior to aquifer storage and recovery (asr). CSIRO land and water science report, Flinders University and CSRO, February 2006. pp.1 - 154.

[57] F. Benitez, L. Acero and I. Leal. Application of microfiltration and ultrafiltration processes to cork processing wastewaters and assessment of the membrane fouling. Separ. Purif. Technol., 50 (2006) 354 – 364.

[58] D. Gallegos. Determination of optical water quality requirements in the Indian river near Ft. Pierce, FL, with emphasis on the impact of colored water discharges. Technical report, South Florida, U.S., 1993.

[59] J. Cho, G. Amy and J. Pellegrino. Membrane filtration of natural organic matter: initial comparison of rejection and flux decline characteristics with ultrafiltration and nanofiltration membranes, Wat. Res., 33 (1999) 2517 – 2526.

[60] G. Artug. Modelling and Simulation of Nanofiltration Membranes. PhD thesis, Cuvillier Verlag G¨ottingen, Germany, 2007.

[61] K. Boussu, C. Vandecasteele and B. Van Der Bruggen. Relation between membrane characteristics and performance in nanofiltration. J. Membr. Sci., 310 (2008) 51 – 65.

[62] M. Tokhy, H.F. Shaalan, A.M. Sharaky, N.M. El-Monem and G.A. Bazedi. Performance analysis of upgrading of secondary treated wastewater by nanofiltration, World Appl. Sci. J., 25 (2013) 384 – 390.

[63] J. Chen and L. Guanghua. Marine reverse osmosis desalination plant - a case study. Desalination, 174 (2005) 299 – 303.

[64] The Dow Chemical Company. Rosa System Design Software, 2013. http://www.dow.com/en-us/water-and-process-solutions/resources/design-software/rosa-software. Accessed 06/05/2015.

[65] N. Li, A. Fane,W. Ho and T. Matsuura. Advanced Membrane Technology and Applications. Wiley, New Jersey, U.S., 2008.

[66] K.L. Tu, L.D. Nghiem and A. Chivas. Boron removal by reverse osmosis membranes in seawater desalination applications. Separ. Purif. Technol., 75 (2010) 87 – 101.

[67] P.P. Mane, P. Park, H. Hyung, J. Brown, and J. Kim. Modeling boron rejection in pilot- and full scale reverse osmosis desalination processes. J. Membr. Sci., 338 (2009) 119 – 127.

[68] E. Vasquez-Alvarez and J. M. Pinto. Efficient MILP formulations for the optimal synthesis of chromatographic protein purification processes. J. Biotech., 110 (2004) 295 – 311.

[69] E.M. Polykarpou, P.A. Dalby and L.G. Papageorgiou. A novel efficient optimization system for purification process synthesis. Biochem. Eng. J., 67 (2012) 186 – 193.

[70] Y. Zhou and R.S.J. Tol. Evaluating the costs of desalination and water transport. Wat. Resour. Res., 43 (2004) 1 – 16.

[71] Energie- en Milieu-Informatiesysteem. Coagulation and floculation, 2010. URL http://emis.vito.be/techniekfiche/coagulation-and-flocculation?language=en. Accessed 10/05/2014.

[72] R.H. Perry and D.W Green. Perry's Chemical Engineers' Handbook. McGraw-Hill, New York, U.S., 8th edition, 2007. pp.2640.

[73] KLM Technology Group. General process plant cost estimation, 2014. URL http://kolmetz.com/pdf/egd2/engineering_design_guidelines_general_plant_cost_estima

ting_rev_web.pdf. Accessed 05/05/2015.

[74] Environmental Protection Agency. Standards of Performance for Greenhouse Gas Emissions From New Stationary, Sources: Electric Utility Generating Units. 79 (2014) 1 – 91.

[75] R. McGuckin, A. Contreras and J. G. Jacangelo. Toolbox for Water Utility Management and Greenhouse Gas Emission Management. Water Research Foundation, U.S., 2013. pp. 15 - 119.

[76] M. Blaikie, C. Pelekani, G. Hijos, J. Artal and M. Kumar. Innovative design: Commissioning and early operational performance of the Adelaide desalination plant. South Australian Water Corporation, (2013) 1-8.

[77] S. Sethi. Transient permeate flux analysis, cost estimation and design optimization in crossflow membrane filtration. PhD thesis, Rice University, Houston, Texas, U.S., 1997.

[78] S. Adham, K. Chiu, G. Lehman, K. Howe, A. Marwah, C. Mysore, J. Clouet, Z. Do – Quang and O. Cagnard. Optimization of Membrane Treatment of Direct and Clarified Water Filtration, American Water Works Association Foundation and U.S. EPA, 2006.

[79] European Commission, Integrated Pollution Prevention and Control. Reference Document on Best Available Technologies in Common Waste Water and Waste Gas Treatment/Management Systems in the Chemical Sector, 2003. http://eippcb.jrc.ec.europa.eu/reference/BREF/cww_bref_0203.pdf. Accessed on 10/02/2016

[80] L.K. Wang, N.K. Shammas, W.A. Selke and D.B. Aulenbach, editors. Handbook of Environmental Engineering. Flotation Technology. Humana Press, 2010.

[81] C.T. Whitman, G.T. Mehan, G.H.Grubbs, S.E. Frace, D.F. Andreson, W.Anderson, G.Jett, Y.Guilaran, J.Freeman. Development Document for Final Effluent Limitations Guidelines and Standards for the Iron and Steel Manufacturing Point Source Category. U.S. Environmental Protection Agency, 2002.

[82] University of New Hampshire, Membrane Filtration Systems. 2016. http://web.utk.edu/~qhe2/MembraneModule/Costs.html. Accessed on 10/02/2016

[83] American Water Works Association Research Foundation, Lyonnaise des Eaux, Water Research Commission of South Africa. Water Treatment Membrane Processes, McGraw Hill, U.S.,1996.

