ON THE DEGENERACY OF THE WATER/WASTEWATER ALLOCATION PROBLEM IN PROCESS PLANTS

Débora C. Faria and Miguel J. Bagajewicz(*)

University of Oklahoma, 100E. Boyd, Norman – OK 73019, USA

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(*) Corresponding Author

Abstract

Several methodologies to design water systems in process plants are based on minimizing freshwater consumption. The objective is the appropriate one when water is scarce and costs are not a big issue. It has also been used as a substitute for cost in the belief that water and final treatment costs overwhelm other fixed capital and operating costs of regeneration processes. Among graphical and algorithmic methods, the popular "Pinch Technology"-based procedure has early proponents and contemporary advocates who consider and defend it as a good method to provide "insights" into the right answer. In this paper, we show that the minimum freshwater problem has sometimes a large number of alternative degenerate solutions, something that graphical and algorithmic procedures can hardly identify systematically. We provide a mathematical programming method to identify these solutions and to point out those that make more economical sense. We also provide means to identify suboptimal solutions that are very close to the optimum economical one. We illustrate these degeneracies in several cases of single and multiple contaminants.

1. Introduction

Water allocation problems (WAP) started to be of interest in the early eighties and have been extensively studied thereafter. Bagajewicz (2000) presents a review of the most popular method presented until 2000. In general, these approaches can be divided in two big classes: mathematical programming-based methods and methods based on graphical, heuristic or algorithmic procedures. In addition, even though the seminal paper by Takama et al. (1980) advocates cost minimization, most of the methods proposed later (Wang and Smith, 1994, 1995; Olesen and Polley, 1997; Kuo and Smith, 1998; Savelski and Bagajewicz, 2001a; Feng and Sieder, 2001; Hallale, 2002; Wang et al., 2003; El-Halwagi et al., 2003; Zheng et al., 2006; Relvas et al., 2008; among others), focus on minimizing freshwater consumption. Although the reason has hardly been made explicit, we believe the assumption is made in analogy to pinch technology-based methods for heat exchangers, that is, that most cost effective solutions would feature minimum consumption. In other words, the underlying assumption is that freshwater costs are the dominant costs.

While mathematical programming-based methods have also been used to solve the minimum freshwater consumption problem, they are the appropriate tool for a variety of cost objectives (Savelski and Bagajewicz, 2001b; Koppol et al., 2003; Guanaratnam, 2005; Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007), to handle forbidden matches (Savelski and Bagajewicz, 2001b; Alva-Argáez et al., 2007; Putra and Amminudin, 2008), to add the cost of regeneration units (Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007) and for maximizing profitability (Faria and Bagajewicz, 2006; Lim et al., 2006, 2007; Wan Alwi and Manan, 2006, 2007; Faria and Bagajewicz, 2009a). Important efforts to solve the WAP to global optimality were presented (Karuppiah and Grossmann, 2006a,b; Bergamini et al., 2008).

The proponents and current advocates of the use of simplified procedures ("Pinch Technology", "sources and sinks", etc), claim that these methods provide quick "insights" into the right answer. They are successful in single component cases to correctly predict minimum freshwater consumption and can even be extended to the case of *total water systems*, where partial regeneration and recycle from end-of-pipe treatment is added (see a discussion in Faria and Bagajewicz, 2009b). In the case of multicomponent systems, they are not rigorous, but several heuristics that reasonably obtain minimum freshwater consumption have been proposed. These methods, however, encounter some difficulties when the objective is cost. Despite the successes in predicting freshwater consumption and above and beyond the difficulties in obtaining good solutions when minimum cost is sought, the issue of obtaining the corresponding network has been considered as secondary, despite indications that several alternative configurations featuring the same freshwater consumption (degenerate solutions), might exist. Bagajewicz et al. (2000) presented an algorithmic procedure that combines mathematical programming and necessary optimality conditions (Savelski and Bagajewicz, 2003). They applied their methodology to a large multiple contaminant example and, in addition to what they consider the optimum solution, four sub-optimum ones were presented. Putra and Amminudin (2008) approached the existence of what they call "class of good solutions". These solutions are different design options that find the same optimum (or near optimum solutions), but show different perspectives concerning cost, layout (complexity) or efficiency of the regeneration processes. They find the "class of good solutions" by fixing the maximum number of connection to an operation or existence of regeneration-recycling, and then minimizing the freshwater consumption. They find four “good solutions” and compare them with three others found by previous works (Kuo, 1996; Alva-Argaéz, 1999; Gunaratnam, 2003). Although their point of analyzing different options is valid, their procedure is not able to effectively generate a considerable number of alternatives. In reality, there is no systematic way known so far to predict beforehand how many alternative solutions a problem has. In addition, it is unclear if such degeneracy exists for the case of minimizing total costs.

