

# Planning Model for the Design and/or Retrofit of Industrial Water Systems

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**ABSTRACT:** Planning models for industrial water systems are needed to address future environmental regulations, increasing costs of freshwater, variability on the quality of the available freshwater source, and bottlenecks caused by expansion of the capacity plant, among other reasons. In this paper, we present a method to address an increase in plant capacity associated with new water-using units planned to be added through time and/or an increase in the mass load of existing water-using units. We compare this method with two ad-hoc alternatives, which exhibit good performance for the examples shown.

## 1. INTRODUCTION

Retrofit designs in water systems are important to be addressed systematically in many situations, such as adjusting the system to new environmental regulations, increased costs of freshwater, variability and/or changes on the quality of the available freshwater source, bottlenecks caused by expansion of the capacity plant, etc. Because these plants already have a water system installed, a model to find the best retrofit solution should consider its operability as well as its economic aspects. In addition, a timeline that takes into account when new constraints and requirements will take place needs to be considered, so that one can consider and decide upon actions that anticipate or simply actions that respond to these changes. While retrofit of water systems is likely to be a more common activity than a grass-roots design, in the latter case, the aforementioned adjustment of the design to time-varying situations (new regulations, changes in costs, etc.), requires asking the question whether one should design once and for the worst case or plan adaptations of the system, that is, a first design followed by retrofits in the future.

Industrial water systems have been thoroughly researched ever since the seminal paper by Prof. Umeda<sup>1</sup> presented the first version. There are a few books,<sup>2–6</sup> two review papers directly devoted to the field,<sup>7,8</sup> and one annotated review prepared by our friend, the late Jacek Jezowski.<sup>9</sup>

Citing all work done is virtually impossible (there are more than 300 papers published), so we limit this reference section to what is relevant to our paper's theme and technique. The field exhibits two distinctive approaches. On one hand, there are the proponents of graphical/algorithmic approaches, one of which is the widely known "Water Pinch",<sup>10,11</sup> but there are several others like the Water Source Diagrams method,<sup>12,13</sup> Sources/Sinks, recycle/reuse-based methods,<sup>14</sup> Cascade Diagrams,<sup>15</sup> necessary condition driven algorithmic-based methods,<sup>16–18</sup> etc. On the other hand, the problem has been also solved by writing all the material balance equations for all units and using mathematical programming<sup>19–25</sup> (although some efforts using stochastic methods are worth mentioning<sup>26</sup>). A few models also cover simultaneous heat integration.<sup>27–30</sup>

Several arguments have been made about the advantages of each approach. Researchers that advocate the use of graphical/algorithmic approaches, notably the Water Pinch methods or similar, claim that the methods provide "good insights", but they mostly restrict this statement to the problem of minimizing freshwater consumption for single component systems.<sup>8</sup> After targeting and in the design phase, these graphical and algorithmic methods are only capable of obtaining one solution that satisfies minimum freshwater consumption. However, when the problem is multicomponent, the insights and the designed networks are obtained using heuristics failing to guarantee optimums. In recent work, we pointed out the degenerate nature of the problem showing that even for single components there is a large number of alternative solutions.<sup>31</sup> Finally, we also discussed issues of appropriate modelling and pointed out that mathematical programming seems to be, in our opinion, the only way to move the field forward when detailed models are to be used.<sup>32</sup> We discuss some more about the issue of detailed modeling below.

We now focus our attention on methodologies for the retrofit design of existing water networks, which are only a few. Some are devoted to targeting<sup>33</sup> and other graphical/algorithmic approaches<sup>34–37</sup> that are hardly amenable to be used in planning. In direct relation to our work are the methods based on mathematical programming,<sup>38,39</sup> because they are the ones that can be used for planning without introducing simplifying assumptions and can readily handle cost objectives.

This paper is organized as follows: We first present the problem definition followed by the model. We illustrate with examples and wrap up presenting our conclusions. In this paper, only the case of retrofit due to an increase in plant capacity is presented. Specifically, we address the installation of new water-using units and/or the increase in the mass load of

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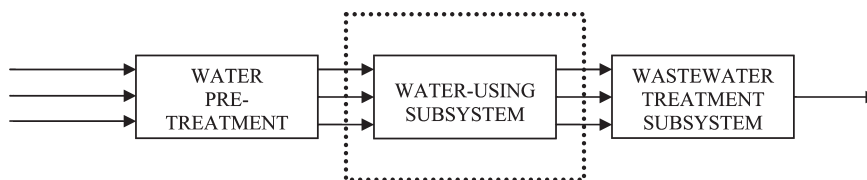


Figure 1. Industrial water system without recycles.

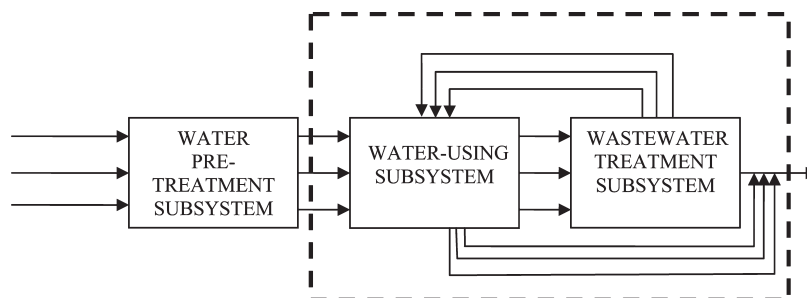


Figure 2. Industrial water system with recycles from the wastewater treatment subsystem.

existing water-using units, which is usually caused by modifications of process conditions for economic reasons or for changes in raw materials processed.

## 2. PROBLEM STATEMENT

Several different models have been proposed for water systems. The issue of the appropriate architecture has been discussed in detail by Faria and Bagajewicz.<sup>32</sup> While Takama et al.<sup>1</sup> proposed to consider two subsystems (water-using units and water treatment units), several papers that followed (starting from Wang and Smith<sup>10</sup>) proposed to solve the water-using subsystem independently (as in Figure 1), assuming that pretreatment and post-treatment will happen on its own. Many of the works that followed included recycles from the water post-treatment (as in Figure 2)

While extensions of these concepts to include recycles to and from pretreatment have been proposed (and solved<sup>32</sup>), the system we refer to in this paper corresponds to the dotted box in Figure 2.

Our planning model can be stated as follows:

Given a water-using system that is supposed to function at different periods of time, each period with its own specifications for discharge concentration limits, its own freshwater and treatment costs, its own freshwater quality, and/or its own new or increased capacity water using units, it is desired to determine where, when, and what capacity of connections are needed, as well as which, when, and what capacity of treatment processes (if any) need to be installed to obtain an optimum network.