[84] A. Cipollina, G. Micale, and L. Rizzuti, editors. Seawater Desalination: Conventional and Renewable Energy Processes. Springer - Verlag, Heidelberg, Germany, 6th edition, 2009. pp. 103 - 106.

[85] American Water Works Association, editor. Reverse Osmosis and Nanofiltration, M46. American Water Works Association, U.S., 2nd edition, 2007. pp.117 - 118.

[86] World Health Organization. Guidelines for Drinking - water Quality. World Health Organization, Malta, 4th edition, 2011. pp.1 - 564.

[87] N. Bastaki. Performance of advanced methods for treatment of wastewater: UV TiO2, RO and UF. Chem. Eng. Process., 43 (2004) 935–940.

[88] A. Hassan, M. Al-Sofi, A. Farooque, A. Dalvi, A. Jamaluddin, N. Kither, A. Al-Amoudi, and I. Al-Tisan. A nanofiltration membrane pretreatment of SWRO feed and MSF make-up. Technical Report No 3807/98008-I, Saudi Arabia, 1999. pp.1 - 19.

[89] US Interior Reclamation Department. Water treatment primer for communities in need, 2013. URL http://www.usbr.gov/pmts/water/publications/primer.html. Accessed on 16/07/2013.

[90] M.C. Mickley, R. Hamilton, L. Gallegos, and J. Truesdall. Membrane concentrate disposal. Technical report, American Water Works Association Research Foundation and American Water Works Association, Colorado, U.S., 1993. pp.52.

[91] U.S. Energy Information Administration. Electric Power Monthly. 2013. URL http://www.eia.gov/electricity/monthly/epm_table_grapher.cfm?t=epmt_5_6_a. Accessed 05/04/2015.

[92] UNESCO Centre for Membrane Science and Technology. Emerging trends in desalination: A review. Technical report, National Water Commission, Canberra,

Australia, 2008. pp.1 - 96.

[93] National Physical Laboratory. Physical properties of sea water, 2015. URL http://www.kayelaby.npl.co.uk/general_physics/2_7/2_7_9.html. Accessed 02/05/2015.

[94] US Inflation Calculator. Inflation Calculator, February 2016. http://www.usinflationcalculator.com/. Accessed 10/02/2016.

[95] AmericanWaterWorks Association, editor. Desalination of Seawater, M61. AmericanWaterWorks Association,U.S., 1st edition, 2011. pp.1 - 99.

[96] E. Rosenthal. GAMS - A User's Guide. GAMS Development Corporation, Washington, DC, U.S., 2012.

[97] V. Lazarova, K.H. Choo, and P. Cornel. Water - energy Interaction in Water Reuse. IWA Publishing, London, UK, 1st edition, 2012. pp.228.

[98] S. Lattemann. Development of an Environmental Impact Assessment and Decision Support System for Seawater Desalination Plants. Taylor & Francis Group, LLC, US, 1st edition, 2010. pp.1 - 105.

[99] US Environmental Protection Agency. Regulatory Information By Sector, 2015. http://www2.epa.gov/regulatory-information-sector. Accessed 10/05/2015.

[100] M. Chowdhury, M.G. Mostafa, T.K. Biswas, and A.K. Saha. Treatment of leather industrial effluents by filtration and coagulation processes. Wat. Resour. Ind., 3 (2013) 11 – 22.

[101] K.Wang, B. Liu, H.D. Zhang and W. Zhao. Commissioning and operation of Heze some leather wastewater treatment plant, In: Proceedings of the 2014 International Conference on Mechatronics Engineering and Electrical Engineering (CMEEE 2014), Sanya, Hainan, P.R. China, 17 – 19 October 2014.

[102] A.V. Nieuwenhuijzen and J.V. Graaf, editors. Handbook on Particle Separation Processes, IWA Publishing, 2011, pp.8.

[103] C. Kaznaer, T. Wintgens and P. Dillon, editors, Water Reclamation Technologies for Safe Managed Aquifer Recharge, European Commission and IWA

Publishing, 2012, pp. 16 – 18

[104] P. Fox, S. Houston, P. Westerhoff, J.E. Drewes, M. Neilor, W.Yanko, R.Baird, M.Rincon, R.Arnoid, K.Lansey, R. Bassett, C.Gerba, M.Karpiscak, G. Amy and M. Reinhard. Soil Aquifer Treatment for Sustainable Water Reuse, AWWA Research Foundation and U.S. Environmental Protection Agency. 2001, pp.146 – 163.

[105] K.J.Howe and M.M. Clark. Coagulation Pretreatment for Membrane Filtration, AWWA Research Foundation, U.S., 2002

[106] Global B2B Marketplace. Alum, 2015. http://manufacturer.ec21.com/alum_flocculant.html. Accessed 03/05/2015.

[107] M.I. Al-Hamdi. Competition for Scarce Groundwater in the Sana'a Plain, Yemen. A study on the incentive systems for urban and agricultural water use. PhD thesis, Delft University of Technology, The Netherlands, 2000.

[108] J.M. Alhumoud, H. Al-Humaidi, I.N. Al-Ghusain and A.M. Alhumous. Cost/Benefit Evaluation of Sulaibiya Wastewater Treatment Plant in Kuwait. Int. Bus. Econ. Res. J., 9 (2010) 271 – 281.

[109] V. Lazarova, T. Asano, A. Bahri and J. Anderson. Milestones in Water Reuse. The Best Success Stories, IWA Publishing, UK, 2013, pp.6 – 20.

[110] N. Voutchkov. Considerations for selection of seawater filtration pretreatment system. Desalination, 261 (2010) 354 – 364.