In this paper, an automatic method to find alternative solutions is proposed. The search for alternative solutions is done in a matter in which a new network configuration (connections among freshwater source, water using units, regeneration processes and sink) is successively found with respect to a certain objective function or a preset conditions (minimum freshwater consumptions for example) that will characterize degenerate solutions for the given condition. At each new search, the networks previously found are excluded from the set of feasible solutions. In a problem with high degeneracy, the optimum solution (objective function value) may be repeated for many of the found structures and the alternative solutions provide a more flexible scope in the decision making process. On the other hand, when the problem is not highly degenerate, the alternative solutions can provide non-optimum solutions in which other criteria (much lower investment costs, easier operability, etc.) can be improved.

The paper is organized as follows: we first present the general mathematical model for the WAP, a *complete integrated water system*, as presented by Faria and Bagajewicz (2009b). Next, a method to identify degenerate and near-optimum solutions is presented, and then several examples are presented.

Mathematical Model

A general non-liner model to solve the water allocation problem is given by the following set of equations:

Water balance at the water-using units

$$\sum_{w} FWU_{w,u} + \sum_{u^*} FUU_{u^*,u} + \sum_{r} FRU_{r,u} = \sum_{s} FUS_{u,s} + \sum_{u^*} FUU_{u,u^*} + \sum_{r} FUR_{u,r} \quad \forall u \qquad (1)$$

where $FWU_{w,u}$ is the flowrate from freshwater source *w* to unit *u*, $FUU_{u^*,u}$ is the flowrate between unit *u** and *u*, $FRU_{r,u}$ is the flowrate from regeneration process *r* to unit *u*, $FUS_{u,s}$ is the flowrate from unit *u* to sink *s* and $FUR_{u^*,r}$ is the flowrate from unit *u* to regeneration process *r*.

Water balance at the regeneration processes

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

where $FWR_{w,r}$ is the flowrate from freshwater source *w* to the regeneration process *r*, $FRR_{r^*,r}$ is the flowrate from regeneration process *r** to regeneration process *r* and $FRS_{r,s}$ is the flowrate from regeneration process *r* to sink *s*. In fact, we assume here that the set of regeneration processes existing in the system is formed by the set of water pre-treatments and the set of wastewater treatments. If one wants to differentiate between these two categories of regeneration processes, two subsets for the regeneration processes set can be easily created and different constraints applied to each subset.

Contaminant balance at the water-using units

$$\left.\begin{aligned}&\sum_{w}\left(CW_{w,c}\ FW_{w,u}\right)+\sum_{u^*}\left(FUU_{u^*,u,c}C^{out}_{u^*,c}\right)+\sum_{r}\left(FRU_{r,u,c}CR^{out}_{r,c}\right)+\Delta M_{u,c}\\&\qquad=\sum_{u^*}\left(FUU_{u,u^*,c}C^{out}_{u,c}\right)+\sum_{s}\left(FUS_{u,s,c}C^{out}_{u,c}\right)+\sum_{r}\left(FUR_{u,r,c}C^{out}_{u,c}\right)\qquad\forall u,c\end{aligned}\right\}\tag{3}$$

where $CW_{w,c}$ is the concentration of contaminant *c* in the freshwater source *w*, $\Delta M_{u,c}$ is the mass load of contaminant *c* extracted in unit *u*, $C^{out}_{u,c}$ is the outlet concentration of contaminant *c* in unit *u*, and $CR^{out}_{r,c}$ is the outlet concentration of the not treated contaminant *c* in regeneration *r* .

