20th International Congress on Modelling and Simulation, Adelaide, Australia, 1–6 December 2013
www.mssanz.org.au/modsim2013

An MILP Model for Cost - Effective Water Treatment Synthesis

M. N. Koleva, E. M. Polykarpou [a] and L. G. Papageorgiou [b]

[a]*UCL School of Energy and Resources, 220 Victoria Square, Adelaide, South Australia, Australia, 5000*
[b]*Centre for Process Systems Engineering, Dept. of Chemical Engineering, UCL, Torrington place, London, United Kingdom, WC1E 7JE*
Email: m.koleva@ucl.ac.uk

Abstract: Water is a precious and scarce resource, essential for sustaining nature, human life and industry. Efficient water treatment is recognised as the only method to sustain safe supplies of water in the future. So far scientific work has focused solely on the performance optimization of individual water purification units due to overall process complexity. A whole - systems approach in the area will be of a significant benefit to industry by increasing overall process efficiency and decreasing plant costs.

This work addresses the current gap by considering synthesis of water treatment trains using mixed integer linear programming (MILP). The model accounts for the most common contaminants found in water, secondary treated wastewater, seawater or brackish water. Such major pollution indicators are chemical oxygen demand (COD), biochemical oxygen demand (BOD), total dissolved solids (TDS), total suspended solids (TSS), turbidity and coliforms. The water source is treated to meet potable, process or reclaimed water standards. The set of candidate steps is selected to reflect the most extensively utilised industrial processes such as coagulation-flocculation, membrane filtration and UV disinfection at various operating conditions. The overall number of trains is minimised based on efficiency removal factors and final water purity specifications. The former takes into account the physicochemical properties of the contaminants and the respective regression models for rejection or retention of an addressed impurity in a certain candidate.

A particular case of desalination for drinking water supply is studied. The model is tested for the standard level of contaminants in seawater, TDS and TSS, to be removed by a set of up to 34 candidate trains. For production of ca. 600 m^3/h water the model identifies an optimum solution of overall 6 trains consisting of ultrafiltration (UF), nanofiltration(NF) and reverse osmosis (RO). The objective function minimised is the annual operating cost as a function of pumps electricity consumption, membrane cleaning and replacement practices. Overall, the results obtained agree with the recent trends in industrial desalination process synthesis and hence, the model can provide a valuable guidance in water purification processes design.

Keywords: *Water purification, MILP, efficiency removal factors, operating cost*

1 INTRODUCTION

With the view of population reaching 8 billion worldwide by 2025 water demand increases to ensure food, energy, personal uses and ecosystems supply (United Nations Water (2012)). Current efforts in research extensively focus on integrated water resources management and design of optimum water treatment processes to ensure safe and affordable water usage.

In particular, the synthesis of separation processes for industrial applications in preliminary design stage can have a significant impact on capital investment costs and annual operating costs associated with those processes. Therefore, there is an increasing interest in developing systematic and rational methods for optimising separation components and their interconnections (Nishida et al. (1992)). Such problems have two main objectives, of finding the nature of the separations and their optimum sequence, and optimum design variables for every separation method.

Purification of water, secondary treated wastewater, seawater and brackish water processes exhibit similarities with regard to the equipment that performs the separation. Hence, a general model can be built for different water sources and end users including a pool of various separation technologies that can be selected appropriately in order to achieve the final specifications.Tchobanoglous et al. (2003) discusses the removal of organic and inorganic colloidal, suspended and dissolved solids in water and secondary wastewater effluents, and the employed unit operations such as coagulation - flocculation, filtration, membrane filtration, ion exchange. Recently the spotlight in separation technology has shifted from conventional to non-conventional equipment. In particular pressure-driven membrane processes are preferred because of their efficiency and no need of fluid phase change (Chan and Tsao (2003)). In addition, seawater desalination by membrane processes such as nanofiltration, reverse osmosis and electrodialysis finds extensive recognition worldwide (Lior (2013)).

