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Profit-based grassroots design and retrofit of water networks in process plants

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ABSTRACT

In this paper, we present a methodology for the grassroots design and/or retrofit of water utilization systems using mathematical optimization to maximize net present value (NPV) and/or return of investment (ROI) instead of minimizing freshwater consumption. The examples show that the solutions where savings and/or profit are maximized can be different from those where freshwater is minimized. They also differ from each other when ROI or NPV are used. In addition, when the NPV objective is used, the optimum solutions also vary depending on the interest rate used to calculate the discount factor.

1. Introduction

Water usage in the process industry especially water reuse and regeneration is a very well known and studied problem. Several review papers were recently written on the subject (Liu, Lucas, & Mann, 2004; Yoo et al., 2006), and a book (Mann & Liu, 1999). In order to design these systems, the tendency has been to minimize freshwater usage, sometimes as a true objective and sometimes as a substitute for a cost objective function using the assumption that freshwater costs is the dominant portion of the cost function.

Despite the aforementioned tendency to focus on freshwater consumption there are several articles that deal with minimizing cost objectives for grassroots design. Total annualized cost is used as the objective function by Chang and Li (2005), Guanaratnam, Alva-Argáez, Kokossis, Kim, and Smith (2005), Karuppiah and Grossmann (2006), and Alva-Argáez, Kokossis, and Smith (2007).

Articles that discuss profitability objectives explicitly for grassroots design are: Zhelev (2005), Wan Alwi and Manan (2006), Wan Alwi, Manan, Samingin, and Misran (2007), Lim, Park, Lee, and Park (2006), and Lim, Park, and Park (2007).

Zhelev (2005) uses a grid diagram analogous to Water Pinch, but targets optimum profitability. The case study used is for an energy recovery project and examples on water network systems are not explored. It analyzes three options that generates the same energy saving and then seeks for the maximum profit.

Wan Alwi and Manan (2006) search for a cost-effective grassroots design for water network involving a single contaminant. Their method is applied both for municipal and industrial sites and is not based on mathematical optimization. Instead they suggest a hierarchical procedure where a sequence of priority water management steps is established: after a payback limit is set, several water network options are investigated. In this sequential procedure, the maximum water recovery of each option is determined and the plot of investment vs. annual savings is generated. If the total payback period does not agree with the one previously set, some processes can be replaced in order to achieve the desired payback period. Wan Alwi et al. (2007) extend their previously presented hierarchical method to account for other steps of the hierarchy, which includes process changes.

Lim et al. (2006) consider an economic evaluation of a freshwater consumption-optimized water network. They analyze the profitability of the optimized network having the conventional water network as a baseline and applying incremental costs and benefits to rearrange the given network to a more operational friendly one. No regeneration processes are considered. Some insights of major contributors to the costs and benefits are presented. However, these findings cannot be necessarily generalized since they are based on a specific case example. In a second paper, Lim et al. (2007), the optimized water network is found directly by optimizing the net present value (NPV) using an NLP model (using MINOS). The formulation of the NPV equation is based in the principal contributors of the incremental costs and benefits found in their previous work. The addition of regeneration processes is not considered either and a maximum allowed flowrate is imposed for each water-using unit. Their results confirm that a network obtained

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Nomenclature

Parameters

FW^{old} existing system freshwater consumption
$C_m^{\max,in}$ maximum inlet of water-using unit "m"
$C_m^{\max,out}$ maximum outlet concentration of water-using unit "m"
$C_{w,j}$ concentration of the water source
$CR_{r,j}^{fixed}$ fixed outlet concentration of contaminant "j" in regeneration process "r"
$XNC_{r,j}$ connective parameter to indicate the treatment of contaminant "j" in regeneration process "r"
$\Delta m_{m,j}$ mass load of contaminant "j" in unit "m"
α cost of freshwater
eop cost of the end of pipe treatment
af annual factor
df discount factor
I discount rate
OP hours of operation per year.
OPN operational cost of the new regeneration processes
$ICUN_m$ investment costs of connection between a water-using unit "m" and the new regeneration process
$ICNU_m$ investment costs of connection between the new regeneration process and a water-using unit "m"
$ICUU_{m,m^*}$ investment costs of connection between the water-using unit "m" and water-using unit "m^*"
$ICNS$ investment costs of connection between the new treatment process and the sink
ICS pre-factor of the investment costs of the new regeneration process
ROI return on investment
FCI fixed capital cost
$U_{WU}^{(w,m)}$ maximum flowrate allowed between freshwater source "w" and water-using unit "m"
$U_{UU}^{(m,m*)}$ maximum flowrate allowed between water-using unit "m" and water-using unit "m^*"
$U_{UN}^{(m,r)}$ maximum flowrate allowed between water-using unit "m" and regeneration process "r"
$U_{NU}^{(r,m)}$ maximum flowrate allowed between regeneration process "r" and water-using unit "m"
$U_{NN}^{(r,r*)}$ maximum flowrate allowed between regeneration process "r" and regeneration process "r^*"
$U_{US}^{(m)}$ maximum flowrate allowed between freshwater source "w" and the sink
$U_{NS}^{(r)}$ maximum flowrate allowed between regeneration process "r" and the sink

Variables

$FW_{w,m}$ flowrate between the freshwater source "w" and water-using unit "m"
FUU_{m,m^*} flowrate between water-using unit "m" and water-using unit "m^*"
$FNU_{r,m}$ flowrate between the regeneration process "r" and water-using unit "m"
$FUN_{m,r}$ flowrate between water-using unit "m" and the regeneration process "r"
FNN_{r,r^*} flowrate between regeneration process "r" and regeneration process "r^*"
FNS_s flowrate between the regeneration process "r" and the sink
FS_m flowrate between water-using unit "m" and the sink
$C_{m,j}^{out}$ outlet concentration of contaminant "j" in unit "m"
$CR_{r,j}^{out}$ outlet concentration of contaminant "j" in regeneration process "r"
$CR_{r,j}^{in}$ inlet concentration of contaminant "j" in regeneration process "r"
$RegCap$ regeneration capacity (it is a parameter in the last part of the methodology)

Binaries (variables for MINLP model and parameters for NLP model)

$YWU_{w,m}$ new connections between freshwater source "w" and water-using unit "m^*"
YUU_{m,m^*} new connections between water-using unit "m" and water-using unit "m^*"
YNU_m new connections between the regeneration process "r" and water-using unit "m"
YUN_m new connections between the water-using unit "m" and the regeneration process "r"
YNS new connections between the regeneration process "r" and the sink
YUS new connections between water-using unit "m" and the sink
YNN_{r,r^*} new connections between the regeneration process "r" and regeneration process "r^*"

Indexes

j contaminants
m (or m^*) water-using units
r (or r^*) regeneration processes
w freshwater source

minimizing costs or freshwater consumption is not necessarily the most profitable ones.

In turn, retrofit projects for water systems are motivated by the need for capacity increase, product quality improvement, and environmental regulations, among others. In particular, one of the important issues concerning retrofit projects of water/wastewater systems are new environmental targets. Sometimes, there are economic incentives that come from cost reductions. While performing a retrofit to meet environmental targets could be mandated, retrofits to reduce freshwater costs as well as water treatment costs are not. In the latter case, profit drives the decision-making. Setting aside the need to approach the retrofit problem trying to meet environmental targets or maximize savings, the cost and finances management point of view (maximum profit) is still very important in any industrial competitive environment.

In retrofit projects there is the same need for profitable alternatives. A cost-effective retrofit project looking at reducing the environmental impact should have a precise description of the plant, be realizable in practice and the pollution impact should be fully defined in practical terms (Nourai, Rashtchian, & Shayegan, 2001). Even if the physical features are very well defined, relatively precise cost estimation is still primordial to reach the best retrofit alternative. This important implication is discussed in detail by Taal, Bulatov, Klemes, and Sterhlik (2003), who conclude that the use of complex methods does not guarantee the success of a retrofit design if reliable cost estimation is not available.

Bagajewicz, Rivas, and Savelski (2000) proposed a retrofit method that minimizes total cost (including cost with freshwater, capital cost and pumping cost) using mathematical programming. Later, Tan and Manan (2004) adapted the mass exchangers networks retrofit methodology presented by Fraser and Hallale (2000). This is a systematic methodology in which the targets are obtained before the network is designed. However, the targeting involves grassroots targets obtained using water pinch analysis. The retrofit is proposed by comparing the existing network and the suggestions inferred by the targeting technique. The design rules applied follows the ones presented by Wang and Smith (1994) for a single contaminant. Later, Tan and Manan (2006) presented another systematic methodology for the retrofit of single contaminant water networks through the optimization of existing regeneration units. The methodology is based on pinch analysis and the addition of new regeneration processes is not allowed. As the majority of graphical methods, the procedure consists of two stages, with a targeting step followed by the network design step. The problem is solved maximizing savings in operating cost under certain limits on minimum payback period and/or maximum capital expenditure. Tan, Manan, and Foo (2007) extended their approach to consider the optimum capacity and/or outlet concentration of the regeneration process as targets. This is also done using a two-step technique (targeting and design) based on pinch analysis. The procedure assumes both mass transfer and non-mass transfer based water-using units, a single contaminant network and only one type of regeneration.

Finally, Hul, Ng, Tan, Chiang, and Foo (2007) presented LP and MILP models to handle the retrofit of water networks where only source-sink type units are considered (fixed flowrates and outlet concentrations). Their approach evaluates different criteria in the optimization of water networks: Maximum water recovery with and without investment limits; wastewater reduction targets; processes constraint as forbidden connections; and, the combination of these criteria. The model cannot be applied for mass transfer type of water-using units. To handle their combined objective they use, fuzzy optimization.

Although successful methodologies have been presented by previous work, there is a lack of a methodology that can provide alternative designs so one can analyze them in a more comprehensive and profit related way and have a better understanding of the opportunities of each option as well as the costs and benefits.

In this paper we extend limited previous work (Faria & Bagajewicz, 2006) on a procedure for the grassroots design and retrofit of single and multicomponents water networks using cost, consumption and profitability as objectives. In both cases, the addition of regeneration process is allowed. The paper is organized as follows: We first present the Problem Statement, then we show the Mathematical Models followed by the Solution Methodology. Finally, examples are presented and discussed.

2. Problem statement

To define the problem we use definitions that are similar to those used in previous work. We just state them here for completeness:

Grassroots: Given

- a set of process systems in need of water for washing operations,
- a set of freshwater sources of different pollutants concentration, and
- a set of potential regeneration processes to be installed,

it is desired to determine what freshwater use is needed in each process, what water reusing connections are needed and what capacity of regeneration processes (if any) is needed to maximize profit or minimize cost.

We assume that any regeneration process has a fixed outlet concentration of at least one contaminant (sometimes a maximum capacity limitation for this process is added). This is particularly true for certain operations, like the removal of solids. Additionally, capital for investment may be limited.

Retrofit: Given

- an existing water network (water-using units, freshwater sources, regeneration processes and end-of-pipe treatment),
- a set of new processes in need of water for washing operations to be added (if any),
- a set of required capacity expansions of existing processes,
- a set of regeneration processes that are available for installation (if needed), and
- new freshwater sources available,

it is desired to determine what re-piping and what capacity of a new treatment process (if any) is needed to maximize targets (profit or savings).

Maximum inlet and outlet concentrations as well as fixed mass loads of the water-using units and freshwater concentrations are used. The economic parameters include the cost of freshwater, operational costs of the end-of-pipe treatment and the regeneration process, the capital cost of the new potential connections and the new potential regeneration processes.