The planning model is based on the classical version of the water allocation problem as originally proposed by Doyle and Smith.<sup>19</sup> To this model, we added the time dimension and the specifications for each period of time and made a few modifications to the equations. That is, for different points in time, one may have different instances that can be caused by an increase in mass loads, a planned addition of water-using units in the future, a future reduction of discharge limits, etc. In essence, the planning model resembles the capacity expansion problem<sup>40</sup> and its MILP version developed for supply chains.<sup>41</sup>

Without a planning model, one could solve the problem first for the current needs and then solve a retrofit problem for the next instance in time where different constraints are imposed. Another option would be to solve the problem with consideration of this specific future situation (worst case scenario). Because the feasible space of a planning model includes as special cases the feasible solutions of these alternative procedures, the planning model is guaranteed to provide a better answer. Nevertheless, we will compare the three alternatives.

## 3. MATHEMATICAL MODEL

The mathematical model we present here has been around for a very long time, and their simplifying assumptions are mostly the same as those originally proposed by the Water Pinch method:<sup>10,11</sup>

- (1) Each water using unit has a maximum inlet and maximum concentration and a fixed load picked up for each contaminant.
- (2) Each water treatment unit either has a fixed contaminant removal ratio or a fixed outlet concentration independent of inlet conditions or flow rate.

We now present the equations of the model and later discuss the shortcomings of the model and the reasons why using it are enough to make our point.

**Water Balance at the Water-Using Units.** The water balance through the units has to be done for every analyzed period of time.

$$\begin{aligned} & \sum_w \text{FWU}_{w,u,t} + \sum_{u^*} \text{FUU}_{u,u^*,t} + \sum_r \text{FRU}_{r,u,t} \\ &= \sum_s \text{FUS}_{u,s,t} + \sum_{u^*} \text{FUU}_{u,u^*,t} + \sum_r \text{FUR}_{u,r,t} + \text{FUL}_{u,t} \quad \forall u, t \end{aligned} \quad (1)$$

In this balance,  $\text{FWU}_{w,u,t}$  is the flow rate from water source  $w$  to water-using unit  $u$  at time  $t$ ;  $\text{FUU}_{u,u^*,t}$  is the flow rate from water-using unit  $u$  to water-using unit  $u^*$  at time  $t$ ;  $\text{FRU}_{r,u,t}$  is the flow rate from regeneration process  $r$  to water-using unit  $u$  at time  $t$ ;  $\text{FUS}_{u,s,t}$  is the flow rate from water-using unit  $u$  to wastewater discharge  $s$  at time  $t$ ;  $\text{FUR}_{u,r,t}$  is the flow rate from water-using

unit  $u$  to regeneration process  $r$  at time  $t$ , and  $FUL_{u,t}$  is the water loss in unit  $u$  at time  $t$ .

**Water Balance at the Regeneration Processes.** The water balance through the regeneration processes for every time is also needed.

$$\sum_w FWR_{w,r,t} + \sum_u FUR_{u,r,t} + \sum_{r^*} FRR_{r^*,r,t} = \sum_u FRU_{r,u,t} + \sum_{r^*} FRR_{r,r^*,t} + \sum_s FRS_{r,s,t} + FRL_{r,t} \quad \forall r, t \quad (2)$$

In this balance,  $FWR_{w,r,t}$  is the flow rate from water source  $w$  to regeneration process  $r$  for time  $t$ ;  $FRR_{r,r^*,t}$  is the flow rate from regeneration unit  $r$  to regeneration process  $r^*$  for time  $t$ ; and  $FRL_{r,t}$  is the water loss in regeneration  $r$  at time  $t$ .

**Contaminant Balance at the Water-Using Units.**

$$\begin{aligned} \sum_w (CW_{w,c}FWU_{w,u,t}) + \sum_{u^*} ZUU_{u^*,u,c,t} + \sum_r ZRU_{r,u,c,t} \\ + \Delta M_{u,c,t} = \sum_{u^*} ZUU_{u^*,u,c,t} + \sum_s ZUS_{u,s,c,t} \\ + \sum_r ZUR_{u,r,c,t} + ZUL_{u,c,t} \quad \forall u, c, t \end{aligned} \quad (3)$$

Here,  $CW_{w,c}$  is concentration of contaminant  $c$  in water source  $w$ ;  $ZUU_{u^*,u,c,t}$  is the mass flow of contaminant  $c$  from water-using unit  $u$  to water-using unit  $u^*$  at time  $t$ ;  $ZRU_{r,u,c,t}$  is the mass flow of contaminant  $c$  from regeneration process  $r$  to water-using unit  $u$  at time  $t$ ;  $ZUS_{u,s,c,t}$  is the mass flow of contaminant  $c$  from water-using unit  $u$  to wastewater discharge  $s$  at time  $t$ ; and  $ZUR_{u,r,c,t}$  is the mass flow of contaminant  $c$  from water-using unit  $u$  to regeneration process  $r$  at time  $t$ . Finally,  $\Delta M_{u,c,t}$  is the load of contaminant  $c$  picked up in unit  $u$  and interval  $t$ ; and  $ZUL_{u,c,t}$  is the mass flow of contaminant  $c$  from water-using unit  $u$  associated with the water loss.

**Maximum Inlet Concentration at the Water-Using Units.** Aside from driving force restrictions, this constraint is also used to limit the total flow rate through the unit to be larger than a certain minimum.

$$\begin{aligned} \sum_w (CW_{w,c}FWU_{w,u,t}) + \sum_{u^*} ZUU_{u^*,u,c,t} \\ + \sum_r ZRU_{r,u,c,t} \leq C_{u,c,t}^{\text{in,max}} \left( \sum_w FWU_{w,u,t} + \sum_{u^*} FUU_{u^*,u,t} \right. \\ \left. + \sum_r FRU_{r,u,t} \right) \quad \forall u, c, t \end{aligned} \quad (4)$$

Here,  $C_{u,c,t}^{\text{in,max}}$  is the maximum allowed inlet concentration of contaminant  $c$  in water-using unit  $u$  for time  $t$ .

**Maximum Outlet Concentration at the Water-Using Units.** This is established by mass transfer driving force considerations (see the paper by Wang and Smith<sup>10</sup> for details of how this is derived from driving force considerations).

$$\begin{aligned} \sum_w (CW_{w,c}FWU_{w,u,t}) + \sum_{u^*} ZUU_{u^*,u,c,t} + \sum_r ZRU_{r,u,c,t} \\ + \Delta M_{u,c,t} \leq C_{u,c,t}^{\text{out,max}} \left( \sum_{u^*} FUU_{u^*,u,t} + \sum_r FUR_{u,r,t} \right. \\ \left. + \sum_s FUS_{u,s,t} \right) \quad \forall u, c, t \end{aligned} \quad (5)$$

Here  $C_{u,c,t}^{\text{out,max}}$  is the maximum allowed outlet concentration of contaminant  $c$  in water-using unit  $u$  for time  $t$ .