Numerous simulations, lab-based, pilot plant and industrial scale experiments have been performed in regression analyses by modelling and optimization of technologies performance such as coagulation - flocculation (Khayet et al. (2010)), carbon adsorption (Barkat et al. (2009)), microfiltration (Benitez et al. (2006)), ultrafiltration (Muthukumaran et al. (2010)), micellar-enhanced ultrafiltration (Landaburu-Aguirre et al. (2013)), nanofiltration (Boussu et al. (2008)), reverse osmosis (Khayet et al. (2010)), forward osmosis (Fang et al. (2013)), membrane distillation (Khayet et al. (2010)), ultraviolet treatment (Hijnen et al. (2005)). Economic appraisal of systems as an essential part of optimization has been discussed in various publications. For instance, Pickering and Wiesner (1993) proposed a cost model for low pressure membrane filtration, Lu et al. (2006) suggested an MINLP cost model for RO systems in desalination processes, Tsiakis and Papageorgiou (2005) considered optimal cost effective design of electrodialysis desalination plants. Research has also focused on MINLP modelling for water network synthesis (Tokos and Pintarich (2009),Khor et al. (2012)). Yet optimal synthesis of water purification processes has not been thoroughly explored.

In the present work a whole - system approach for the preliminary design of water treatment flowsheet is proposed with seawater desalination for production of potable water as a final product. Lastly, the results from the MILP model are discussed together with the computational performance.

2 PROBLEM DEFINITION

The mathematical representation of the problem to be solved is summarised below and has a particular focus on seawater desalination.

Given:

- a set of contaminants $(i : 1, 2, ..., I)$
- a set of technologies $(t : 1, 2, ..., T)$
- parameters: pressures (P_t), recoveries (Y_t) and efficiencies (η_{FP_t})
- continuous variables: contaminants concentrations $c_{i,t}$, flowrates Q_t, operating pump costs FP_t, membrane cleaning costs CC_t and membrane replacement costs RC_t

Determine:

- process flowsheet and minimal annual operating cost (OP)

The model assumes that no recycling is taking place, and one - stage and one - pass membrane configurations.

3 PURIFICATION EFFICIENCY

For any separation process contaminant removal efficiency to meet a given design purity specification, classifies as an essential performance criterion. Therefore, a core technological efficiency parameter in seawater desalination is the removal of major indicators such as TDS and TSS (Acton (2013)). Since the focus of the study is primarily on the pre-treatment and desalination sections, a reasonable starting point is to consider those major contaminant groups.

The removal efficiency of downstream water purification processes can be measured by removal, rejection, retention or deactivation coefficients as functions of the contaminants' physicochemical properties $(P_{i,t})$ (1) such as molecular weight and hydrophobicity, feed temperature, pressure and concentration, technology characteristics, etc (Benjamin and D.F.Lawler (2013), Scott and Hughes (1996), Xu et al. (2005)). It can take values between 0 and 1 as the former refers to no separation from contaminant and the latter refers to 100% separation achieved.

$$R_{i,t} = f(P_{i,t}) = 1 - \frac{c_p}{c_f}, \qquad \forall i, t \qquad (1)$$

In equation (1), c_p (mg/L) is the contaminant concentration in the permeate and c_f (mg/L) is the contaminant concentration in the feed. Each technique is associated with the rejection of an individual or multiple contaminants. It is assumed that a particular technique removes insignificant amounts of other, untargeted by the technique, contaminants and that in the presence of those contaminants in a mixture with targeted contaminants, the rejection coefficients still fairly accurately predict the removal efficiency of the targeted pollutants. The removal efficiency is represented in the form of regression models based on ANOVA analysis for each of the considered techniques in the current case study. The rest of the models are available in published literature (Khayet et al. (2010), Barkat et al. (2009), Landaburu-Aguirre et al. (2013), Khayet et al. (2010), Fang et al. (2013), Khayet et al. (2010), Hijnen et al. (2005)).