3. Mathematical model

The constraints of the mathematical model for both grassroots design and retrofit of water networks with multiple contaminants are the following standard ones:

Material and component balances:

Balance of water in the units:

$$\sum_{w \in W} FW_{w,m^*} + \sum_{r \in R} FNU_{r,m^*} + \sum_{m \neq m^* \in M} FUU_{m,m^*} = \sum_{r \in R} FUN_{m^*,r} + FS_{m^*} + \sum_{m \neq m^*; m \in M} FUU_{m^*,m} \quad \forall m^* \in M \tag{1}$$

Balance of water in treatment/regeneration processes:

$$\sum_{m \in M} FUN_{m,r^*} + \sum_{r \neq r^*; r \in R} FNN_{r,r^*} = FNS_{r^*} + \sum_{m \in M} FNU_{m,r^*} + \sum_{r \neq r^*; r \in R} FNN_{r^*,r} \quad \forall r^* \in R \tag{2}$$

Balance of contaminant in the units:

$$\sum_{w \in W} FW_{w,m^*} * C_{w,j} + \sum_{r \in R} FNU_{r,m^*} * CR^{out}_{r,j} + \sum_{m \neq m^*; m \in R} FUU_{m,m^*} * C^{out}_{m,j} + \Delta m_{m^*,j} = \left(\sum_{r \in R} FUN_{m^*,r} + FS_{m^*} + \sum_{m \neq m^*; m \in M} FUU_{m^*,m} \right) * C^{out}_{m^*,j} \quad \forall m^* \in M, \ \forall j \in J \tag{3}$$

Limit of inlet concentration of contaminants in the units:

$$\sum_{w \in W} FW_{w,m^*} * C_{w,j} + \sum_{r \in R} FNU_{r,m^*} * CR^{out}_{r,j} + \sum_{m \neq m^*; m \in M} FUU_{m,m^*} * C^{out}_{m,j} \leq$$

$$\times\left(\sum_{r\in R} FUN_{m^*,r}+FS_{m^*}+\sum_{m\neq m^*;m\in M} FUU_{m^*,m}\right) * C^{\max,in}_{m^*,j}\quad \forall m^*\in M,\ \forall j\in J \tag{4}$$

Limit of outlet concentration of contaminants in the units:

$$C^{out}_{m^*,j}\le C^{\max,out}_{m^*,j}\quad \forall m^*\in M,\ \forall j\in J \tag{5}$$

Balance of contaminants in treatment/regeneration processes: A material balance at the inlet of the regeneration process is needed to identify the outlet concentrations of the contaminants that are not being treated by the respective regeneration process. Additionally, an equation using a connective binary parameter $XNC_{r,j}$ equal to one if treatment/regeneration process r treats contaminant j; and, 0 otherwise, is necessary To establish what is the outlet concentration of that particular contaminant.

$$\sum_{m\in M} FUN_{m,r^*} * C^{out}_{m,j}+\sum_{r\neq r^*;r\in R} FNN_{r,r^*} * CR^{out}_{r^*,j} = CR^{in}_{r^*,j} * \left(\sum_{m\in M} FUN_{m,r^*}+\sum_{r\neq r^*;r\in R} FNN_{r,r^*}\right)\quad \forall r^*\in R,\ \forall j\in J \tag{6}$$

$$CR^{out}_{r,j}=CR^{in}_{m,j} * (1-XNC_{r,j})+CR^{fixed}_{m,j} * XNC_{r,j}\quad \forall r\in R,\ \forall j\in J \tag{7}$$

Existence of new connections: Binary variables (Y) are used to determine if a new connection is established and the following classical “big M” constraints are used to count the capital cost of the new connections.

$$FW_{w,m}\le U^{(w,m)}_{WU} * YWU_{w,m}\quad \forall w\in W,\ \forall m\in M \tag{8}$$

$$FUN_{m,r}\le U^{(m,r)}_{UN} * YUN_{m,}\quad \forall m\in M,\ \forall r\in R \tag{9}$$

$$FNU_{r,m}\le U^{(r,u)}_{NU} * YNU_{r,m}\quad \forall m\in M,\ \forall r\in R \tag{10}$$

$$FUU_{m^*,m}\le U^{(m^*,m)}_{UU} * YUU_{m^*,m}\quad \forall m^*\in M,\ \forall m\in M \tag{11}$$

$$FNN_{r^*,r}\le U^{(r^*,r)}_{NN} * YNN_{r^*,r}\quad \forall r^*\in R,\ \forall r\in R \tag{12}$$

$$FS_m\le U^{(m)}_{MS} * YMS_m\quad \forall m\in M \tag{13}$$

$$FNS_r\le U^{(r)}_{NS} * YNS\quad \forall r\in R \tag{14}$$

When connections already exist the binary variables are set to one and the respective capital cost set to zero.

Treatment/regeneration capacity: The flowrate through the treatment/regeneration unit is limited by the unit capacity:

$$\sum_{m\in M} FUN_{m,r^*}+\sum_{r\neq r^*;r\in R} FNN_{r,r^*}\le RegCap_{r^*}\quad \forall r^*\in R \tag{15}$$

As in the case of existing connections, the capacities of an existing treatment/regeneration processes are set and the capital cost parameters are zero. For the cases in which the new regeneration processes can be added, the regeneration capacity ($RegCap_r$) is in some instances treated as a variable (design mode) or as a parameter (evaluation mode), as described below.

3.1. Objective functions

We consider the case of retrofit because it is more general and we then show how the objectives reduce to the grassroots case. Let FW^{old} be the existing system freshwater consumption, which is a fixed value and assume that operational costs are direct function of flowrates (freshwater and regenerated flowrate); then, the following objective function maximizes net savings:

$$Max\left[\left(\begin{array}{l}\sum_{w\in W}\left(FW^{old}_w-\sum_{m\in M} FW_{w,m}\right) * \alpha_w\\ +\sum_{r\in R_{ex}} OPN^{old}_r * \left(\sum_{m\in M_{ex}} FUN^{old}_{m,r}+\sum_{r*\in R_{ex}} FNN^{old}_{r^*,r}\right)\\ -\sum_{r\in R_{new}} OPN^{new}_r * \left(\sum_{m\in M_{new}} FUN_{m,r}+\sum_{r^*\in R_{new}} FNN_{r^*,r}\right)\end{array}\right) * OP-FCI * af\right] \tag{16}$$

In the case of grassroots design, we have $FW^{old}=0$, $FNN^{old}_{r^*,r}=0$ and $FUN^{old}_{m,r}=0$, which makes the problem one of minimizing costs.

The first part of the equation represents the savings obtained from freshwater and end of pipe treatment flowrate reduction. In this expression, FW_m and α are the flowrate and cost of freshwater, respectively. The model can be extended to make these costs function of inlet concentrations of pollutants. The next term is devoted to regeneration costs, where OPN^{new}_r and OPN^{old}_r are the operational cost of the regeneration processes (new and old), $FUN_{m,r}$ are the flowrates between the water-using units and the regeneration process r and $FNN_{r^*,r}$ are the flowrates between two regeneration processes. Finally, OP represents the hours of operation per year. The last term is the annualized capital cost invested in the retrofit, where FCI is the fixed capital cost and af is any factor that annualizes the capital cost (usually $1/N$, where N is the number of years of depreciation). The fixed capital of investment is calculated using the sum of the piping costs and the new regeneration units costs as follows:

$$FCI=\sum_{m\in M}\left(\begin{array}{l}\sum_{w\in W} YWU_{w,m} * ICWU_{w,m}+\sum_{r\in R}(YUN_{m,r} * ICUN_{m,r}+YNU_m * ICNU_m)\\ +\sum_{m^*\neq m,m^*\in M} YUU_{m,m^*} * ICUU_{m,m^*}+YUS_m * ICUS_m\end{array}\right) +\sum_{r\in R}\left(\sum_{r^*\neq r;r^*\in R} YNN_{r,r^*} * ICNN_{r,r^*}+YNS_r * ICNS_r+ICN_r * (RegCap_r)^{0.7}+YNS_r * ICNS_r\right) \tag{17}$$

The first term represents the capital costs with connections between the regeneration process and water-using units, and the capital cost associated to connections between two water-using units and end-of-pipe treatment. The second term corresponds to the capital costs of the connection between two new regeneration processes, between the new regeneration processes and the end of pipe treatment and the capital cost of the new regeneration treatments. The cost of the regeneration units is assumed to be a function of the regeneration process capacity only.

Note that for the retrofit case and a single source of water, when there is no capital investment to depreciate ($af=0$), $OPN_{FT}^{old}=OPN_{FT}^{new}$ (unchanged end of pipe treatment) and no regeneration is used, then Eq. (16) reduces to minimizing freshwater consumption. However, even if the end of pipe treatment cost does not change, when regeneration is present, even if $OPN_r^{new}=OPN_r^{old}$ the objective is not equivalent to minimizing freshwater consumption. Indeed, under these conditions, Eq. (16) becomes

$$Min\left[\left(\sum_{w\in W}\sum_{m\in M}FW_{w,m}*\alpha_w+\sum_{r\in R_{new}}OPN_r^{old}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\right)\right] \quad (18)$$

which can be rewritten as follows when water from the final treatment is not recycled but entirely disposed of (the usual assumption in many methods):

$$Min\left[\left(\sum_{w\in W}\sum_{m\in M}FW_{w,m}*(\alpha_w+OPN_{FT}^{old})+\sum_{r\in R_{new};r\neq FT}OPN_r^{old}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\right)\right] \quad (19)$$

This last expression cannot be argued to be equivalent to minimizing freshwater consumption. The reason stems from the costing, which in this expression is not tied to the amount of pollutant removal, but to flows. In other words, if the operating costs would be only the cost of chemicals needed to remove the pollutants, then this would be a fixed amount because the amount of pollutants to remove in the whole network is fixed. However, even if the same amount of chemicals is used, the treatment units may receive water at different concentrations, and therefore require to manipulate larger or smaller flows. The operating cost related to moving fluids, which is what we use, can therefore vary. This invalidates arguments that freshwater consumption minimization is a valid economic goal when regeneration is used.

An alternative objective function for retrofit is the net present value (*NPV*)

$$Max\left[\begin{pmatrix}\sum_{w\in W}\left(FW_w^{old}-\sum_{m\in M}FW_{w,m}\right)*\alpha_w\\ +\sum_{r\in R_{ex}}OPN_r^{old}*\left(\sum_{m\in M_{ex}}FUN_{m,r}^{old}+\sum_{r^*\in R_{ex}}FNN_{r^*,r}^{old}\right)\\ -\sum_{r\in R_{new}}OPN_r^{new}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\end{pmatrix}*OP*df-FCI\right] \quad (20)$$

where the discount factor *df* is the sum over *N* years of the different discount factors, that is

$$df=\sum_{n=1}^{N}\frac{1}{(1+i)^n} \quad (21)$$

Finally, the return of investment (ROI) for retrofit is given by

$$Max\frac{\begin{pmatrix}\sum_{w\in W}\left(FW_w^{old}-\sum_{m\in M}FW_{w,m}\right)*\alpha_w\\ +\sum_{r\in R_{ex}}OPN_r^{old}*\left(\sum_{m\in M_{ex}}FUN_{m,r}^{old}+\sum_{r^*\in R_{ex}}FNN_{r^*,r}^{old}\right)\\ -\sum_{r\in R_{new}}OPN_r^{new}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\end{pmatrix}*OP}{FCI} \quad (22)$$

In the case of grassroots design $FW_w^{old}=0$, $FNN_{r^*,r}^{old}=0$ and $FUN_{m,r}^{old}=0$, which in the case of Eq. (20), makes the problem one of minimizing the net present costs (NPC). In the case of ROI, Eq. (22) turns into a minimization of operating costs per unit capital invested. One would not use ROI in a grassroots context because there is no profit to talk about, and therefore Eq. (22) leads to such an unusual concept. Thus, for grassroots design we redefine ROI with respect to a reference network, which we call return on extra investment (ROEI). We will present details of this together with the examples.