Maximum inlet concentration at the water-using units

$$\left.\begin{aligned}&\sum_{w}\left(CW_{w,c}\ FW_{w,u}\right)+\sum_{u^*}\left(FUU_{u^*,u,c}C^{out}_{u^*,c}\right)+\sum_{r}\left(FRU_{r,u,c}CR^{out}_{r,c}\right)\\&\qquad\leq C^{in,max}_{u,c}\left(\sum_{w}FUW_{w,u}+\sum_{u^*}FUU_{u^*,u}+\sum_{r}FRU_{r,u}\right)\qquad\forall u,c\end{aligned}\right\}\tag{4}$$

where $C^{in,max}_{u,c}$ is the maximum allowed concentration of contaminant *c* at the inlet of unit *u*.

Maximum outlet concentration at the water-using units

$$C^{out}_{u^*,c}\leq C^{out,max}_{u,c}\quad\forall u,c\tag{5}$$

where $C^{out,max}_{u,c}$ is the maximum allowed concentration of contaminant *c* at the outlet of unit *u*.

Flowrate trough the regeneration processes

$$FR_r=\sum_{w}FWR_{w,r}+\sum_{u}FUR_{u,r}+\sum_{r^*}FRR_{r^*,r}\quad\forall r\tag{6}$$

where FR_r is the flowrate through the regeneration process *r*.

Contaminant balance at the regeneration processes

$$FR_{r,c}CR^{in}_{r,c}=\sum_{w}\left(FWR_{w,r}CW_{w,c}\right)+\sum_{u}\left(FUR_{u,r}C^{out}_{u,c}\right)+\sum_{r^*}\left(FRR_{r^*,r}CR^{out}_{r^*,c}\right)\qquad\forall r,c\tag{7}$$

$$CR_{r,c}^{out} = CR_{r,c}^{in}(1 - XCR_{r,c}) + CRF_{r,c}^{out}\ XCR_{r,c} \qquad \forall r,c \tag{8}$$

where $CR_{r,c}^{in}$ is the concentration of contaminant *c* at the inlet of regeneration process *r*, $CRF_{r,c}^{out}$ is the outlet concentration of contaminant *c* in regeneration process *r* and $XCR_{r,c}$ is a binary parameter that indicates if contaminant *c* is treated by regeneration process *r*. We assume that $CRF_{r,c}^{out}$, the concentration of the treated contaminant is known and constant.

Maximum inlet concentration of the regeneration processes

$$CR_{r,c}^{in} \le CR_{r,c}^{in,max} \qquad \forall r,c \tag{9}$$

where $CR_{r,c}^{in,\max}$ is the maximum concentration of contaminant *c* allowed at the inlet of regeneration process *r*.

Maximum allowed discharge concentration

$$\sum_{u}\left(FUS_{u,s,c}C_{u,c}^{out}\right) + \sum_{r}\left(FRS_{r,s,c}CR_{r,c}^{out}\right) \le C_{s,c}^{discharge,max}\left(\sum_{u} FUS_{u,s} + \sum_{r} FRS_{r,s}\right) \qquad \forall s,c \tag{10}$$

where $C_{s,c}^{discharge,max}$ is the maximum allowed concentration at sink *s*.

Minimum flowrates

It is well known that many solutions of the water problem may include small flowrates that are impractical. To avoid these we use the following constraints:

$$FWU_{w,u} \ge FWU_{w,u}^{Min}\ YWU_{w,u} \qquad \forall w,u \tag{11}$$
$$FWR_{w,r} \ge FWR_{w,r}^{Min}\ YWR_{w,r} \qquad \forall w,r \tag{12}$$
$$FUU_{u,u*} \ge FUU_{u,u*}^{Min}\ YUU_{u,u*} \qquad \forall u,u* \tag{13}$$
$$FUS_{u,s} \ge FUS_{u,s}^{Min}\ YUS_{u,s} \qquad \forall u,s \tag{14}$$
$$FUR_{u,r} \ge FUR_{u,r}^{Min}\ YUR_{u,r} \qquad \forall u,r \tag{15}$$
$$FRU_{r,u} \ge FRU_{r,u}^{Min}\ YRU_{r,u} \qquad \forall r,u \tag{16}$$
$$FRR_{r,r*} \ge FRR_{r,r*}^{Min}\ YRR_{r,r*} \qquad \forall r,r* \tag{17}$$
$$FRS_{r,s} \ge FRS_{r,s}^{Min}\ YRS_{r,s} \qquad \forall r,s \tag{18}$$