**Treated Flow Rate and Capacity of the Regeneration Processes.** The flow rate treated by the regeneration processes is computed using eq 6 and 7 for every period.

$$FR_{r,t}^{\text{in}} = \sum_w FWR_{w,r,t} + \sum_u FUR_{u,r,t} + \sum_{r^*} FRR_{r^*,r,t} \quad \forall r, t \quad (6)$$

$$FR_{r,t}^{\text{out}} = \sum_u FRU_{r,u,t} + \sum_{r^*} FRR_{r,r^*,t} + \sum_s FRS_{r,s,t} \quad \forall r, t \quad (7)$$

In these equations,  $FR_{r,t}^{\text{in}}$  and  $FR_{r,t}^{\text{out}}$  are, respectively, the inlet and outlet flow rate through regeneration process  $r$  for time  $t$ . In turn, eq 8 gives the capacity of the installed regeneration process, which consequently constrains the flow rates of every time after the regeneration process is installed.

$$FR_{r,t}^{\text{in}} \leq \sum_{t^* \leq t} \text{RegCap}_{r,t^*} + \text{ECap}_r \quad \forall r, t \quad (8)$$

Here,  $\text{RegCap}_{r,t}$  is the capacity of regeneration process  $r$  installed for time  $t$ , and  $\text{ECap}_r$  is the existing capacity of regeneration process  $r$ . Finally, eq 9 gives the time in which the regeneration process is installed, and eq 10 controls the maximum allowed number of regeneration process  $r$  to be installed.

$$\text{RegCap}_{r,t} \leq \text{RegCap}_r^{\text{max}} YR_{r,t} \quad \forall r, t \quad (9)$$

$$\sum_t YR_{r,t} \leq \text{max} YR_r \quad \forall r \quad (10)$$

Here,  $\text{RegCap}_r^{\text{max}}$  is the maximum allowed capacity expansion of regeneration process  $r$  in each period of time;  $YR_{r,t}$  is the binary variable related to the existence and installation timing of regeneration process  $r$ ; and  $\text{max} YR_r$  is maximum number of expansions of regeneration process  $r$ .

**Contaminant Balance at the Regeneration Processes Mixer.** The mass flows of contaminants feeding the regeneration unit  $ZR_{r,c,t}^{\text{in}}$  are computed in eq 11 using also contaminant mass flows from other units ( $ZUR_{u,r,c,t}$ ) and from other regeneration processes ( $ZRR_{r^*,r,c,t}$ ). These contaminant mass flows are defined later.

$$\begin{aligned} ZR_{r,c,t}^{\text{in}} = \sum_w (FWR_{w,r,t} CW_{w,c}) + \sum_u ZUR_{u,r,c,t} \\ + \sum_{r^*} ZRR_{r^*,r,c,t} \quad \forall r, c, t \end{aligned} \quad (11)$$

In turn, eq 12 also establishes a balance between the flow of contaminant coming out of the regeneration unit ( $ZR_{r,c,t}^{\text{out}}$ ) and the mass flows to units ( $ZRU_{r,u,c,t}$ ), the mass flows to other regeneration units ( $ZRR_{r,r^*,c,t}$ ), and the discharged water ( $ZRS_{r,s,c,t}$ ).

$$\begin{aligned} ZR_{r,c,t}^{\text{out}} = \sum_u ZRU_{r,u,c,t} + \sum_{r^*} ZRR_{r,r^*,c,t} \\ + \sum_s ZRS_{r,s,c,t} \quad \forall r, c, t \end{aligned} \quad (12)$$

**Performance of the Regeneration Processes.** We include two classes of regeneration processes: those that have defined (and fixed) outlet concentration and those that are based on a removal efficiency. Equations 13 and 14 are used to represent both cases by introducing a binary variable  $XCR_{r,c}$  that

defines when regeneration process  $r$  has its performance defined by a fixed outlet concentration ( $XCR_{r,c} = 1$ ) or by efficiency ( $XCR_{r,c} = 0$ ).

$$CR_{r,c,t}^{\text{out}} = CR_{r,c,t}^{\text{in}} \varphi_{r,c,t} (1 - XCR_{r,c}) + CR_{r,c}^{\text{out}} XCR_{r,c} \quad \forall r, c, t \quad (13)$$

$$\varphi_{r,c,t} = f(CR_{r,c,t}^{\text{in}}, FR_{r,t}^{\text{in}}) \quad \forall r, c, t \quad (14)$$

In eq 13,  $CR_{r,c,t}^{\text{out}}$  is the outlet concentration of regeneration process  $r$  for time  $t$ ;  $CR_{r,c,t}^{\text{in}}$  is the inlet concentration of regeneration process  $r$  for time  $t$ ; and  $\varphi_{r,c,t}$  is the efficiency of regeneration process  $r$  for time  $t$ . In eq 13,  $f(CR_{r,c,t}^{\text{in}}, FR_{r,t}^{\text{in}})$  defines the efficiency. In some cases, this efficiency can be defined as a constant, which is the option used in this paper.

#### Maximum Allowed Discharge Concentration.

$$\sum_u ZUS_{u,s,c,t} + \sum_r ZRS_{r,s,c,t} \leq CS_{s,c,t}^{\text{max}} \left( \sum_u FUS_{u,s,t} + \sum_r FRS_{r,s,t} \right) \quad \forall s, c, t \quad (15)$$

Here,  $CS_{s,c,t}^{\text{max}}$  is the maximum discharge concentration of disposal  $s$  at time  $t$ .

#### Minimum and Maximum Flow Rates.

$$FIJ_{i,j,t} \geq FIJ_{i,j}^{\text{min}} \sum_{t^* \leq t} YIJ_{i,j,t^*} \quad \forall (i,j) \in \left\{ \begin{array}{l} (w,u), (w,r), (u,u^*), (u,r), \\ (u,s), (r,u), (r,r^*), (r,s) \end{array} \right\}, t \quad (16)$$

$$FIJ_{i,j,t} \leq \sum_{t^* \leq t} \text{Cap}FIJ_{i,j,t^*} + \text{E} \text{Cap}FIJ_{i,j} \quad \forall (i,j) \in \left\{ \begin{array}{l} (w,u), (w,r), (u,u^*), (u,r), \\ (u,s), (r,u), (r,r^*), (r,s) \end{array} \right\}, t \quad (17)$$

where  $\text{E} \text{Cap}FIJ_{i,j}$  is the existing capacity of the connection between process  $i$  and process  $j$ ; and  $\text{Cap}FIJ_{i,j,t^*}$  is the capacity of the connection between process  $i$  and process  $j$  to be installed in time  $t$ .