3.2. Solution methodology

The methodology consists of maximizing Net Savings first (Eq. (16)) subject to the set of constraints given by Eqs. (1)–(15) and then calculating *NPV* (Eq. (20)) and *ROI* (Eq. (22)). To do this, we first determine the range of feasible freshwater consumption, which is defined as the interval from the minimum possible freshwater consumption of the network to its maximum freshwater consumption, which we consider is the consumption under no reuse conditions. The freshwater consumption under no reuse conditions, which is the maximum value of the range, considers the water-using units are operating under their minimum flowrate. The minimum consumption is obtained using the conventional minimum freshwater consumption model, that is, the same model as above (Eqs. (1)–(15)) and the following objective:

$$Min\sum_{w\in W}\sum_{m\in M}FW_{w,m} \quad (23)$$

In turn, the maximum freshwater consumption, given by the consumption of a conventional network in which no reuse exists

Table 1
Limiting process water data.

Process number	Mass load of contaminant	C_{in} (ppm)	C_{out} (ppm)
1	2 kg/h	0	100
2	5 kg/h	50	100
3	30 kg/h	50	800
4	4 kg/h	400	800

and the all the water-using units are fed by freshwater and operate at their minimum freshwater consumption (FW^{old} for the retrofit case, which is the flowrate of the existing network) can be obtained by simple construction.

Subsequently, when savings (Eq. (16)) are maximized for fixed freshwater consumption inside the aforementioned range, the respective capital investments (Eq. (17)) are calculated and the corresponding *NPV* (Eq. (20)) and *ROI* (Eq. (22)) are obtained. When plotting these results (Savings, FCI, NPV or ROI vs. Freshwater flowrate), different points correspond to different networks and also different capacities of the new regeneration process (if any) are found. Once the networks are identified, they are ranked according to different criteria. Finally, incremental analysis is performed.

These models are MINLP formulations that have been solved using DICOPT (CONOPT/CPLEX) as the solver in the GAMS platform.

4. Single contaminant example

The following one component example was adapted from Example 1 of Wang and Smith (1994). The limiting process data for this problem are shown in Table 1 and it has a freshwater consumption without reuse (conventional network configuration) of 112.5 ton/h.

The cost of freshwater is α_i (\$/ton) = 0.3 and the system operates OP (h/year) = 8600. The freshwater concentration was assumed to be equal to zero. The end of pipe treatment has an operating cost OPN_r (\$/ton) = 1.0067 and an investment cost ICN_r (\$/ton$^{0.7}$) = 19,400.

A potential new regeneration process is available for the grassroots design and the retrofit case. Its capital cost is *ICN* (\$/ton$^{0.7}$) = 16,800 and the operational cost is assumed to be *OCN* (\$/ton) = 1.00. Only one regeneration unit with outlet concentration of 10 ppm is considered. Finally, in the profitability analysis a 10 years period (af = 0.1) is used.

4.1.1. *Grassroots design case*

The costs of connections for the superstructure of this network are presented in Table 2. Other cost data were presented above.

The feasible range of freshwater usage of this system is determined to be between the minimum freshwater consumption (20 ton/h) and the consumption required by a network with no reuse (112.5 ton/h). Fig. 1 gives the optimum annualized total cost profile obtained when it is minimized (Eq. (16)) through the range of freshwater usage. This MINLP problem has 59 constraints, 38 continuous variables and 29 binary variables.

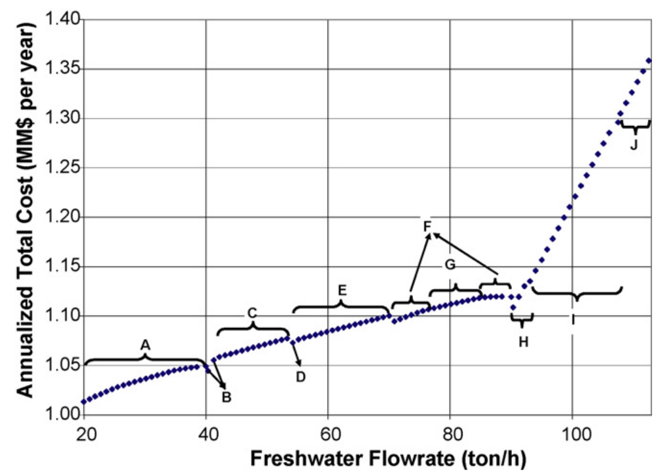

Fig. 1. Annualized total cost as a function of freshwater flowrate for the grassroots design.

Ten different networks were found as optimum as a function of freshwater consumptions as shown by those profiles. The networks are summarized in Table 3, by indicating their connections and the minimum freshwater consumption they can reach. Network A represents the optimum solution when annualized total cost is minimized. For this case, it also represents the network that is able to reach the minimum consumption. Fig. 2 shows networks A, B, H and I (we ignore the rest) because they will become relevant in the discussion that follows. Network B exhibits one interesting feature: it is disconnected and exhibits a loop involving two units and a regeneration without discharge. Usually, because of possible build up of undesired contaminants, one would tend to disregard such a network. For the sake of completeness, we consider it acceptable, assuming that all these other contaminants are somehow taken care of in the regeneration unit.

If freshwater consumption is not a primordial issue (i.e. when freshwater is largely available and is cheap) and/or there are limitations in the investments, one may want to analyze this graph together with the FCI graph. Fig. 3 shows the fixed capital cost profiles of the networks presented in Fig. 1 along the range of freshwater usage. Although the costs of connections are constant for each network, the capital cost of the regeneration process and the end-of-pipe treatment vary. In fact as one increases the other decreases (Fig. 4). From the FCI graph we can note that network C is the one in which the highest investment cost is required. If budget is an important issue for the project, network C may become an unattractive option. The effects of budgets limitations will be further discussed later.

The same solutions are obtained when the NPC (Eq. (20)) is directly optimized (Fig. 5). Variation on the rate of discount points at different optimal networks. The difference between the minimum and maximum NPC when a 5% rate of discount is used is around MM\$2.6. When a 20% rate of discount is used, this difference reduces to approximately MM\$1.3. Although larger discount

Table 2
Capital costs of the connections.

	Unit 1	Unit 2	Unit 3	Unit 4	Reg.	End of pipe treatment
FW	\$39,000	\$76,000	\$47,000	\$92,000	–	–
Unit 1	–	\$150,000	\$110,000	\$45,000	\$145,000	\$83,000
Unit 2	\$50,000	–	\$134,000	\$40,000	\$37,000	\$102,500
Unit 3	\$180,000	\$35,000	–	\$42,000	\$91,000	\$98,000
Unit 4	\$163,000	\$130,000	\$90,000	–	\$132,000	\$124,000
Reg.	\$33,000	\$130,000	\$50,000	\$98,000	–	\$45,000

Table 3
Networks for grassroots design (reuse of end-of-pipe wastewater not allowed).

Network	Connections	Min consumption
A	W-U1, U1-U3, U1-U4, U2-U4, U3-U4, N1-U2, N1-U3, U3-EoPT, U4-N1, EoPT-S	20 ton/h
B	W-U1, W-U3, U1-U3, U2-U4, N1-U2, U3-EoPT, U4-N1, EoPT-S	40 ton/h
C	W-U1, W-U2, W-U3, U1-U3, U2-U4, U3-U4, N1-U2, U4-N1, U4-EoPT, EoPT-S	40 ton/h
D	W-U1, W-U2, W-U3, U1-U3, U2-U4, N1-U2, U3-N1, U4-EoPT, EoPT-S	54 ton/h
E	W-U1, W-U2, W-U3, U1-U3, U2-U4, U3-U4, N1-U2, U3-N1, U4-EoPT, EoPT-S	54 ton/h
F	W-U1, W-U2, U1-U3, U1-U4, U2-U4, N1-U3, U2-N1, U3-EoPT, U4-EoPT, EoPT-S	70 ton/h
G	W-U1, W-U2, W-U3, U1-U3, U1-U4, U2-U4, N1-U3, U2-N1, U3-EoPT, U4-EoPT, EoPT-S	70 ton/h
H	W-U1, W-U2, U1-U3, U2-U4, U3-EoPT, U4-EoPT, EoPT-S	90 ton/h
I	W-U1, W-U2, U1-U3, U2-U4, U3-U4, U4-EoPT, EoPT-S	92.5 ton/h
J	W-U1, W-U2,W-U3, U1-U4, U2-U4, U3-U4, U4-EoPT, EoPT-S	107.5 ton/h

Abbreviations—W: freshwater, Ui: Unit *i*, N1: Treatment/Regeneration unit 1, EoPT: End of Pipe treatment, S: sink.

rates are unlikely, we investigated their effect to analyze if the optimal solution might change (Fig. 6) and it does in favor of solutions with lower FCI as one might expect.

We now analyze the cost and profitability of the network options previously suggested in comparison to the initial investments needed. For that, a typical rate of discount of 9% is considered. In both cases (annualized total cost and NPC), network A shows the lowest objective value. However, if one considers also the initial investment (FCI), additional conclusions can be obtained. Fig. 7 shows the annualized total cost vs. FCI and NPC vs. FCI. The optimum capacities of the regeneration process and end-of-pipe treatment for each of the networks are presented in Table 4.

4.1.2. *Evaluation of budget limitations*

Considering the solutions previously obtained, note that if the budget is constrained to be lower than $1,190,000, the optimum solution (minimum NPC) is network B instead network A. Network B has a NPC of $7,112,219 (for a 9% discount rate). This network does not use the whole budget since it has an FCI around $1,134,000.

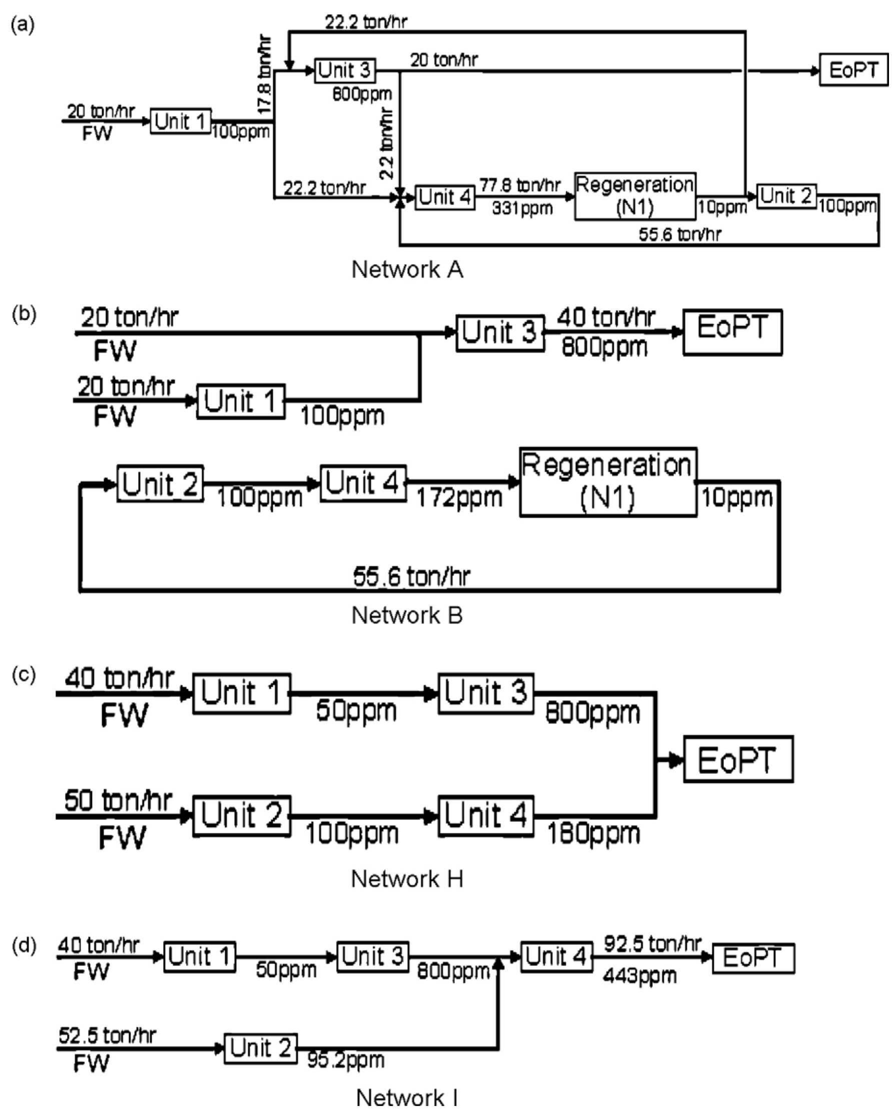

Fig. 2. Selected networks from Table 3.