which uses a set of binary variables ($YWU_{w,u}$, $YWR_{w,r}$ $YUU_{u,u*}$, $YUS_{u,s}$, $YUR_{u,r}$, $YRU_{r,u}$, $YRR_{r,r*}$ and $YRS_{r,s}$) that are equal to one when the corresponding flowrate is different from zero and zero otherwise.

Maximum flowrates

To ensure that the connections do not surpass maximum values, we use the following constraints:

$$FWU_{w,u} \le FWU_{w,u}^{Max}\ YWU_{w,u} \quad \forall w,u \tag{19}$$

$$FWR_{w,r} \le FWR_{w,r}^{Max}\ YWR_{w,r} \quad \forall w,r \tag{20}$$

$$FUU_{u,u*} \le FUU_{u,u*}^{Max}\ YUU_{u,u*} \quad \forall u,u* \tag{21}$$

$$FUS_{u,s} \le FUS_{u,s}^{Max}\ YUS_{u,s} \quad \forall u,s \tag{22}$$

$$FUR_{u,r} \le FUR_{u,r}^{Max}\ YUR_{u,r} \quad \forall u,r \tag{23}$$

$$FRU_{r,u} \le FRU_{r,u}^{Max}\ YRU_{r,u} \quad \forall r,u \tag{24}$$

$$FRR_{r,r*} \le FRR_{r,r*}^{Max}\ YRR_{r,r*} \quad \forall r,r* \tag{25}$$

$$FRS_{r,s} \le FRS_{r,s}^{Max}\ YRS_{r,s} \quad \forall r,s \tag{26}$$

Objective functions

Minimum freshwater consumption:

$$Min \sum_{w} \left(\sum_{u} FWU_{w,u} + \sum_{r} FWR_{w,r} \right) \tag{27}$$

Minimum total annual cost:

$$Max \left[OP \left(\sum_{w} \alpha_w \left(\sum_{u} FWU_{w,m} + \sum_{r} FWR_{w,r} \right) + \sum_{r} OPN_r\, FR_r \right) - af\ FCI \right] \tag{28}$$

where OPN_r are the operational cost of the regeneration processes, OP is the hours of operation per year. The last term is the annualized capital cost, 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:

$$\left. \begin{aligned} FCI = \sum_{u} & \left(\begin{aligned} & \sum_{w} YWU_{w,u}\ CCWU_{w,u} + \sum_{r} YUR_{u,r}\ CCUR_{u,r} \\ & + \sum_{u* \ne u} YUU_{u,u*}\ CCUU_{u,u*} + \sum_{s} YUS_{u,s}\ CCUS_{u,s} \end{aligned} \right) \\ + \sum_{r} & \left(\begin{aligned} & \sum_{w} YWR_{w,r}\ CCWR_{w,r} + \sum_{r* \ne r} YRR_{r,r*}\ CCRR_{r,r*} + \\ & \sum_{u} YRU_{u}\ CCRU_{u} + \sum_{s} YRS_{r,s}\ CCRS_{r,s} + CCR_r \left(FR_r \right)^{0.7} \end{aligned} \right) \end{aligned} \right\} \tag{29}$$

which uses a set of capital cost parameters to assign cost to the connections ($CCWU_{w,u}$, $CCWR_{w,r}$ $CCUU_{u,u*}$, $CCUS_{u,s}$, $CCUR_{u,r}$, $CCRU_{r,u}$, $CCRR_{r,r*}$ and $CCRS_{r,s}$) and to the regeneration processes (CCR_r).