#### Capacity of Connections.

$$\text{Cap}FIJ_{i,j,t} \leq FIJ_{i,j}^{\text{max}} YIJ_{i,j,t} \quad \forall (i,j) \in \left\{ \begin{array}{l} (w,u), (w,r), (u,u^*), (u,r), \\ (u,s), (r,u), (r,r^*), (r,s) \end{array} \right\}, c, t \quad (18)$$

Here,  $FIJ_{i,j}^{\text{max}}$  is the maximum allowed capacity expansion of connections in each period of time; and  $YIJ_{i,j,t}$  is a binary variable that is used later in assessing capital cost.

#### Contaminant Mass Loads.

$$ZIJ_{i,j,c,t} = FIJ_{i,j,t} \text{Cout}_{i,j,t} \quad \forall i \in \{U, R\}, j \in \{U, R, S\}, c, t \quad (19)$$

$$ZR_{r,c,t}^{\text{in}} = FR_{r,t}^{\text{in}} CR_{r,c,t}^{\text{in}} \quad \forall r, c, t \quad (20)$$

$$ZR_{r,c,t}^{\text{out}} = FR_{r,t}^{\text{out}} CR_{r,c,t}^{\text{out}} \quad \forall r, c, t \quad (21)$$

**Objective Functions.** We have four different objective functions. Equation 22 represents freshwater consumption.

$$FW_t = \sum_w \sum_u FWU_{w,u,t} \quad (22)$$

In turn, eq 23 represents operating cost.

$$\text{Opcost}_t = \left( \sum_w \alpha_w FW_{w,t} + \sum_r \text{OPN}_{r,t} FR_{r,t}^{\text{in}} \right) \quad (23)$$

Such operating cost is proportional to the freshwater consumption  $FW_{w,t}$  (through the unit cost  $\alpha_w$ ) and the flow rate of the water treatment units  $FR_{r,t}^{\text{in}}$  (through the unit cost  $\text{OPN}_{r,t}$ ).

Finally, eq 24 computes capital costs and eq 25 computes net present cost.

$$\begin{aligned} \text{FCI}_t &= \left( \sum_{(i,j) \in \left\{ \begin{array}{l} (w,u), (u,u^*), (u,r), \\ (u,s), (r,u), (r,r^*), (r,s) \end{array} \right\}} YIJ_{i,j,t} \text{FCC}_{i,j} + \text{Cap}FIJ_{i,j,t} \text{VCC}_{i,j} \right) \\ &\quad + \sum_r YR_{r,t} \text{FCRP}_r + \text{VCRP}_r \text{RegCap}_{r,t}^{0.7} \end{aligned} \quad (24)$$

$$\text{NPC} = \sum_t \text{DF}_t (\text{Opcost}_t + \text{FCI}_t) \quad (25)$$

In these equations,  $\text{FCC}_{i,j}$  is the fixed cost of connections between different units ( $u$  and  $r$ ), and  $\text{VCC}_{i,j}$  is the corresponding variable cost. Similarly,  $\text{FCRP}_r$  and  $\text{VCRP}_r$  are the fixed cost and variable cost coefficient for regeneration units, respectively. Finally,  $\text{DF}_t$  is the very well-known discount factor.

The above model (without the time dimension) lacks some features that are of importance. First, as pointed out by Faria and Bagajewicz,<sup>32</sup> the appropriate architecture requires using pre-treatment units and considering recycling the discharge stream, if any, so that the model can represent zero-liquid discharge systems. Also, the equipment and piping connection cost functions used are simplified and could be improved to reflect a more complex relationship with the variables. Finally, although the models include water losses/gains, without a better modeling of  $t$ , the internals of the units, the losses are arbitrary and usually fixed parameters. The same can be said for the contaminant mass losses, and that is why we set them to zero in our models. Much better models are needed to use flow rate and inlet concentration-dependent loads and or removal rates, especially because these can vary differently for different contaminants (as opposed to

**Table 1. Limiting data**

process ( $u$ )	contaminant	mass load (kg/h)	$C_{\text{in}}$ (ppm)	$C_{\text{out}}$ (ppm)
1 – distillation	HC	0.675	0	15
	H <sub>2</sub> S	180	0	400
	salts	1.575	0	35
2 – HDS	HC	4.08	20	120
	H <sub>2</sub> S	425	300	12500
	salts	6.12	45	180
3 – desalter	HC	12.32	120	220
	H <sub>2</sub> S	2.52	20	45
	salts	532	200	9500

Table 2. Regeneration Processes Data

process (r)	contaminant	CRF <sub>r,c</sub> <sup>out</sup> (ppm) or $\phi_{r,c,t}$ (%)	C <sub>in,max</sub> (ppm)	OPN <sub>r</sub> (\$/t)	VCRP <sub>r-</sub> (\$/t <sup>0.7</sup> )
1 – R1	HC	10	500	0.30	8500
	H <sub>2</sub> S	NA	200		
	salts	NA	200		
2 – R2	HC	0	20	0.50	10500
	H <sub>2</sub> S	0	200		
	salts	0	200		
3 – R3	HC	0%	NA	1.00	16800
	H <sub>2</sub> S	0.999%	NA		
	salts	0%	NA		
4 – R4	HC	10	NA	1.0067	34200
	H <sub>2</sub> S	10	NA		
	salts	10	NA		

Table 3. Increasing Mass Load of Hydrocarbons

process	1 – distillation	2 – HDS	3 – desalter
mass load	1.467 kg/h	10.08 kg/h	18.32 kg/h

being constant). These are, incidentally, considerations that are not done in any of the existing models, beyond the simplifying assumptions of assuming the mass loads and the water gain/losses as known parameters.

We believe that adding all of these features would certainly improve the results, as the removal of simplifying assumptions in any model will, but does not change the main conclusions of our paper, which are that the appropriate approach for time-varying input data for water network problems is the use of planning models and not at the very least the alternatives illustrated in our examples.

#### 4. RESULTS

To illustrate the methodology, we use the refinery example from Wang and Smith<sup>10</sup> with the addition the two pretreatment units. For simplicity, we treat these as regeneration units because our model allows these to be fed by freshwater, thus generalizing the model. This is discussed in more detail by Faria and Bagajewicz.<sup>32</sup> Table 1 presents the limiting data for the base case, which represents the first period of time analyzed.