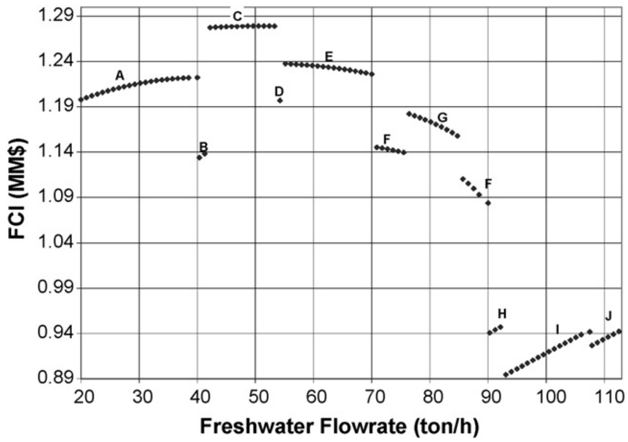

Fig. 3. FCI as a function of freshwater flowrate grassroots design.

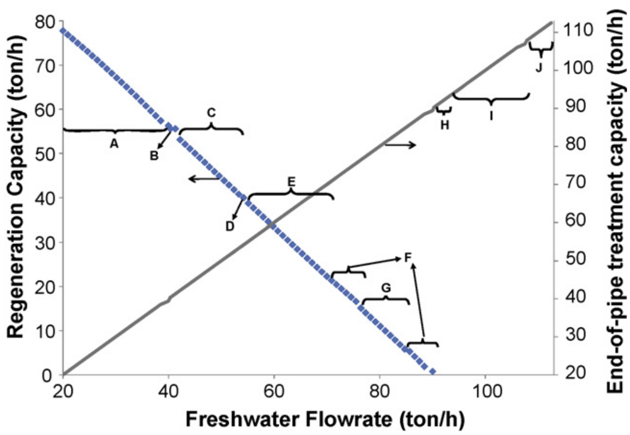

Fig. 4. Regeneration and end-of-pipe treatment capacities as a function of freshwater consumption.

Due to its isolated loop without discharge (or any other reason), one may not consider network B. In this case other options can be analyzed. To better organize this information we calculate the marginal values of annualized total cost and NPC and show them in Fig. 7. Network B is chosen as the reference network because it is the optimum solution for a $1,190,000 budget limit case. Thus, marginal values of the other suggested networks can be calculated by simply computing the change in costs (cost of a given network minus

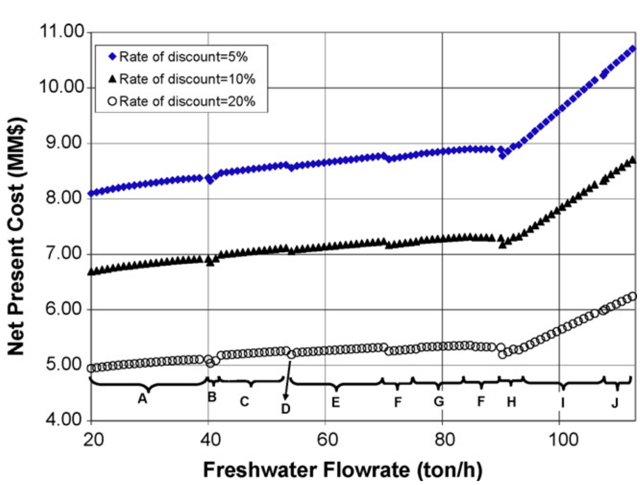

Fig. 5. NPC using different rates of interest as a function of freshwater flowrate in the grassroots design.

Table 4
Regeneration and end-of-pipe treatment capacity of the networks analyzed in Fig. 5.

	Regeneration capacity	EOP capacity
Network A	77.8 ton/h	20 ton/h
Network B	55.6 ton/h	40 ton/h
Network C	55.6 ton/h	40 ton/h
Network D	40 ton/h	54 ton/h
Network E	40 ton/h	54 ton/h
Network F	22.3 ton/h	70 ton/h
Network G	22.3 ton/h	70 ton/h
Network H	–	90 ton/h
Network I	–	92.5 ton/h
Network J	–	107.5 ton/h

the optimum network). The first quadrant contains the solutions that do not give any advantages in terms of the analyzed objective, the second shows networks in which the budget constraint is violated, but they provide a better solution in terms of the objective function and, the third one is always empty since the graph is done using the optimum solution of a budget limited case. Finally, the last quadrant provides information of networks that require a lower investment, but result in a larger objective function. The second and fourth quadrants are the ones with interest in this analysis and will be discussed further.

First, we note that networks C, D, E, F and G do not give any advantage in terms of either annualized total cost or NPC. Then, we look at the issue of how much we are losing for not having a higher budget (second quadrant). In this case we can see that with a $64,000 investment higher (which represents only $8,000 more than the budget), we would be able to decrease the annualized cost by $30,000 and NPC by $177,000 (network A).

Now if we look the graph considering the former discussion (how much more you are investing to gain a certain delta in NPC—fourth quadrant) and assuming that no more money can be put in this project (the maximum is $1,190,00), another interesting point can be made. In this case, network H would give a annualized total cost $64,000 higher and would increase the NPC by $343,000. On the other hand, network H has a lower investment ($193,000 lower than network B and $249,285 lower than the budget).

A similar analysis can also be done considering a measurement of return on investment. Because this is a grassroots design, no direct profit can be calculated. However, it is known that one important objective function used by previous works (Hallale and Fraser, 1998, 2000a, 2000b) is the minimization of capital cost (FCI). To evaluate this choice, one can now consider the optimum solution obtained when FCI is minimized (Eq. (17)) and use it as a reference solution. Thus, the Return on Extra Investment (ROEI) can be calculated as follows:

$$ROEI = \frac{OperatingCost^{ref} - OperatingCost}{FCI - FCI^{ref}} \quad (23)$$

This analysis is important when freshwater is not an important issue and capital cost is the main concern. In this case, one may think at first that the minimum capital of investment is the best choice. However, we show that some better opportunities can be missed.

For this example, network I presents the minimum FCI and accordingly is the reference network. Fig. 8 shows the ROEI as function of the freshwater flowrate considering the optimum ranges found from the minimization of annualized total cost (Figs. 1–4).

The maximum ROEI as function of incremental FCI is shown in Fig. 9. Because of its negative value (−457%), network J was excluded from the figure. Now, from the ROEI point of view, the optimum network is network H, which gives a 67% return on extra investment. This network also corresponds to the one with the lowest extra investment. Note that network J represents a bad choice from the

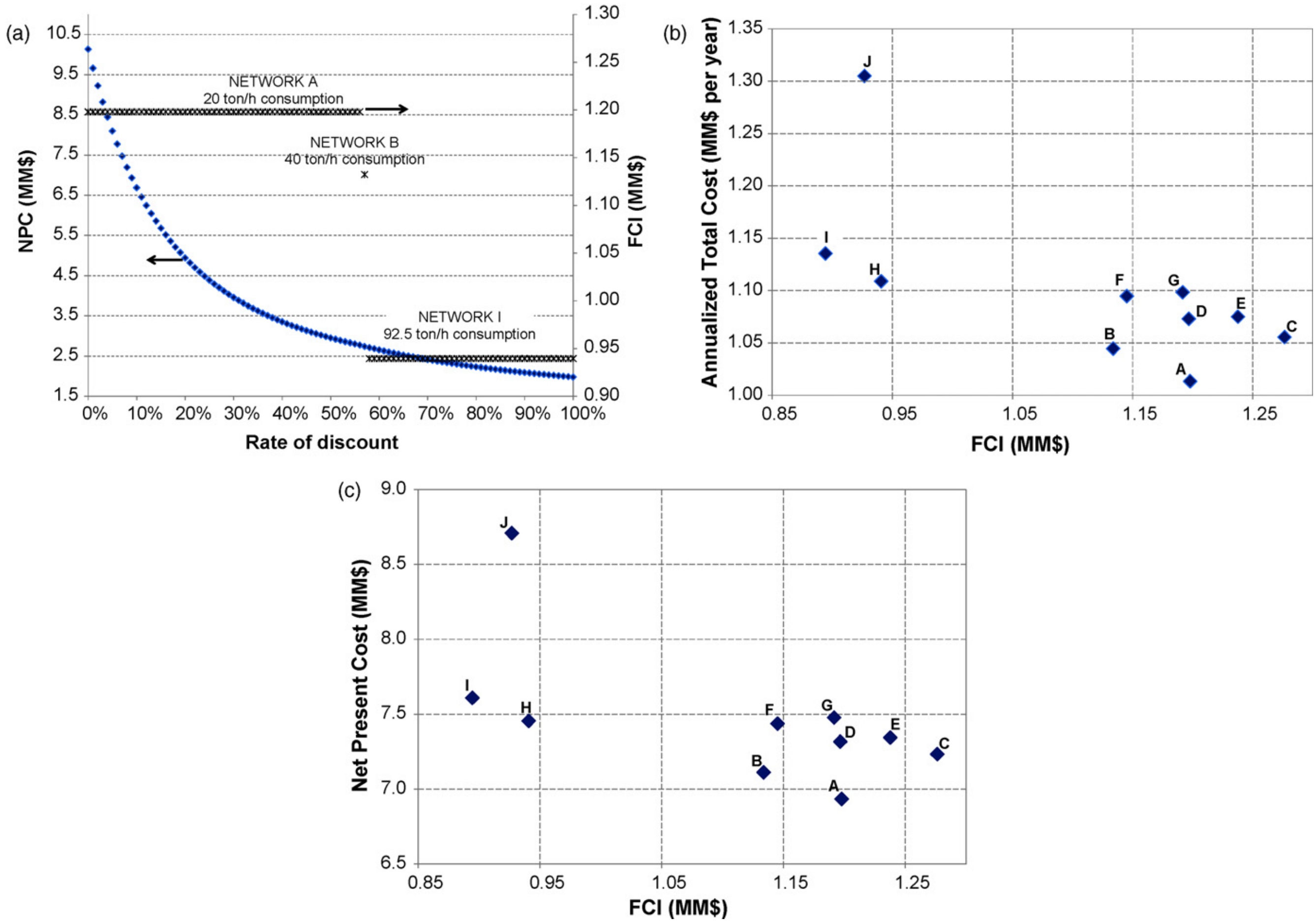

Fig. 6. (a) NPC and FCI as a function of rate of discount; (b) Annualized total cost as function of FCI; (c) NPC as a function of FCI.

return on extra investment perspective since it has a higher FCI and a higher operating cost.

Table 5 summarizes the results (the FCI, Total cost, NPC and ROEI are calculated at the minimum freshwater consumption). One can see the importance of looking at this problem from a more comprehensive view of the opportunities, which allows the designer to make a decision based on the level of importance and priorities of the project, current financial situation of the company, available budget, etc.