The separation efficiency of COD and colour from water by microfiltration (MF) is shown in equation (2) based on experimental work (Benitez et al. (2006)):

$$R_{i,t} = 0.126 + 0.001 \cdot T + 0.097 \cdot TMP, \qquad \forall t \in MF \qquad (2)$$

where T $(°C)$ and TMP (MPa) is the transmembrane pressure. For removal of turbidity by ultrafiltration (UF), equation (3) holds (Muthukumaran et al. (2010)) and the rejection is expressed as a function of the transmembrane pressure.

$$R_{i,t} = 0.959 - 1.510 \cdot TMP, \qquad \forall t \in UF \qquad (3)$$

It has been reported that turbidity and total suspended solids are roughly related (Gallegos (1993)). Hence, equation 3 can give an approximate estimation of suspended solids removal in seawater. The performance characteristics of nanofiltration membranes are affected by solute properties, solution pH and membrane characteristics such as pore size, hydrophobicity and surface roughness (Artug (2007)). Since seawater contains a large amount of dissolved organic matter (Duursma and Dawson (1981)), the retention of dissolved uncharged organic compounds, for nanofiltration (NF) can be approximated using contaminants hydrophobicity (H) and molecular weight cut - off $(MWCO)$ (Boussu et al. (2008)):

$$R_{i,t} = 0.01 \cdot (5.730 - 0.710 \cdot log(H) - 0.002 \cdot MWCO)^2, \qquad \forall t \in NF \qquad (4)$$

Seawater desalination reverse osmosis (RO) rejection coefficient for salt is represented in equation (5) as a function of the pressure (Chen and Guanghua (2005)):

$$R_{i,t} = 0.01 \cdot (89 + 34 \cdot P - 0.3 \cdot P^2), \qquad \forall t \in RO \qquad (5)$$

The TDS of interest in equation 5 are composed of K, Na, Mg, Ca, Ba, Sr, CO_3, HCO_3, NO_3, Cl, F, SO_4 and NH_4.

4 MATHEMATICAL MODEL

The mathematical optimization model for the case study is presented in the following section.

4.1 Concentrations constraints

The concentration of pollutant, i, after the first step is calculated by equation (6a). When a technique, t, is selected, the binary variable, $E_t = 1$, and the contaminant is reduced from an initial concentration of c_1 based on equation (1). Equation (6c) shows the interconnection between two potential candidates and equations (6d) and (6e) are disjunctions used to maintain the linearity of the model. A similar formulation is implemented in previous works for biochemical processes (Vasquez-Alvarez and Pinto (2004), Polykarpou et al. (2012)).

$$c_{p_{i,t}} = E_t \cdot c_1 \cdot (1 - R_{i,t}) + (1 - E_t) \cdot c_1, \qquad \forall t = 1, i \tag{6a}$$
$$c_{p_{i,t}} = c^{'}_{f_{i,t}} \cdot (1 - R_{i,t}) + c^{''}_{f_{i,t}}, \qquad \forall t > 1, i \tag{6b}$$
$$c_{p_{i,t-1}} = c^{'}_{f_{i,t}} + c^{''}_{f_{i,t}}, \qquad \forall t > 1, i \tag{6c}$$
$$c^{'}_{f_{i,t}} \leq E_t \cdot c_1, \qquad \forall t > 1, i \tag{6d}$$
$$c^{''}_{f_{i,t}} \leq (1 - E_t) \cdot c_1, \qquad \forall t > 1, i \tag{6e}$$

In the set above, $c_{p_{i,t}}$ (mg/L) is the pollutant concentration in the permeate, $c^{'}_{f_{i,t}}$ (mg/L) is the contaminant concentration in feed provided a candidate is selected and $c^{''}_{f_{i,t}}$ (mg/L) is the contaminant concentration when a candidate is not selected.

4.2 Flowrates constraints

The permeate flowrate, Q_p, is calculated using (7b). When a candidate is selected, the flowrate is reduced to $Q_f \cdot Y_t$ based on system recovery, Y, otherwise it takes the value of the feed. The first equation from (7) gives the initial mass balances starting from initial flowrate, Q_1 and every subsequent one is calculated from (7b).

$$Q_{p_t} = E_t \cdot Q_1 \cdot Y_t + (1 - E_t) \cdot Q_1, \qquad \forall t = 1 \tag{7a}$$
$$Q_{p_t} = Q^{'}_{f_t} \cdot Y_t + Q^{''}_{f_t}, \qquad \forall t > 1 \tag{7b}$$
$$Q_{p_{t-1}} = Q^{'}_{f_t} + Q^{''}_{f_t}, \qquad \forall t > 1 \tag{7c}$$
$$Q^{'}_{f_t} \leq E_t \cdot Q_1, \qquad \forall t > 1 \tag{7d}$$
$$Q^{''}_{f_t} \leq (1 - E_t) \cdot Q_1, \qquad \forall t > 1 \tag{7e}$$

To express the relation between the candidate trains, equation (7c) is inserted. For instance, provided a train is selected, the permeate from the previous train becomes the feed of the candidate of interest.