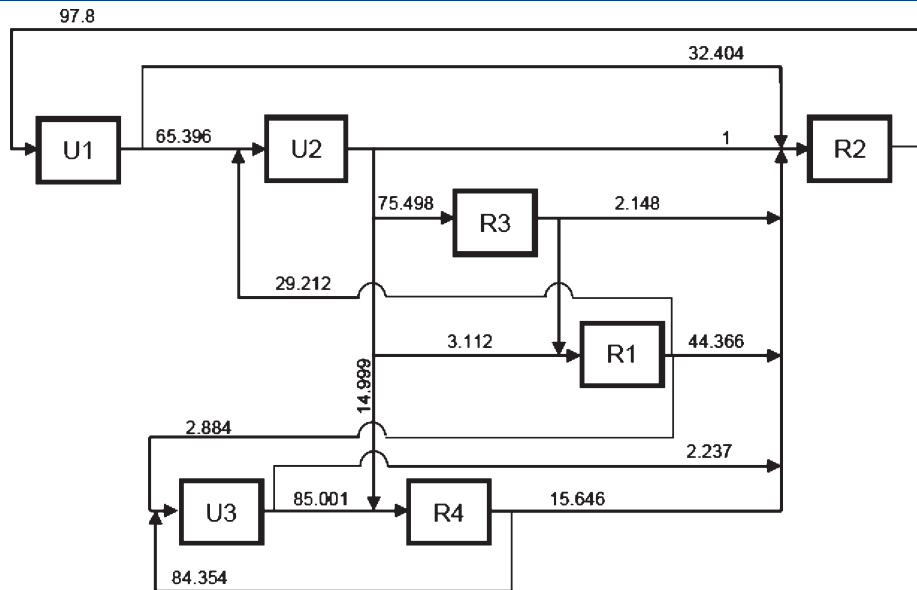


Figure 3. Worst case design (example 1).

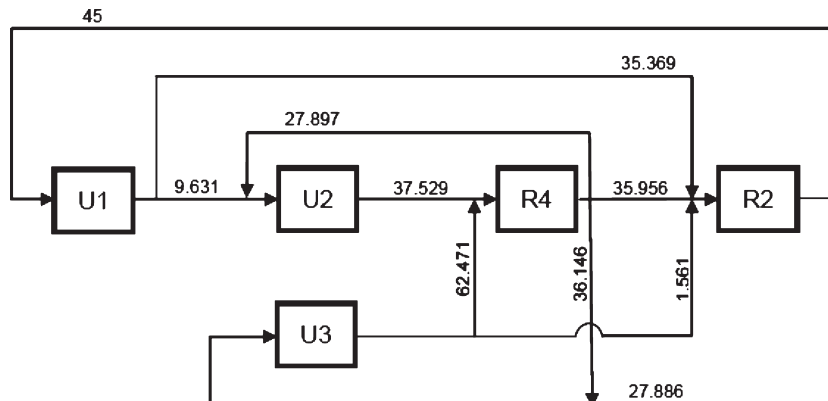


Figure 4. Design for the first period (example 1).



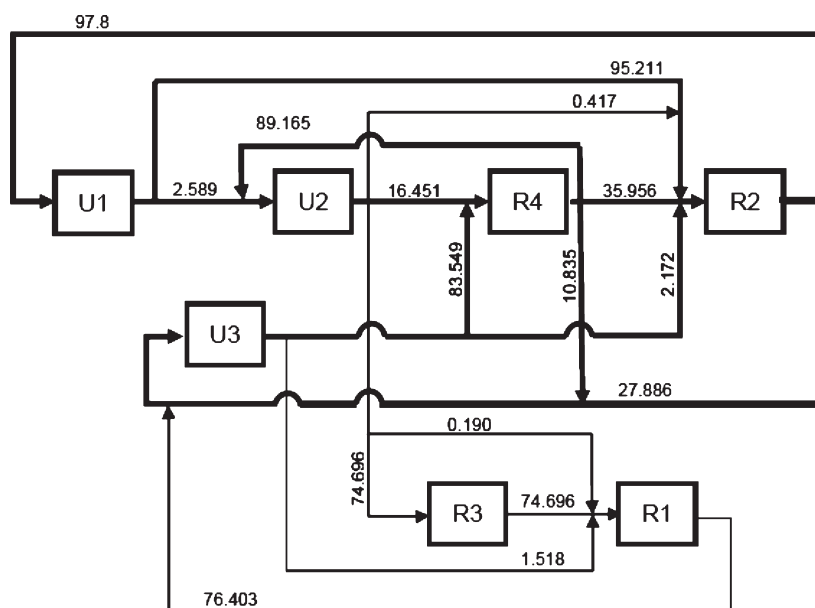


Figure 5. Retrofit design (example 1).

One external freshwater source with 200 ppm of HC, 3 ppm of  $H_2S$ , and 150 ppm of salts is considered to feed this system. Besides the regeneration process (foul water stripper R3) and end-of-pipe treatment (R4) included by Wang and Smith, there also available two water pretreatment units (R1 and R2). The end-of-pipe treatment (R4) is able to bring the concentration down to environmental limits (10 ppm for all contaminant) and is allowed to recycle. The data for these regeneration processes are presented in Table 2. Finally, the system operates 8600 h/year, and we assume an interest rate of 10%.

We solve all our case studies to global optimality using our recently developed bound contraction procedure.<sup>43–45</sup>

**4.1. Increase in Mass Load of Existing Units.** In this first case, it is considered that due to future changes in production planning, the mass loads of hydrocarbon will increase in all water-using units as shown in Table 3. For this example, we assume the costs of connections ( $F_{IJC_{ij}}$  and  $V_{IJC_{ij}}$ ) are independent of the distances and are only functions of the flow rates.

The changes will happen after 5 years, and we want to determine which regeneration processes should be installed and when. To solve this problem, one could use alternatives other than building a planning model: (1) Solve the problem for the “worst case”, that is, the one with the largest mass loads. (2) Solve the problem for the first period and then retrofit the plant after 5 years, which is, solve for the first period, fix the decided connections and set their cost as zero, and then run for the latter case.

To compare the advantages of the planning model, both alternatives were solved. The design for the worst case gives a total cost of \$3,777,798, which consists of \$1,644,939 of capital cost and \$2,132,859 of operating cost. This solution is presented in Figure 3 and was found to have global optimality in 1.5 CPUs. Note that assuming the design using the worst case, one would consider that this network would be built at the beginning of the operation. Thus, in addition to this cost, we still need to compute the operating cost of the periods (4 years) before the changes. Minimizing this operating cost, considering the design obtained for current conditions, we found it to be \$1,162,048. This solution was found to have global optimality in 1.6 CPUs. Thus,

adding the cost to calculate the net present cost, we found a NPC of \$4,129,360.

In the second alternative (design for current conditions and retrofit later), we first solve the problem minimizing total cost for the first period. This network is presented in Figure 4 and has a total cost of \$2,251,176, of which \$1,072,004 is capital cost and \$1,179,173 is operating cost. This solution was found to have global optimality in 39.3 CPUs.