4.1.3. Retrofit case

For the retrofit case, a conventional network (no water reuse) in which no regeneration process exists is assumed. That is, the current network has only the connection between the water source and units and between units and the end of pipe treatment. The investment costs of new connections and available new regeneration processes are needed. The costs previously presented are used in this case as well. However, the capital cost of existing connec-

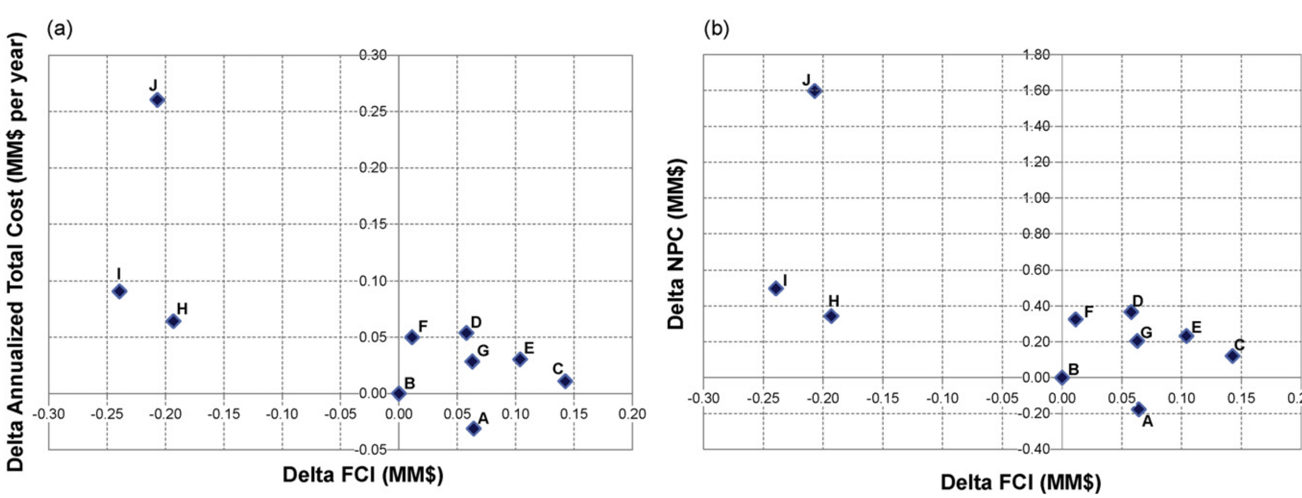

Fig. 7. (a) Marginal annualized total cost. (b) Marginal (grassroots case when reuse of end-of-pipe wastewater is not allowed).

Table 5
Summary of results—grassroots case.

Network	Minimum freshwater consumption	FCI	Total cost	NPC	ROEI
A	20 ton/h	$1,197,873	$1,013,429	$6,935,050	50%
B	40 ton/h	$1,133,814	$1,044,597	$7,112,219	48%
C	40 ton/h	$1,276,442	$1,055,516	$7,233,376	31%
D	54 ton/h	$1,196,702	$1,073,030	$7,317,272	31%
E	54 ton/h	$1,237729	$1,074,983	$7,344,497	28%
F	70 ton/h	$1,145,154	$1,094,624	$7,437,454	26%
G	70 ton/h	$1,191,666	$1,098,383	$7,478,235	22%
H	90 ton/h	$940,715	$1,108,829	$7,455,456	67%
I	92.5 ton/h	$894,431	$1,135,385	$7,609,375	Reference
J	107.5 ton/h	$926,861	$1,304,944	$8,709,560	−513%

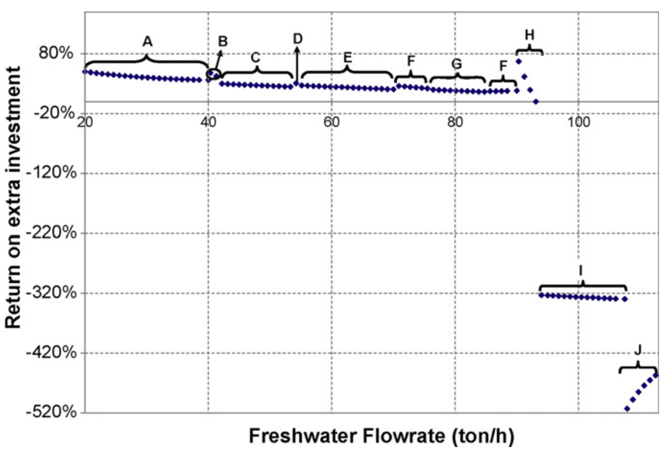

Fig. 8. Return on extra investment—grassroots case.

tions (between freshwater and water-using units and water-using units and end of pipe treatment) and processes (in this case the end of pipe treatment) are set to zero.

The feasible range of freshwater usage found for the studied water network is between 20 ton/h (the minimum flowrate using a regeneration process) and 112.5 ton/h (flowrate of the current network). Fig. 10 depicts the savings as a function of flowrate, where networks A through D make use of a regeneration unit and networks E, F and G do not use regeneration. Note that each point corresponds to a different regeneration unit capacity (when this applies).

The ranges of freshwater, where each network is the economical optimal solution (maximum Net Savings—Eq. (16)), are shown in Table 6. Selected configurations (networks A, C, E and F) are presented in Fig. 11. The thicker lines in the figures represent new connections and the values inside the boxes represent altered flowrates and concentration. The flowrates and concentrations shown in the figures correspond to the operating conditions to reach the maximum savings of each network.

The FCI and the ROI profiles corresponding to the savings presented in Fig. 10 are shown in Figs. 12 and 13, respectively. Savings and FCI go down in a discontinuous manner. The ROI, however, increases. Therefore, one can conclude that maximizing savings does not necessarily generate the most profitable solution from the ROI point of view. *Indeed, the most profitable option from the ROI point of view happens at the limit of 95 ton/h (Network F), where no regeneration process is needed. Conversely, Network A exhibits the highest savings.*

We now concentrate on using the net present value (NPV) as mean of looking at profitability. The same solutions are obtained either savings (Eq. (16)) or NPV (Eq. (20)) is optimized. In this case, note that we are looking at true profitability of the retrofit, as opposed to using the net present cost as in the case of grassroots design. Fig. 14 shows the NPV profiles of all the aforementioned solutions for different discount rates. The optimum solution varies according to the discount rate used. The 20% rate of discount gives network E as the one with maximum NPV. On the other hand, the 10% rate of discount shows network A as having the maximum NPV. However, networks C and F also exhibit fairly good NPVs. For the 5% discount rate case, network A would be the best network from the NPV profitability based point of view. A better evaluation of what happens with the optimum solutions from the NPV point of view as function of rate of discount is shown in Fig. 15. We remind the reader that each point has a different regeneration unit capacity (when this applies).

4.1.4. Operability range of the networks

Here we intend to show the operability range (feasible variations of freshwater consumption) of each network and their relation with

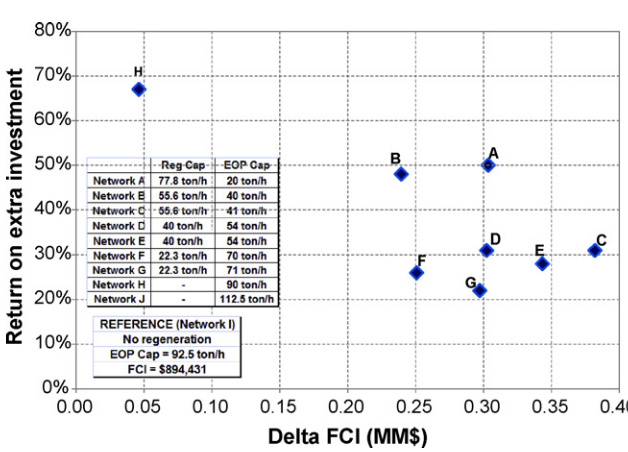

Fig. 9. Return on extra investment—grassroots case.

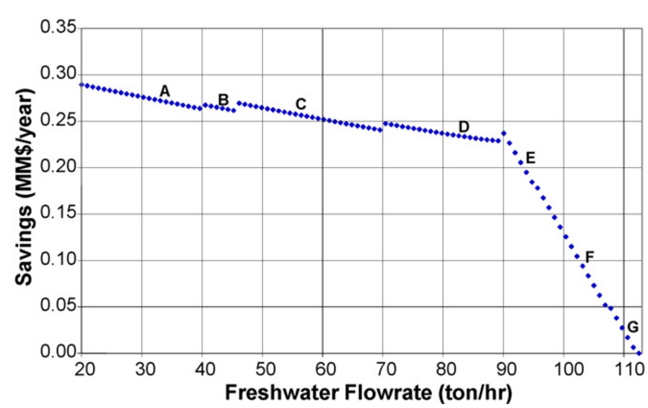

Fig. 10. Savings as a function of freshwater flowrate for the retrofit design.

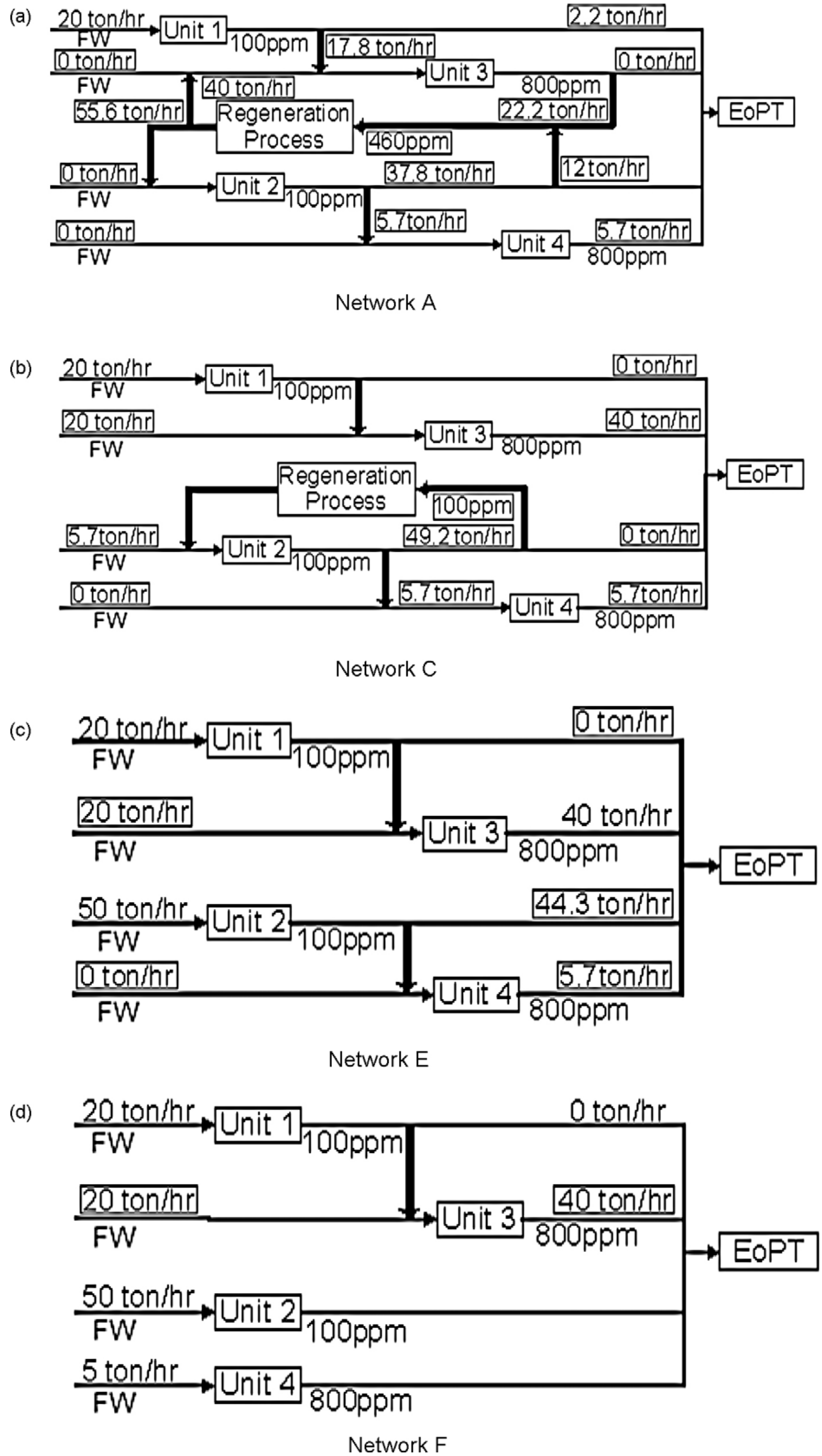

Fig. 11. Selected networks for the retrofit example.

a chosen regeneration capacity. This can help in identifying adequate capacities of the regeneration process in each network and better understand the tradeoff between freshwater savings and cost with regeneration.