4.3 Operating costs constraints

The operating costs for the feed pumps FP_t are expressed in the following set of equations where bilinear tranformation was performed to linearize equation 8a:

$$FP_t = \frac{a \cdot C_e \cdot w_t \cdot P_{FP_t}}{\eta_{FP_t}}, \qquad \forall t \tag{8a}$$
$$\omega_t \leq E_t \cdot Q_1, \qquad \forall t > 1 \tag{8b}$$
$$\omega_t \leq Q_{f_t} + E_t \cdot Q_1, \qquad \forall t > 1 \tag{8c}$$
$$\omega_t \geq Q_{f_t} - E_t \cdot Q_1, \qquad \forall t > 1 \tag{8d}$$

where ω_t is a bilinear variable, a is a constant, η_{FP_t} is the efficiency of the feed pump prior to a train, and C_e is the electricity charge and has a value of 0.08 USD/kWh to account for any future increments from the U.S. Energy Information Administration (2013) review and to comply with literature values (Lu et al. (2006)). The maintenance costs are calculated from membrane cleaning (CC_t) costs in (9) and membrane replacement costs (RC_t) in (10):

$$CC_t = b \cdot E_t \cdot C_o \cdot N_u \cdot C_{cm}, \qquad \forall t \tag{9}$$

$$RC_t = \frac{E_t \cdot C_o \cdot N_u \cdot C_m}{c}, \qquad \forall t \tag{10}$$

where b and c are constants, C_o (USD) is the operating cost charge rate during maintenance, C_m (USD) is the membrane replacement cost per module and C_{cm} (USD) is the fixed cost for downtime (Lu et al. (2006)). It is assumed that cleaning or replacement takes place simultaneously for all trains, there are no pressure losses from pump to membrain train, every train contains the same number of membrane modules $N_u = 360$, cleaning is performed every 6 months, replacement is recommended every 5 years, and the annual operation is 300 days a year.

4.4 Target water purity constraints

The final water purity should not exceed the conditions imposed by the following constraint:

$$PS_{i,t} \leq M_i, \qquad \forall i,\ \forall t = T \tag{11}$$

where M_i is a maximum allowable concentration of a contaminant in mg/L. According to the World Health Organization (2011), potable water of good quality contains less than ca. 600 mg/L. No explicit limits for TSS exist in the Drinking Water Quality Guidelines. However, turbidity should be no more than 1 NTU but in practice, it is recommended to achieve less than 0.5 NTU. The relationship between turbidity and TSS given by Gallegos (1993) provides a rough estimate of the maximum allowable TSS concentrations which is 1.34 mg/L. Thus, the final purity specifications used in the model are less than 100 mg/L TDS and less than 1 mg/L TSS.

4.5 Objective function

The objective function of minimizing the annual operating cost (OP) is a sum of the pumps running costs (PC), membrane cleaning costs (CC) and membrane replacement costs (RC) for all the selected technologies.

$$OP = \sum_t (PC_t + CC_t + RC_t), \qquad \forall t \tag{12}$$

5 RESULTS

The model for the case study was tested on GAMS 23.9 (Rosenthal (2012)). The solver used was CPLEX on a Dell PC OptiPlex 9010 Core i5-3570 at 3.4 GHz and 3.89 GB RAM.

5.1 Case study: Seawater Desalination

In total there were 36 candidates - 9 MF, 5 UF, 9 NF and 11 RO trains. The initial flowrate was 5500 m^3/h.