However, because of the future increase in mass load, this network will need to be retrofitted in 5 years. Thus, the retrofit model is run. In this case, the cost of existing connections and regeneration processes are set to zero. In addition to the two available processes that were not used at the beginning of the operations, the existing regeneration processes were also allowed to be expanded. The minimum total cost found for the retrofitted network (Figure 5) is \$2,748,213, which is \$622,409 of capital cost and \$2,125,804 of operating cost. Summing these costs, we have a net present cost of \$3,955,068. Note that regenerations 1 and 3 were added, and regeneration 2 had an expansion of 24.914 t/h. The thicker lines are connections that already existed. However, they may have been expanded when needed.

Now the problem is solved using the planning model. The best found solution has a NPC of \$3,939,928. The planning model chooses to install regenerations 2 (capacity of 97.8 t/h) and 4 (capacity of 100 t/h) at the beginning of operation (Figure 6). After 5 years, the plant is expanded and regenerations 1 (capacity of 76.403 t/h) and 3 (capacity of 74.696 t/h) are installed together with few new connections. In Figure 6b the thicker lines represent connections that already existed, and the dotted lines are connections that are no longer used. The other lines are connections installed during the expansion.

**4.2. Installation of New Units.** In this case, it is assumed that unit 2, HDS, does not exist in the first period and will only be installed after 5 years of operation. We want to determine which regeneration processes and connections should exist, when they should be installed (or expanded), and what their capacities are.

For this example, we assume the cost of connections ( $F_{IJC_{ij}}$  and  $V_{IJC_{ij}}$ ) as also a function of the distances between processes

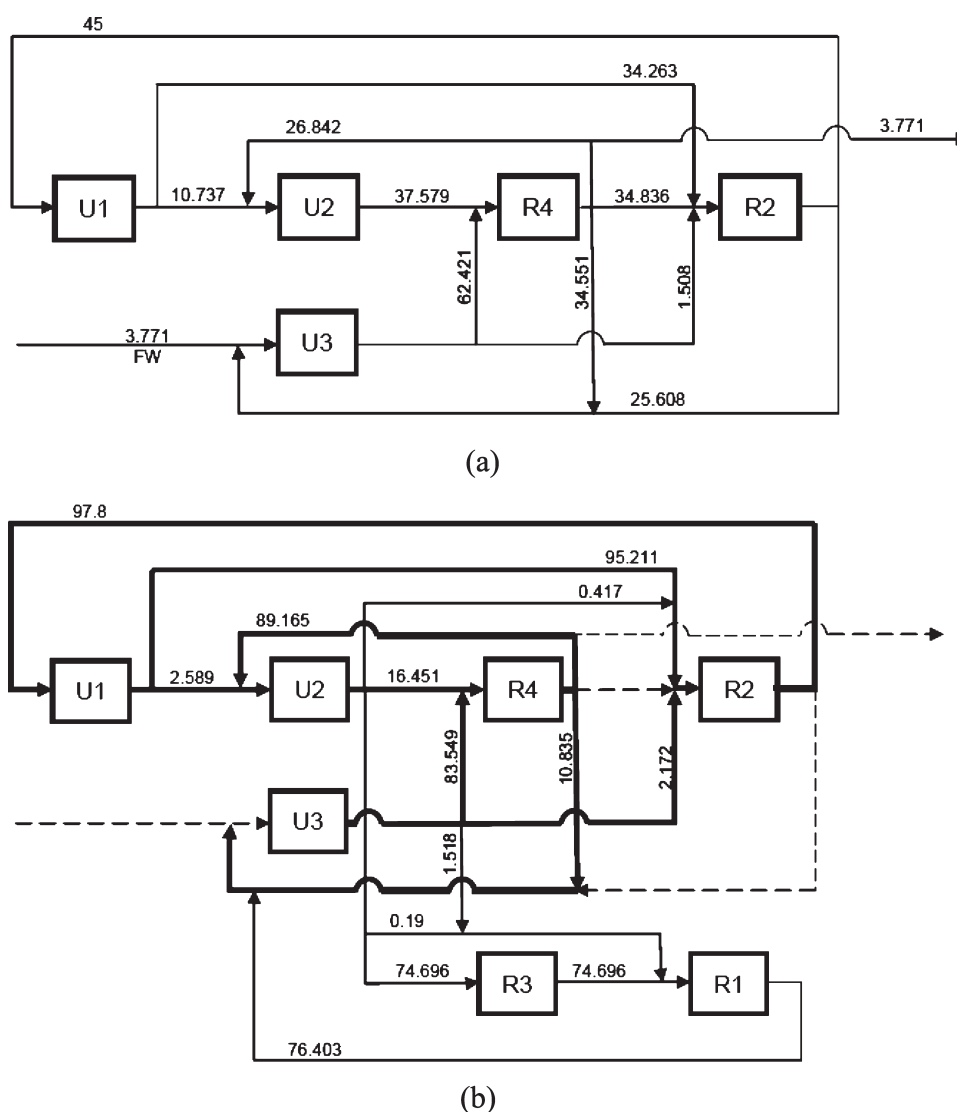


Figure 6. Planning model results (example 1). (a) First period design. (b) Future expansion.

Table 4. Distances between Processes

$d_{ij}$ (m)	U1	U2	U3	R1	R2	R3	R4	S1
FW	100	120	170	30	50	1000	1200	1500
U1	—	30	80	90	150	200	600	700
U2	30	—	60	100	150	180	300	1000
U3	80	60	—	180	130	200	400	800
R1	90	100	180	—	15	800	850	1100
R2	150	150	130	15	—	750	900	1000
R3	200	180	200	800	750	—	30	50
R4	600	300	400	850	900	30	—	30

(Table 4). We calculated these values using eqs 26 and 27, which take into account the distances between processes from Table 3. The coefficients of the constraints are based on an assumed economic velocity of 1 m/s.

$$FIJC_{i,j}(\$) = 125 d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \quad (26)$$

$$VIJC_{i,j}(\$ / t) = 1 d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \quad (27)$$

Table 5. First Period Design (Example 2)

configuration during the first period (years 1–5)				
	unit 1	unit 3	reg 2	reg 4
unit 1	—	—	45.000	—
unit 3	—	—	1.811	56.56
reg 2	45.000	47.702	—	—
reg 4	—	10.669	45.891	—

Table 6. Retrofit Configuration for Example 2 (Years 6–10)

	unit 1	unit 2	unit 3	reg 2	reg 4
unit 1	—	—	—	45.000	—
unit 3	—	—	—	1.811	56.56
unit 2	—	—	—	—	37.091
reg 2	45.000	—	47.702	—	—
reg 4	—	37.091	10.669	45.891	—

As in the previous example, the planning model solution is compared to other two options. The first option solves the problem for the initial situation and uses the retrofit model to add unit 2 after 5 years. This solution is presented in Tables 5 and 6.