To make the operability range analysis, we extend the feasibility range of each network beyond the interval in which they are optimal by solving the same problem again for each of the networks. We fix the network connections (but not the size of the regen-

Table 6
Network and corresponding range of freshwater flowrate (Fig. 10).

Network	Range of freshwater usage (discrete values)	New connections	FCI of new connections
A	20.00–39.621 ton/h	U1-U3, U2-U4, N1-U2, N1-U3, U2-N1, U3-N1	$458,000.00
B	40.556–45.227 ton/h	U1-U3, U2-U4, N1-U2, U2-N1, U3-N1	$408,000.00
C	46.162–69.520 ton/h	U1-U3, U2-U4, N1-U2, U2-N1	$317,000.00
D	70.455–89.141 ton/h	U1-U3, U2-U4, N1-U3, U2-N1	$237,000.00
E	90.076–94.747 ton/h	U1-U3, U2-U4	$150,000.00
F	95.682–106.894 ton/h	U1-U3	$110,000.00
G	107.828–111.566 ton/h	U2-U4	$40,000.00

eration unit yet) and maximize savings (Eq. (16)) for each fixed freshwater flowrate. Unlike the previous problem, an NLP solver (GAMS/CONOPT) can be used here since the binary variables are now fixed. The results are shown in Fig. 16.

Note the existence of overlapping solutions for all networks, which indicates that different networks can operate at certain same freshwater consumption. There is a linear relation between the regeneration capacity and the freshwater flowrate, which is also shown in the top scale of the figure. The interesting point to make here is that at certain freshwater flowrate, the network with maximum saving obeys this linear relationship and, all the other feasible networks with the same freshwater consumption have the same regeneration capacity. Another thing worth pointing out is that to construct the curves the minimum freshwater flowrate obtained for a fixed network may not coincide with the original minimum value of the freshwater usage range at maximum savings. When this happens, one may get isolated points like the one shown in Fig. 16 for network C. This isolated point of network C represents a feasible operating condition of this network where it operates economically worse than at least another network. Since this point does not represent the maximum savings at this freshwater consumption, the regeneration flowrate scale is no longer valid for it. The corresponding ROI and NPV profiles for these extended ranges are shown in Figs. 17 and 18, respectively.

In the next step, we fix the size of the regeneration ($RegCap_r$ is fixed in Eq. (15)) network in addition to the connections. We pick the sizes that correspond to the capacity obtained for the point with maximum savings of each network. Moreover, an additional lower size can be found using information of the other networks. For example, the lower size of network C is the capacity corresponding to the point where at least one other network can reach the same savings (in this case network D). The savings are now linear for the whole feasible freshwater consumption range, as shown in Fig. 19.

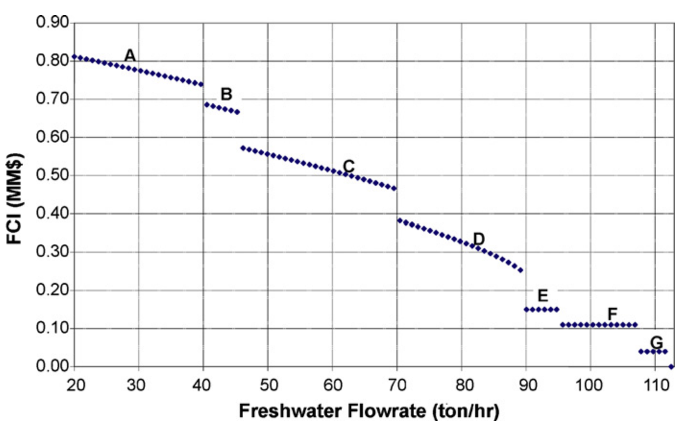

Fig. 12. FCI as a function of freshwater flowrate—retrofit.

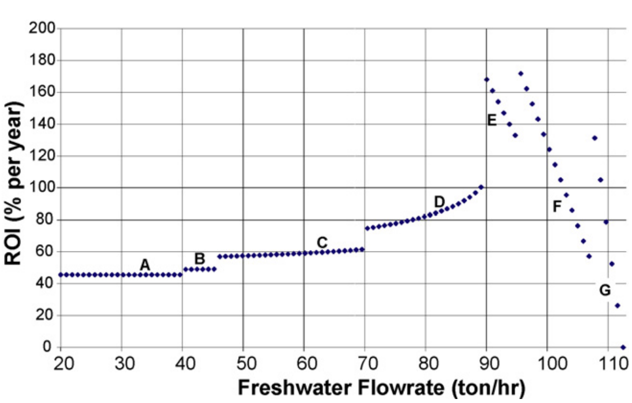

Fig. 13. ROI as a function of freshwater flowrate—retrofit.

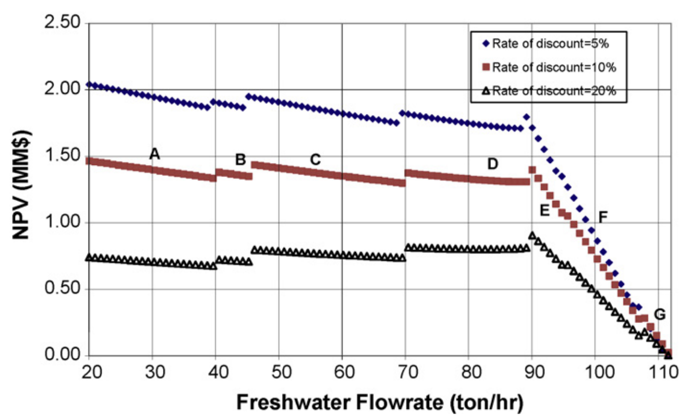

Fig. 14. NPV as a function of freshwater flowrate—retrofit design.

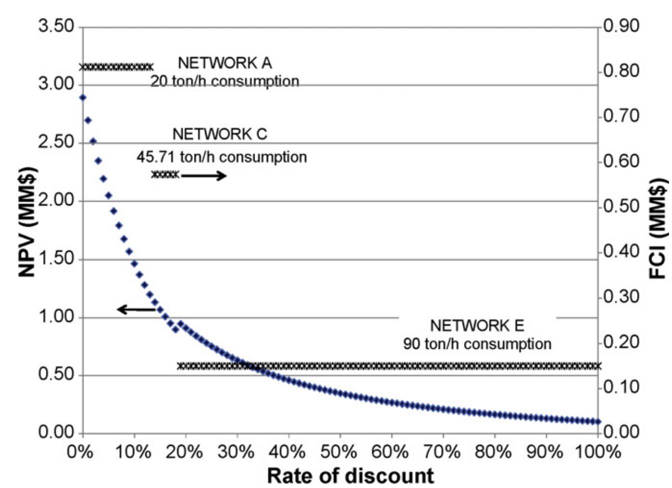

Fig. 15. NPC and FCI as a function of rate of discount—retrofit design.

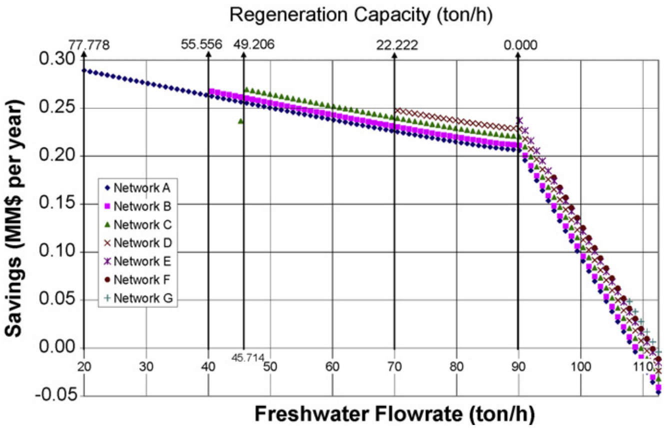

Fig. 16. Savings profile of the suggested networks.

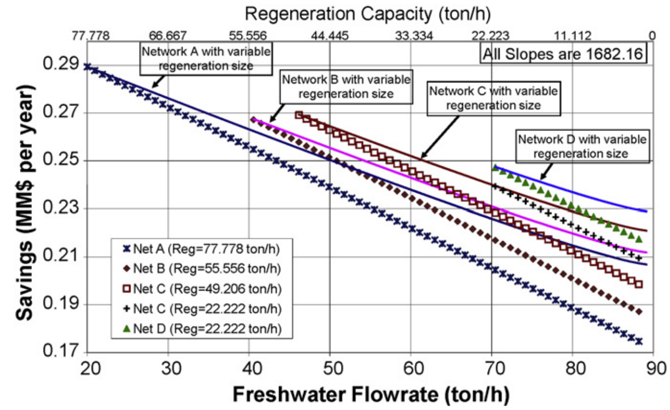

Fig. 19. Savings profile for fixed sizes of the regeneration process—retrofit design.

In this figure, the previous curves of the networks with regeneration are included for reference. The capacities of the regeneration units correspond to where the straight line touches its curved savings profile. Once the regeneration capacity is defined, the minimum freshwater consumption is determined by the freshwater flowrate scale (in the bottom).

This evaluation is useful to define economical limit sizes of the regeneration process for the different networks. For each network, a regeneration process with capacity higher than the maximum values used to construct Fig. 19 does not decrease the freshwater consumption without generating a saving that is lower than one of another network. Consequently, in the best case (when freshwater consumption does not decrease), the operational part of the savings equation does not change while FCI increases. Thus, a higher regeneration capacity generates economic loss.

In Fig. 20 the lower limit of the regeneration capacities are analyzed. One can see that a regeneration process with capacity of 22.222 ton/h will be economically superior when used in network D than when used in network C. This also happens with networks A and B with 22.222 ton/h capacity. If we draw the profile, they will be below of the one in network D. Similarly, a regeneration sys-

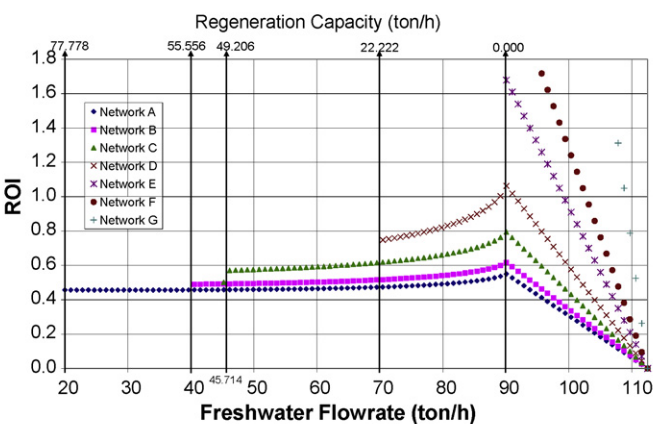

Fig. 17. ROI profile of the suggested networks—retrofit.

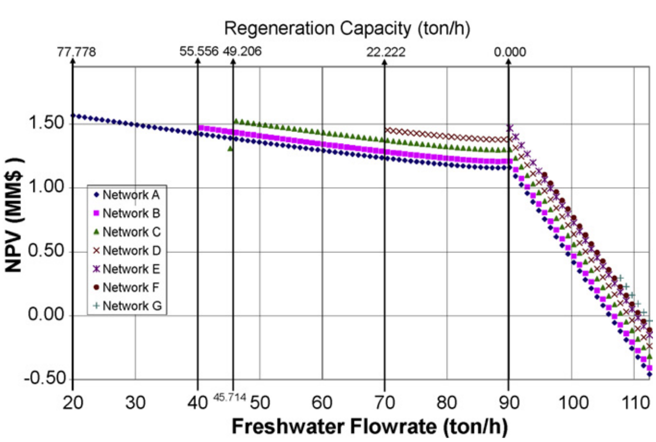

Fig. 18. NPV profile of the suggested networks for 9% rate of discount—retrofit design.