Table 1. Desalination MILP model input

Technology	Pressure $[MPa]$	Temperature [°C]	Hydrophobicity $[-]$	Molecular weight cut-off $[Da]$	Recovery $[-]$	Pump efficiency $[-]$
MF	0.1 - 0.2	20 - 55	-	-	0.95	0.80
UF	0.1 - 0.3	-	-	-	0.90	0.75
NF	0.5 - 1.5	-	0.002 - 1	300 - 1200	0.60	0.85
RO	5.0 - 6.0	-	-	-	0.40	0.75

Source: Lu et al. (2006)

Figure 1 represents the soluton of the MILP model as UF1, UF2 and UF3 operate respectively at 0.10, 0.15 and 0.20 MPa, NF1 and NF2 at hydrophobicity of the components 0.002 and 0.01 at pH7, respectively, and MWCO 300 Da, and RO1 at 5.0 MPa. The final flowrate was estimated at 577 m^3/h with 15.8 mg/L TDS and 0.528 mg/L TSS. For a given option of train re-selection, the model chooses MF1, operating at 0.1 MPa, two times UF1, operating at 0.1 MPa, two times NF1 at 0.6 MPa and one time NF2 at 0.6 MPa.

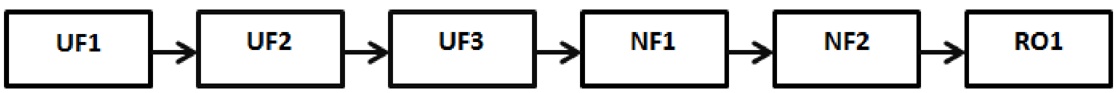

Figure 1. Optimal flowsheet for seawater desalination with option of no train re-selection

The annual running and maintenance cost returned by the solver was 2,913,471.5 USD, approximately 2 times higher than when the train re-selection option was used. In total, the model had 34 discrete variables, 437 continuous variables, and 637 single equations. It took CPLEX a total CPU time 3.77 seconds to return a solution for the no re-selection option and 230.96 seconds for the re-selection option. Majority of the current desalination plants use UF and NF as a pre-treatment to RO (DesalData (2013)). Therefore, the results generally agree with available industrial data.

6 CONCLUSIONS

In the present work, an optimization for the synthesis of water purification processes was presented. The mathematical problem for minimizing the annual operating cost was formulated as an MILP model and was solved for a case study of seawater desalination to meet potable water standards. The solution consists of the process flowsheet along with operating conditions, and an optimum integer solution was obtained. The selected trains demonstrated efficiency parameters with lower pressures, temperatures, hydrophobicity and molecular weight cut - off values in order to both meet the purity and costs constraints. The findings are consistent with literature as such operating and technology conditions result in higher rejection coefficients and require less energy consumption. In early design stages this model would be of a great benefit to estimate the most economically-wise flowsheet configurations.

A future extention of this work will involve expanding the pool of technologies for the presented case study, including conventional and emerging technologies. Furthermore, modelling fluxes to enable accurate determination of trains capacities, membrane fouling and cleaning will be another aspect for future work. Finally, envrionmental impacts on the flowsheet configuration are yet to be addressed.

ACKNOWLEDGEMENT

The authors would like to thank the financial support from the UCL School of Energy and Resources, Australia and BHP Billiton.

REFERENCES

Acton, Q. (2013). *Advances in Oxygen Research and Application*. Atlanta, Georgia, USA: Scholarly Editions.

Artug, G. (2007). *Modelling and Simulation of Nanofiltration Membranes*. Ph. D. thesis.

Barkat, M., D. Nibou, S. Chegrouche, and A. Mellah (2009). Kinetics and thermodynamics studies of chromium (vi) ions adsorption onto activated carbon from aqueous solutions. *Chemical Engineering and Processing*.

Benitez, F., L. Acero, and I. Leal (2006). Application of microfiltration and ultrafiltration processes to cork processing wastewaters and assessment of the membrane fouling. *Separation and Purification Technology 50*.

Benjamin, M. and D.F.Lawler (2013). *Water Quality Engineering: Physical/ Chemical Treatment Processes* (1st ed.). New Jersey: Wiley.

Boussu, K., C. Vandecasteele, and B. V. D. Bruggen (2008). Relation between membrane characteristics and performance in nanofiltration. *Journal of Membrane Science*.

Chan, W.-H. and S.-C. Tsao (2003). Fabrication of nanofiltration membranes with tunable separation characteristics using methods of uniform design and regression analysis. *Chemometrics and Intelligent Laboratory Systems 65*, 241–256.

Chen, J. and L. Guanghua (2005). Marine reverse osmosis desalination plant - a case study. *Desalination 174*.