In the second option, we solve the problem for the complete network (second period on time: years 6–10) and then check the configuration for its performance in the first period on time (years 1–5) obtaining the best operating conditions in this period. The solution obtained for the worst case scenario is presented in Table 7. This network costs \$1,539,292 and has an operating cost of \$1,179,173 per year.

Note that because unit 2 does not exist from year 1–5, the connections to/from unit 2 would not need to be installed in year one. That could reduce the capital cost of the first year and leaves the investment of these connections to year 6.

However, in a second step of this analysis, one needs to check how the configuration found works for the first 5 years. Considering the configuration without the connection to/from unit 2, one finds out that the remaining configuration is infeasible. One reason is because the water balance of unit 1 turns out to be incorrect. For that, one can consider that unit 1 feeds regeneration process 4 directly. This configuration has a capital cost of \$1,521,405 and an operating cost of \$ 937,648. In this case, after 5 years, the connection to/from unit 2 has to be added and replaced. This corresponds to an investment of \$98,667 in year 6. The network from year 6 to year 10 has an operating cost of \$1,179,172. The operating condition for the first 5 years is presented in Table 8

**Table 7. Worst Case Design (Example 2)**

	unit 1	unit 2	unit 3	reg 2	reg 4
unit 1	—	9.631	—	35.369	—
unit 2	—	—	—	—	37.529
unit 3	—	—	—	1.561	62.471
reg 2	45.000	—	27.886	—	—
reg 4	—	27.897	36.146	35.956	—

**Table 11. Summary of Costs for Example 2**

		conventional model + retrofit model		worst case		planning	
		capital cost	operating	capital cost	operating	capital cost	operating
first period (years 1–5)		\$1,197,231	\$888,294	\$1,521,405	\$ 937,648	\$1,553,400.00	\$888,290
second period (years 6–10)		\$529,500.55	\$1,209,419	\$98,666.73	\$1,179,172	\$253,680.00	\$1,179,100

year	DF <sub>i</sub>						
1	1	\$1,197,231	\$888,294	\$1,521,405	\$ 937,648	\$1,553,400.00	\$888,290
2	0.909		\$807,540		\$852,407		\$807,536
3	0.826		\$734,127		\$774,916		\$734,123
4	0.751		\$667,388		\$704,469		\$667,385
5	0.683		\$606,717		\$640,426		\$606,714
6	0.621	\$328,778	\$750,954	\$61,264	\$732,173	\$157,515.32	\$732,128
7	0.564		\$682,685		\$665,612		\$665,571
8	0.513		\$620,623		\$605,102		\$605,064
9	0.467		\$564,202		\$550,092		\$550,058
10	0.424		\$512,911		\$500,084		\$500,053
		\$1,526,009	\$6,835,447.12	\$1,582,669	\$6,962,933.40	\$1,710,915.32	\$6,756,926.41
total		\$8,361,456		\$8,545,603		\$8,354,287	

**Table 8. Design for Example 2 (First 5 Years)**

	unit 1	unit 3	reg 2	reg 4
unit 1	—	—	35.369	9.631
unit 3	—	—	1.561	62.471
reg 2	45.000	27.886	—	—
reg 4	—	36.146	35.957	—

**Table 9. Planning Model Design for Example 2 (First Period Design)**

configuration during the first period (years–5)				
	unit 1	unit 3	reg 2	reg 4
unit 1	—	—	45.000	—
unit 3	—	—	1.811	56.56
reg 2	45.000	47.702	—	—
reg 4	—	10.669	45.891	—

**Table 10. Planning Model Design for Example 2 (Second Period Design)**

configuration during the second period (years 6–10)						
	unit 1	unit 2	unit 3	reg 2	reg 4	S1
FW	—	—	3.771	—	—	—
unit 1	—	10.737	—	34.263	—	—
unit 2	—	—	—	—	37.579	—
unit 3	—	—	—	1.508	62.421	—
reg 2	45.000	—	25.608	—	—	—
reg 4	—	26.842	34.551	34.836	—	3.771



Next, the solution of the planning model is presented in Tables 9 and 10. Finally, Table 11 presents an economic comparison of all results for example 2.

## 5. CONCLUSIONS

We presented a planning model for industrial water systems. We consider two cases: the future increase in the load of contaminants in existing units and the possible addition of new units. We compared the design for the worst case scenario, using the long-term most demanding conditions, and the design for current constraints followed by a retrofit at a later time to a design obtained using a planning model. We concluded that for our examples, similar results in terms of costs and small variations in the structure are obtained. This does not preclude that more significant differences are obtained in other cases. Because the solutions of the other models are in the feasible space of the planning model and because the computational cost of the planning model is small compared to that of the alternative methods, we recommend using the planning model, which will always give a better result. We expect the above planning model to be simple to extend to other situations, like future environmental regulations, increasing costs of freshwater, variability on the quality of the available freshwater source, and others.