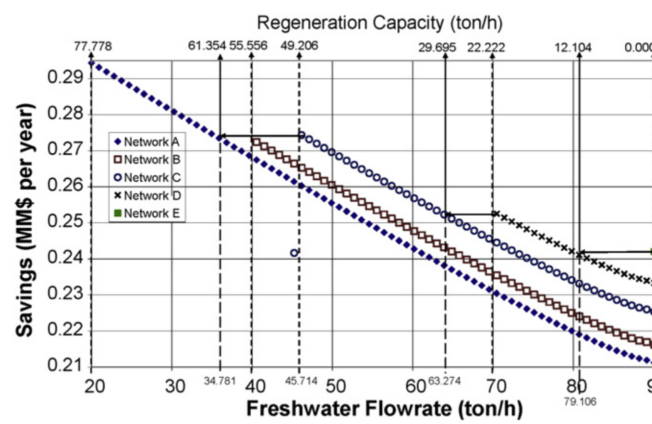

Fig. 20. Analysis of regeneration capacity—retrofit design.

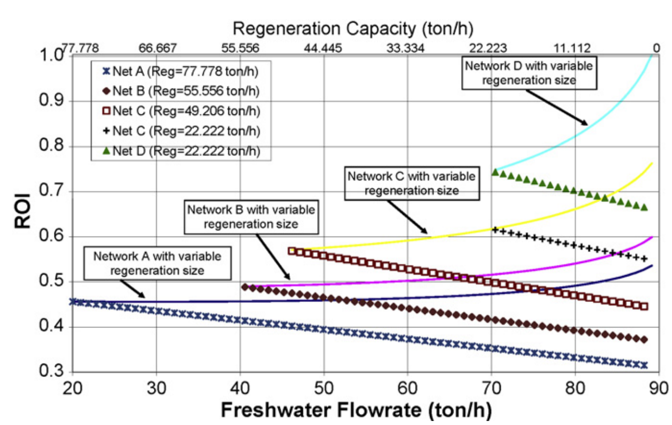

Fig. 21. ROI profile for the limit sizes of regeneration process—retrofit.

Table 7
Summary of results—retrofit design.

Network	Minimum freshwater consumption	FCI	Savings	NPV (i = 10%)	ROI
A	20 ton/h	$811,922	$289,398	$1,465,194	45.6%
B	40 ton/h	$685,473	$267,467	$1,379,189	49.0%
C	45 ton/h	$589,494	$236,631	$1,226,719	50.1%
D	70 ton/h	$381,901	$247,533	$1,373,743	74.8%
E	90 ton/h	$150,000	$236,995	$1,398,400	168.0%
F	95 ton/h	$110,000	$177,996	$1,051,298	171.8%
G	107.5 ton/h	$40,000	$48,499	$282,583	131.2%

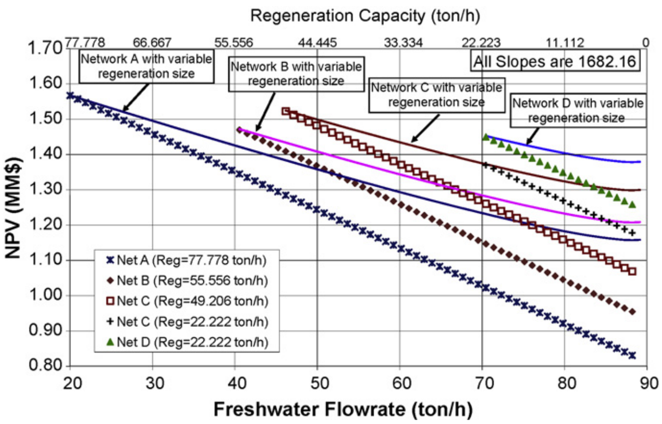

Fig. 22. NPV profile for the limit sizes of regeneration process—retrofit design.

tem with capacity of 49.206 ton/h is economically superior when used in network C than when used by network B and one with 55.556 ton/h capacity is economically superior in network B than in network A. Further, from the economical point of view, network A should not work with a regeneration process with capacity lower than 61.345 ton/h and, as suggested before it should not work with a regeneration process with capacity higher than 77.778 ton/h. This lower capacity limit represents the regeneration capacity in network A that generates the same savings than the maximum following savings generates by other network (in this case, network C). This point is also the upper limit economically optimum of network C (49.206 ton/h). Besides, network B does not present any economical advantages. The only reason that it could be considered is due to freshwater consumption issues when compared to network C. Similarly, the limits for network C are between 49.206 ton/h and 29.695 ton/h (this lower limit generates the same savings as network D at its maximum savings). In turn, network D has the limit between 22.222 ton/h and 12.104 ton/h (this lower limit generates the same savings as the maximum savings in network E—the highest savings between the options without regeneration). Finally, the use of a regeneration process with capacity outside these intervals generates economical losses. This process of thought is illustrated in Fig. 20.

The ROI and NPV profiles of the networks A to D with fixed size of regeneration process are presented in Figs. 21 and 22, respectively. The largest advisable sizes from the savings point of view are used in these profiles. The pattern of straight lines repeats, but they are not parallel anymore.

Table 7 shows the summary of the results for the retrofit case of the single contaminant example. As before, all economics is computed for the minimum freshwater consumption.

5. Multicontaminant example

To address the multicontaminant case, the refinery example presented by Koppol and Bagajewicz (2003) is investigated. It consists

Table 8
Limiting process water data for multicontaminant example.

Process	Contaminant	Mass load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1. CausticTreating	Salts	0.18	300	500
	Organics	1.2	50	500
	H2S	0.75	5000	11000
	Ammonia	0.1	1500	3000
2. Distillation	Salts	3.61	10	200
	Organics	100	1	4000
	H2S	0.25	0	500
	Ammonia	0.8	0	1000
3. Amine Sweetening	Salts	0.6	10	1000
	Organics	30	1	3500
	H2S	1.5	0	2000
	Ammonia	1	0	3500
4. Merox-I Sweetening	Salts	2	100	400
	Organics	60	200	6000
	H2S	0.8	50	2000
	Ammonia	1	1000	3500
5. Hydrotreating	Salts	3.8	85	350
	Organics	45	200	1800
	H2S	1.1	300	6500
	Ammonia	2	200	1000
6. Desalting	Salts	120	1000	9500
	Organics	480	1000	6500
	H2S	1.5	150	450
	Ammonia	0	200	400

Table 9
Capital costs of the connections.

$ ($\times 10^3$)	U1	U2	U3	U4	U5	U6	R1	R2	R3	EOP
W1	23	50	18	63	16	25	–	–	–	–
U1	–	50	110	45	70	42	23	15	11	53
U2	50	–	34	40	11	35	50	12	34	51
U3	110	34	–	42	60	18	18	35	47	62
U4	45	40	42	–	23	34	63	13	50	78
U5	70	11	60	23	–	28	16	21	19	58
U6	42	35	18	34	28	–	25	33	24	22
R1	23	50	18	63	16	25	–	50	31	44
R2	15	12	35	13	21	33	50	–	34	40
R3	11	34	47	50	19	24	31	34	–	52
EOP	53	51	62	78	58	22	44	40	52	–

of six water-using units and four key contaminants, which operates 8600 h/year. Table 8 gives the limiting data of the six water-using units.

The cost of freshwater is $0.32/ton and its concentration is assumed to be zero. The operating cost of the end of pipe treatment is $1.68/ton and its capital cost factor is $30,000/ton$^{0.7}$. The financial analysis of the project is done for a period of 10 years (N = 10 years and af = 0.1). This problem has 215 constraints, 139 continuous variables and 87 binary variables.

5.1. Grassroots case

For the grassroots case all design decisions need to be made. The capital costs of connections between processes are presented in Table 9.

Three intermediary regeneration processes are available (API separator followed by ACA, which reduces organics to 50 ppm; Reverse osmosis, which reduces salts to 20 ppm; and Chevron wastewater treatment, which reduces H_2S to 5 ppm and ammonia to 30 ppm). The capital cost factor ICN_r and the operation cost OPN_r are presented in Table 10.

The range of freshwater usage of this network is defined between its minimum consumption (33.6 ton/h) and its freshwater consumption without reuse (144.8 ton/h). Fig. 23 shows the annualized total cost as function of freshwater consumption when the annualized total cost is minimized (Eq. (16)). The optimum solution from the annualized total cost point of view is network A, which can reach the minimum freshwater consumption.

Table 11 shows the connections of all these networks and their corresponding minimum values of freshwater consumption (even when they are not optimal for those values). Relevant networks (A, B, C and F) are presented in Fig. 24. Note that Table 11 indicates that network A has a connection between the freshwater source and water-using unit 4 (Merox I). In Fig. 24a, however, this connection is not shown because this connection is not active at the specific condition of minimum freshwater consumption.

Fig. 25 shows the regeneration capacities needed as function of the freshwater consumption of the networks previously found. The only regeneration process that is always used through the whole range of freshwater usage is the end-of-pipe treatment. API separator is used up to 120 ton/h freshwater consumption (networks A to E), the reverse osmosis up to about 66 ton/h (networks A and B)

Table 10
Capital cost factor and operation cost for the regeneration processes.

Regeneration process	ICN_r (\$/ton$^{0.7}$)	OPN_r (\$/ton)
1. API separator followed by ACA	25,000	0.12
2. Reverse osmosis	20,100	0.56
3. Chevron wastewater treatment	16,800	1.00

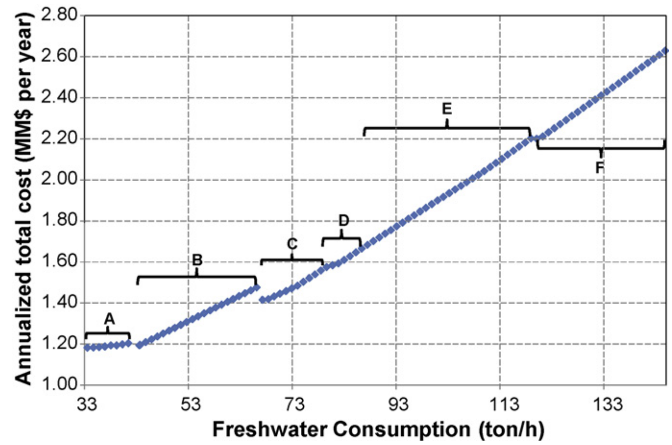

Fig. 23. Annualized total cost as a function of freshwater flowrate for the grassroots case of the multicontaminant example.

and the Chevron wastewater treatment is used only by network A (up to approximately 40 ton/h). Note that only an extremely small capacity of Chevron treatment is needed, what is not acceptable in practice. As another option in which the total cost does not significantly increase, network B can be considered.

The FCI of the networks presented in Fig. 23 as function of the freshwater flowrate is presented in Fig. 26. The discontinuities of the curves are caused by the different piping configurations, and the curvatures are due to the different regeneration capacities for each fixed freshwater consumption.

Fig. 27 shows minimum NPC of those networks for different rates of discount as function of freshwater consumption. Note the optimum solution depends on the discount rate applied. At a 10% discount rate network A is the optimum solution. However, for rates of discount of 15% or 20%, the network B presents the lowest NPC.

Fig. 28 shows the minimum NPC for a rate of discount of 10% of each network as function of FCI. The freshwater consumption where the minimum NPC happens is also presented in the graph.

The return on extra investment is analyzed next. Network G features the minimum FCI operating at its minimum freshwater

Table 11
Network connections and minimum freshwater consumption of the networks—multicontaminant case.