DesalData (2013). Projects/plants.

Duursma, E. and R. Dawson (Eds.) (1981). *Marine Organic Chemistry. Evolution, Composition, Interactions and Chemistry of Organic Matter in Seawater* (4th ed. ed.). Amsterdam, The Netherlands: Elsevier Oceanography Series.

Fang, Y., L. Bian, and X. Wang (2013). Understanding membrane parameters of a forward osmosis membrane based on nonequilibrium thermodynamics. *Journal of Membrane Science*.

Gallegos, D. (1993). 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.

Hijnen, W. M., E. F. Beerendonk, and G. Medema (2005). Inactivation credit of uv radiation viruses, bacteria and protozoan (oo)cysts in water: A review. *Water Research*.

Khayet, M., C. Cojocaru, and M. Carcia-Payo (2010). Eperimental design and optimization of asymmetric flat-sheet membranes prepared for direct contact membrane distillation. *Journal of Membrane Science*.

Khayet, M., C. Cojocaru, and M. Essalhi (2010). Artificial neural network modelling and response surface methodology of desalination by reverse osmosis. *Journal of Membrane Science*.

Khayet, M., A. Y. Zahrim, and N. Hilal (2010). Modelling and optimization of coagulation of highly concentrated industrial grade leather dye by response surface methodology. *Chemical Engineering Journal*.

Khor, C., B. Chachuat, and N. Shah (2012). A superstructure optimization approach for water network synthesis with membrane separation - based regenerators. *Computers and Chemical Engineering 14*.

Landaburu-Aguirre, J., E. Pongracz, A. Sarpola, and R. Keiski (2013). Simultaneous removal of heavy metals from phosphorous rich rel wastewaters by micellar - enhanced ultrafiltration. *Separation and Purification Technology*.

Lior, N. (2013). *Advances in water desalination*, Volume 1. New Jersey: Wiley.

Lu, Y., Y. Hu, D. Xu, and L. Wu (2006). Optimum design of reverse osmosis seawater desalination system considering membrane cleaning and replacing. *Journal of Membrane Science vol.282*.

Muthukumaran, S., D. Nguyen, and K. Baskaran (2010). Performance evaluation of different ultrafiltration membranes for the reclamation and reuse of secondary effluent. *Desalination vol.279*.

Nishida, N., G. Stephanopoulos, and A. Westerberg (1992). A review of process synthesis. *AIChE Journal 27*, 321–351.

Pickering, K. D. and M. R. Wiesner (1993). Cost model for low - pressure membrane filtration. *Journal of Environmental Engineering vol. 119*.

Polykarpou, E. M., P. A. Dalby, and L. G. Papageorgiou (2012). A novel efficient optimization system for purification process synthesis. *Biochemical Engineering Journal 67*.

Rosenthal, E. (2012). *GAMS - A User's Guide*. Washington, DC, USA: GAMS Development Corporation.

Scott, K. and R. Hughes (Eds.) (1996). *Industrial Membrane Separation Technology* (1st ed.). Great Britain: Blackie Academic and Professional.

Tchobanoglous, G., F. Burton, and H. Stensel (2003). *Wastewater Engineering, Treatment and Reuse* (4th ed. ed.). New York: McGraw-Hill.

Tokos, H. and Z. N. Pintarich (2009). Development of a minlp model for the optimization of a large industrial water system. *Optimization and Engineering 13*.

Tsiakis, P. and L. Papageorgiou (2005). Optimal design of an electrodialysis brackish water desalination plant. *Desalination 173*.

United Nations Water (2012). Managing water under uncertainty and risk: The united nations world water development report 4.

U.S. Energy Information Administration (2013). Electric power monthly.

Vasquez-Alvarez, E. and J. M. Pinto (2004). Efficient milp formulations for the optimal synthesis of chromatographic protein purification processes. *Journal of Biotechnology 110*.

World Health Organization (2011). Guidelines for drinking - water quality. Technical report, Malta.

Xu, P., J. Drewes, C. Bellona, G. Amy, T. Kim, M. Adam, and T. Heberer (2005). Rejection of emerging organic micropollutants in nanofiltration - reverse osmosis membrane applications. *Water Environment Research 77*.