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## REFERENCES

- (1) Takama, N.; Kuriyama, T.; Shiroko, K.; Umeda, T. Optimal water allocation in a petroleum refinery. *Comput. Chem. Eng.* **1980**, *4*, 251–258.
- (2) Rossiter, A. P. *Waste Minimization through Process Design*; McGraw-Hill: New York, 1995.
- (3) Mann, J. G.; Liu, Y. A. *Industrial Water Reuse and Wastewater Minimization*; McGraw Hill: New York, 1999.
- (4) El-Halwagi, M. M. *Pollution Prevention through Process Integration: Systematic Design Tools*; Academic Press: San Diego, 1997; 1997.
- (5) El-Halwagi, M. M. *Process Integration*; Elsevier, Inc.: San Diego, 2006.
- (6) Sieniutycz, S.; Jeżowski, J. *Energy Optimization in Process Systems*; Elsevier: Amsterdam, The Netherlands, 2009.
- (7) Bagajewicz, M. J. A review of recent design procedures for water networks in refineries and process plants. *Comput. Chem. Eng.* **2000**, *24*, 2093–2113.
- (8) Foo, D. C. Y. State-of-the-art review of pinch analysis techniques for water network synthesis. *Ind. Eng. Chem. Res.* **2009**, *48*, 5125–5151.
- (9) Jeżowski, J. Review of water network design methods with literature annotations. *Ind. Eng. Chem. Res.* **2010**, *49*, 4475–4516.
- (10) Wang, Y. P.; Smith, R. Wastewater Minimisation. *Chem. Eng. Sci.* **1994**, *40* (7), 981–1006.
- (11) Kuo, W. C. J.; Smith, R. Effluent treatment system design. *Chem. Eng. Sci.* **1997**, *52* (23), 4273.
- (12) Gómez, J.; Savelski, M.; Bagajewicz, M. On a systematic design procedure single component water utilization systems in process plants. *Chem. Eng. Commun.* **2001**, *186*, 183–203.
- (13) Gomes, J. F. S.; Queiroz, E. M.; Pessoa, F. L. P. Design procedure for water/wastewater minimization: single contaminant. *J. Cleaner Prod.* **2007**, *15*, 474–485.
- (14) El-Halwagi, M. M.; Gabriel, F.; Harell, D. Rigorous graphical targeting for resource conservation via material recycle/reuse networks. *Ind. Eng. Chem. Res.* **2003**, *42*, 4319–4328.
- (15) Foo, D. C. Y.; Kazantzi, V.; El-Halwagi, M. M.; Manan, Z. A. Surplus diagram and cascade analysis technique for targeting property-based material reuse network. *Chem. Eng. Sci.* **2006**, *61*, 2626–2642.
- (16) Savelski, M.; Bagajewicz, M. Design of Water utilization systems in process plants with a single contaminant. *Waste Manage.* **2000**, *20* (8), 659–664.
- (17) Savelski, M. J.; Bagajewicz, M. J. Algorithmic procedure to design single component water utilization systems in process plants. *Chem. Eng. Sci.* **2001**, *56*, 1897–1912.
- (18) Savelski, M.; Bagajewicz, M. On the necessary conditions of optimality of water utilization systems in process plants with multiple contaminants. *Chem. Eng. Sci.* **2003**, *58* (23–24), 5349–5362.
- (19) Doyle, S. J.; Smith, R. Targeting water reuse with multiple contaminants. *Trans. Inst. Chem. Eng., Part B* **1997**, *75* (3), 181–189.
- (20) Alva-Argaez, A.; Kokossis, A. C.; Smith, R. A conceptual decomposition of MINLP models for the design of water-using systems. *Int. J. Environ. Pollut.* **2007**, *29*, 177–205.
- (21) Gunaratnam, M.; Alva-Argaez, A.; Kokosis, A.; Kim, J. K.; Smith, R. Automated design of total water systems. *Ind. Eng. Chem. Res.* **2005**, *44*, 588–599.
- (22) Bagajewicz, M.; Rivas, M.; Savelski, M. A robust method to obtain optimal and sub-optimal design and retrofit solutions of water utilization systems with multiple contaminants in process plants. *Comput. Chem. Eng.* **2000**, *24*, 1461–1466.
- (23) Karuppiah, R.; Grossmann, I. E. Global optimization for the synthesis of integrated water systems in chemical processes. *Comput. Chem. Eng.* **2006**, *30*, 650–673.
- (24) Koppol, A. P. R.; Bagajewicz, J. M.; Dericks, B. J.; Savelski, M. J. On zero water discharge solutions in process industry. *Adv. Environ. Res.* **2003**, *8*, 151–171.
- (25) Huang, C.-H.; Chang, C.-T.; Ling, H.-C.; Chang, C.-C. A Mathematical programming model for water usage and treatment network design. *Ind. Eng. Chem. Res.* **1999**, *38*, 2666.
- (26) Jeżowski, J.; Bochenek, R.; Poplewski, G. On application of stochastic optimization techniques to designing heat exchanger- and water networks. *Chem. Eng. Process.* **2007**, *46* (11), 1160–1174.
- (27) Savulescu, L. E.; Sorin, M.; Smith, R. Direct and indirect heat transfer in water network systems. *Appl. Therm. Eng.* **2002**, *22*, 981–988.
- (28) Rodera, H.; Bagajewicz, M. Targeting procedures for energy savings through heat integration across plants. *AIChE J.* **1999**, *45* (8), 1721–1742.
- (29) Bagajewicz, M.; Rodera, H.; Savelski, M. Energy efficient water utilization systems in refineries and process plants. *Comput. Chem. Eng.* **2002**, *26* (1), 56–79.
- (30) Bogataj, M.; Bagajewicz, M. J. Synthesis of non-isothermal heat integrated water networks in chemical processes. *Comput. Chem. Eng.* **2008**, *32*, 3130–3142.
- (31) Faria, D.; Bagajewicz, M. On the degeneracy of the water/wastewater allocation problem in process plants. *Ind. Eng. Chem. Res.* **2010**, *49* (9), 4340–4351.
- (32) Faria Débora, C.; Bagajewicz, M. On the appropriate modeling of process plant water systems. *AIChE J.* **2010**, *56* (3), 668–689.
- (33) Nourai, F.; Rashtchian, D.; Shayegan, J. An integrated framework of process and environmental models, and EHS constraints for retrofit targeting. *Comput. Chem. Eng.* **2001**, *25*, 745–755.
- (34) Fraser, D. M.; Hallale, N. Retrofit of mass exchanger networks using pinch technology. *AIChE J.* **2000**, *46* (10), 2112–2117.
- (35) Tan, Y. L.; Manan, Z. A. Retrofit of water network with optimization of existing regeneration units. *Ind. Eng. Chem. Res.* **2006**, *45*, 7592–7602.
- (36) Tan, Y. L.; Manan, Z. A.; Foo, D. C. Y. Retrofit of water network with regeneration using water pinch analysis. *Process Saf. Environ. Prot.* **2008**, *85* (B4), 305–317.

- (37) Dvarioniene, J.; Stasiskiene, Z. Integrated water resource management model for process industry in Lithuania. *J. Cleaner Prod.* **2007**, *15* (10), 950–957.
- (38) Jödicke, G.; Fischer, U.; Hungerbühler, K. Wastewater reuse: A new approach to screen for designs with minimal total costs. *Comput. Chem. Eng.* **2001**, *25*, 203–215.
- (39) Faria, D. C.; Bagajewicz, M. J. Profit-based grassroots design and retrofit of water networks in process plants. *Comput. Chem. Eng.* **2009**, *33*–2, 436–453.
- (40) Eppen, G. D.; Martin, R. K.; Schrage, L. A scenario approach to capacity planning. *Oper. Res.* **1989**, *37*, 517.
- (41) Sahinidis, N. V.; Grossmann, I. E.; Fornari, R. E.; Chathrathi, M. Optimization model for long range planning in the chemical industry. *Comput. Chem. Eng.* **1989**, *13*, 1049.
- (42) Faria, D.; Bagajewicz, M. Global optimization of water management problems using linear relaxations and bound contraction methods. *Ind. Eng. Chem. Res.*, in press.
- (43) Faria, D.; Bagajewicz, M. A new approach for global optimization of a class of MINLP problems with applications to water management and pooling problems. *AIChE J.*, in preparation.
- (44) Faria, D.; Bagajewicz, M. Novel bound contraction procedure for global optimization of bilinear MINLP problems with applications to water management problems. *Comput. Chem. Eng.*, in preparation.
- (45) Faria, D.; Bagajewicz, M. Global optimization based on sub-spaces search and elimination. applications to generalized pooling and water management problems. *AIChE J.*, submitted.