Network	Connections	Min consumption
A	W-U2, W-U3, W-U4, U1-U4, U2-U5, U5-U6, N1-U1, N1-U5, N1-U6, N3-U4, U1-N3, U2-N1, U2-N2, U3-N1, U4-N1, U5-EoPT, U6-N2, U6-EoPT, N2-N1, EoPT-S	33.6 ton/h
B	W-U2, W-U3, W-U4, U1-U6, U2-U6, U5-U6, N1-U1, N1-U5, N1-U6, U2-N1, U2-N2, U3-N1, U4-N1, U6-N2, U6-EoPT, N2-N1, EoPT-S	43.6 ton/h
C	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U5, U1-U6, U5-U4, U5-U6, N1-U1, U2-N1, U3-N1, U4-N1, U5-N1, U6-N1, U6-EoPT, N1-EoPT, EoPT-S	68.1 ton/h
D	W-U2, W-U3, W-U4, W-U5, W-U6, U1-U6, U3-U6, U5-U6, N1-U1, N1-U5, U2-N1, U4-N1, U6-N1, U6-EoPT, EoPT-S	78.7 ton/h
E	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U6, U2-U5, U3-U6, U5-U6, N1-U6, U2-EoPT, U4-N1, U6-EoPT, EoPT-S	85.8 ton/h
F	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U6, U3-U6, U5-U6, U2-EoPT, U4-EoPT, U6-EoPT, EoPT-S	120.6 ton/h

N1 – API separator; N2 – RO; N3 – Chevron treatment; EoPT – End-of-pipe treatment.

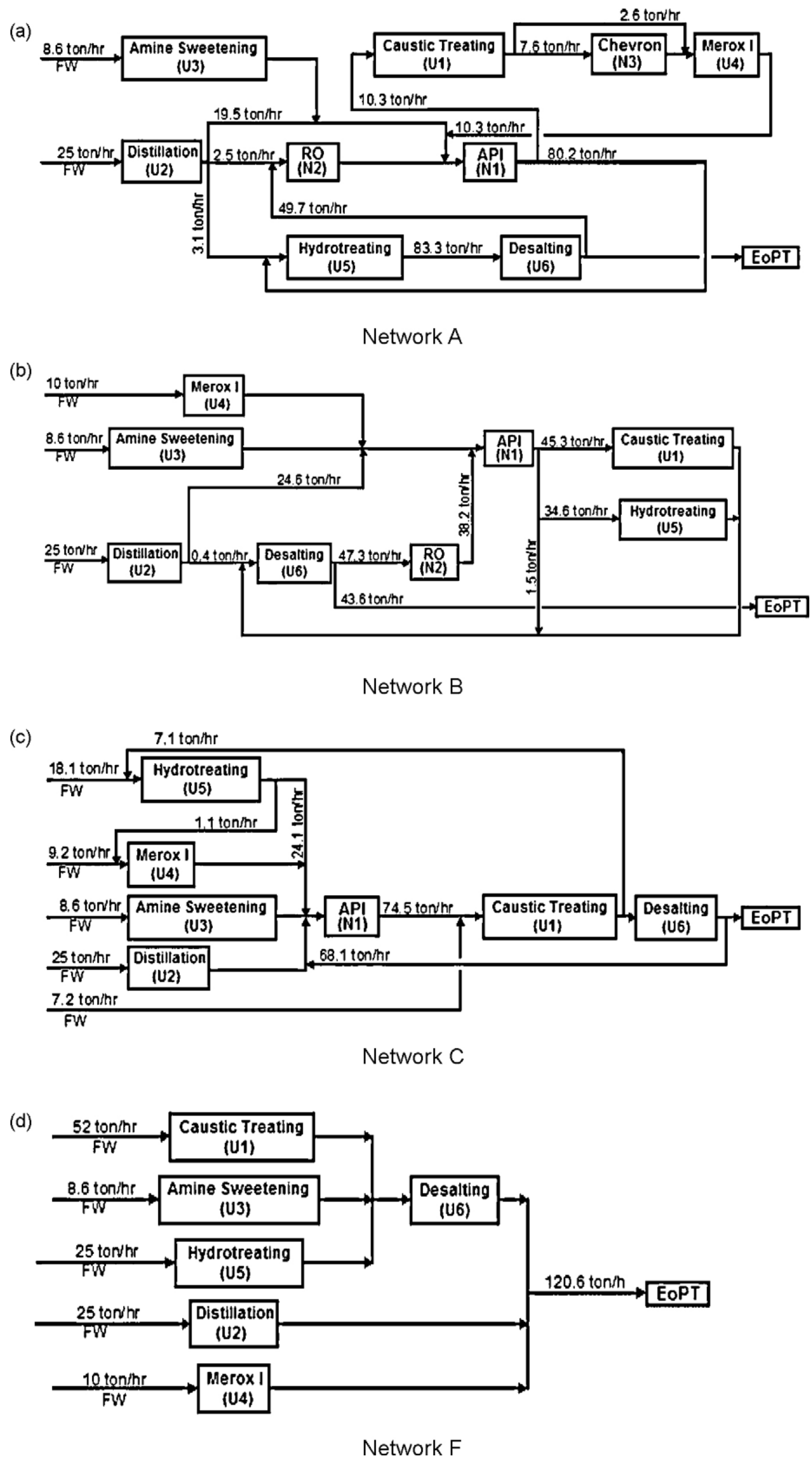

Fig. 24. Selected networks from Table 11.

consumption (120.1 ton/h). This network has a FCI of $1,267,987 and an annualized total cost of $2,200,590. Using this network as reference, the ROEI vs. freshwater consumption was calculated using Eq. (23) and is shown in Fig. 29 . Note that network G generates a negative ROEI. From the ROEI perspective, network C is the optimum solution when it is designed for a freshwater consumption of 68.1 ton/h, which has an API regeneration process with capacity for 74.5 ton/h.

Table 12
Summary of results for the multicontaminant case.

Network	Freshwater consumption	FCI	Total cost	NPC	ROEI
A	33.6 ton/h	$1,917,204	$1,182,217	$8,024,198	155%
B	43.6 ton/h	$1,770,753	$1,194,671	$8,039,440	210%
C	68.1 ton/h	$1,415,986	$1,415,986	$9,246,542	540%
D	79.6 ton/h	$1,505,614	$1,575,265	$10,259,802	273%
E	87.5 ton/h	$1,452,112	$1,683,807	$10,906,119	291%
F	120.6 ton/h	$1,267,987	$2,200,590	$14,010,534	Reference

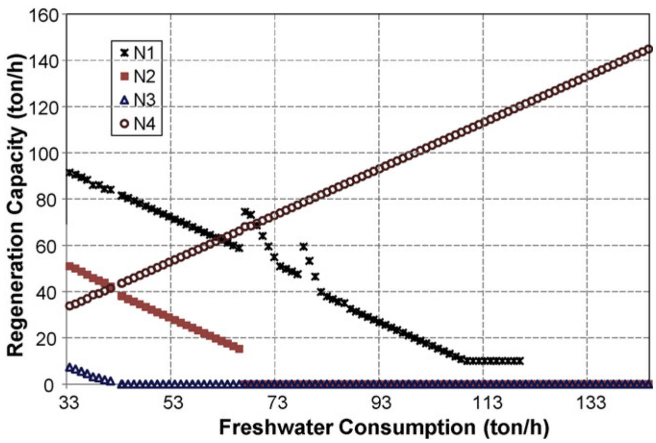

Fig. 25. Regeneration capacities as a function of freshwater flowrate for the grassroots case of the multicontaminant example.

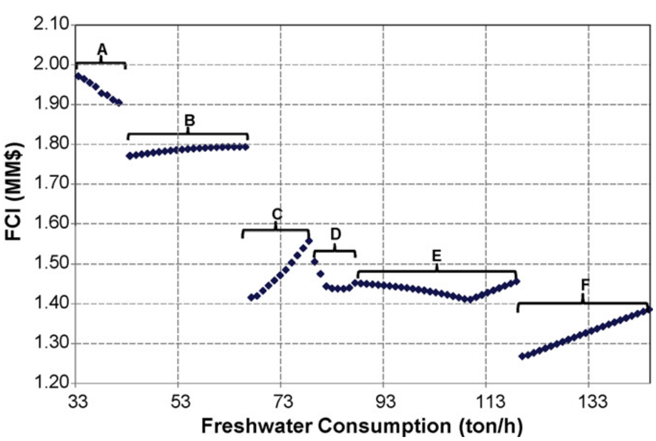

Fig. 26. FCI as a function of freshwater flowrate for the grassroots case of the multicontaminant example.

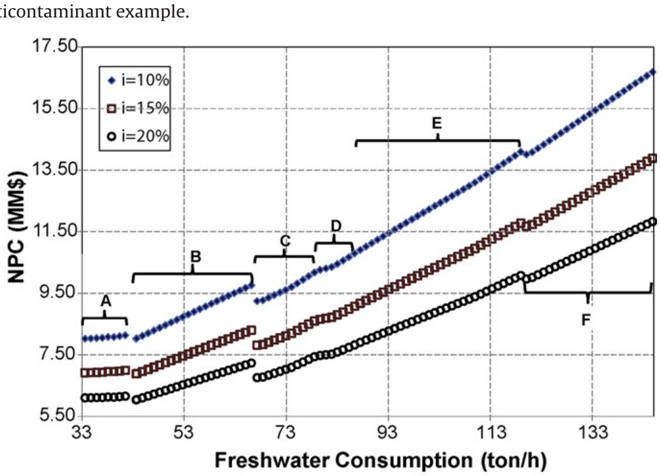

Fig. 27. NPC as a function of freshwater flowrate for the grassroots case of the multicontaminant example.

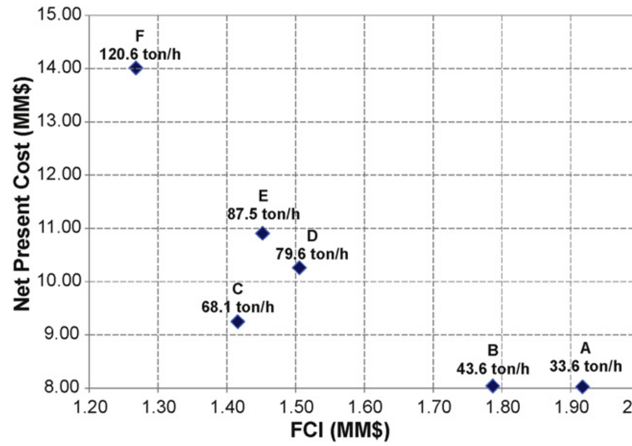

Fig. 28. NPC as a function of FCI for the grassroots case of the multicontaminant example (for rate of discount of 10%).

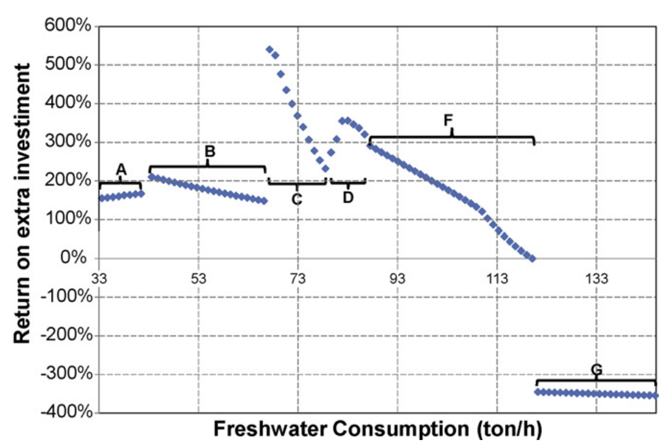

Fig. 29. Savings as a function of freshwater flowrate for the grassroots case of the multicontaminant example.

A summary of the results for the multicontaminant example is presented in Table 12. Costs correspond to minimum freshwater consumption when the network is optimum. Network C has the highest ROEI (540%) when designed for a freshwater consumption of 67.3 ton/h. The optimum solutions of each criterion are bolded.

6. Conclusions

This paper introduced a methodology to perform the grassroots design and retrofit of water/wastewater systems based on mathematical optimization and profitability insights. The results point some important conclusions: Targeting maximum savings (or total annualized cost) does not necessarily generate the most profitable solution. In addition, different measurements for profitability can give different solutions. Moreover, when NPV is used as the measurement, the used discount rate can alter the optimum solution.

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