Degeneracy and Sub-Optimal Solutions

With the exception of Bagajewicz et al. (2000), who presents a procedure to identify optimum and sub-optimum solution using the necessary conditions of optimality from Savelski and Bagajewicz (2003) and Putra and Amminudin (2008), who present an approach to generate what they call "class of good solutions", we know of no other work that has presented a methodology to find degenerate and sub-optimum solutions of water allocation problems. Putra and Amminudin (2008) proposed a two-step approach to find the multiple solutions. In the first step the structure of the network is defined using an MILP model, and then a NLP model is used to find the conditions for the found structure. They claim this strategy renders a global optimum, but they offer no proof of this assertion. Because of the two step strategy proposed, we doubt it is. The "class of good solutions" is found fixing the piping connections, which can be related to the number of water reuse streams, maximum number of connection to an operation or existence of regeneration-recycling, and minimizing the freshwater consumption. Even if degeneracy and sub-optimum solutions can be found using this procedure, there can still exist other alternative solutions for the same piping network.

To ameliorate the above problems, we propose an automatic method to find a significant higher number of options, if not all of them. The search for alternative solutions is done in a matter in which a new network configuration (connections among freshwater source, water using units, regeneration processes and sink) is successively found with respect to a certain objective function. At each new search the previous found network are excluded from the feasible solution. In a problem with high degeneracy, the optimum solution (objective function value) will be repeated for many of the found structures and the alternative solutions provide a more flexible scope in the decision making process. On the other hand, when the problem is not highly degenerated, the alternative solutions can provide non optimum solutions in which present other advantages such as much lower investment costs, easier operability, etc.

The alternative solutions are found as follows:

Step 1. Run the model presented in section 3.
Step 2. Forbid the networks previously found.
Step 3. Go back to Step 1.

To forbid the networks, the following constraint is added to the model:

$$\sum_{(i,j)\in\left\{\begin{matrix}(w,u),(u,u*),(u,r),\\(u,s),(r,u),(r,r*),(r,s)\end{matrix}\right\}} NYIJ_{n,i,j}YIJ_{i,j} + \left(1-NYIJ_{n,i,j}\right)\left(1-YIJ_{i,j}\right) \le CARD(NYIJ)-1 \qquad \forall n < n_{found} \qquad (30)$$

where n corresponds to the n^{th} network previously found, n_{found} is the number of networks previously found and $NYIJ_{n,i,j}$ are the values of the binary variables obtained in run n, which define the configuration of each network. In turn, *CARD(NYIJ)* is the cardinality of the set of binary variables *NYIJ*. Thus, the network exclusion constraints forbid combinations of possible connections found all previous iterations. The left hand side of the equation is used to account for existing (first term) and non-existing connections (second term) in the n^{th} solution. In other words, all the previously found combinations will have the summation equal to *CARD(NYIJ)* and therefore cannot be repeated. Thus, to generate a new network, at least one of the connections needs to be included or excluded.

Results

Results have showed that for some problems present a significant number of degenerate solutions regarding minimum freshwater consumption. On the other hand, there are problems in which degeneracy is not present or is very small. We start with a single contaminant case and then analyze multiple contaminant cases.

Example 1

This example corresponds to the *water-using subsystem* example presented by Wang and Smith (1994), which has four water-using units. The data for this problem is shown in Table 1.

Table 1 – Limiting data of example 1.

Process	Mass Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	2	0	100
2	5	25	75
3	30	80	240
4	40	30	90

We solve the problem minimizing freshwater consumption to global optimality to find the 100 first networks. We use a minimum flowrate of 1 t/h for all connections. Here, the minimum flowrate is not only related to practical issues, but also to avoid the existence of combinations of networks that, in reality, have zero flowrate through the connections. We used the global optimization approach presented by Faria and Bagajewicz (2008, 2009c) with a 1% tolerance gap.

Figure 1 illustrates the freshwater consumption and the number of connections for the first 100 solutions, as they were obtained (not sorted); the first 96 feature the minimum consumption of 90 t/h (ordinate on the left) and the last four exhibit a slightly higher value. The number of connections is also shown (ordinate on the right). All solutions were obtained minimizing freshwater adding the corresponding connections exclusion constraint (30). All the 100 solutions were found using an Intel Xeon 2.67 GHz and 2.5 GB of RAM in 1 hour (wall clock time).

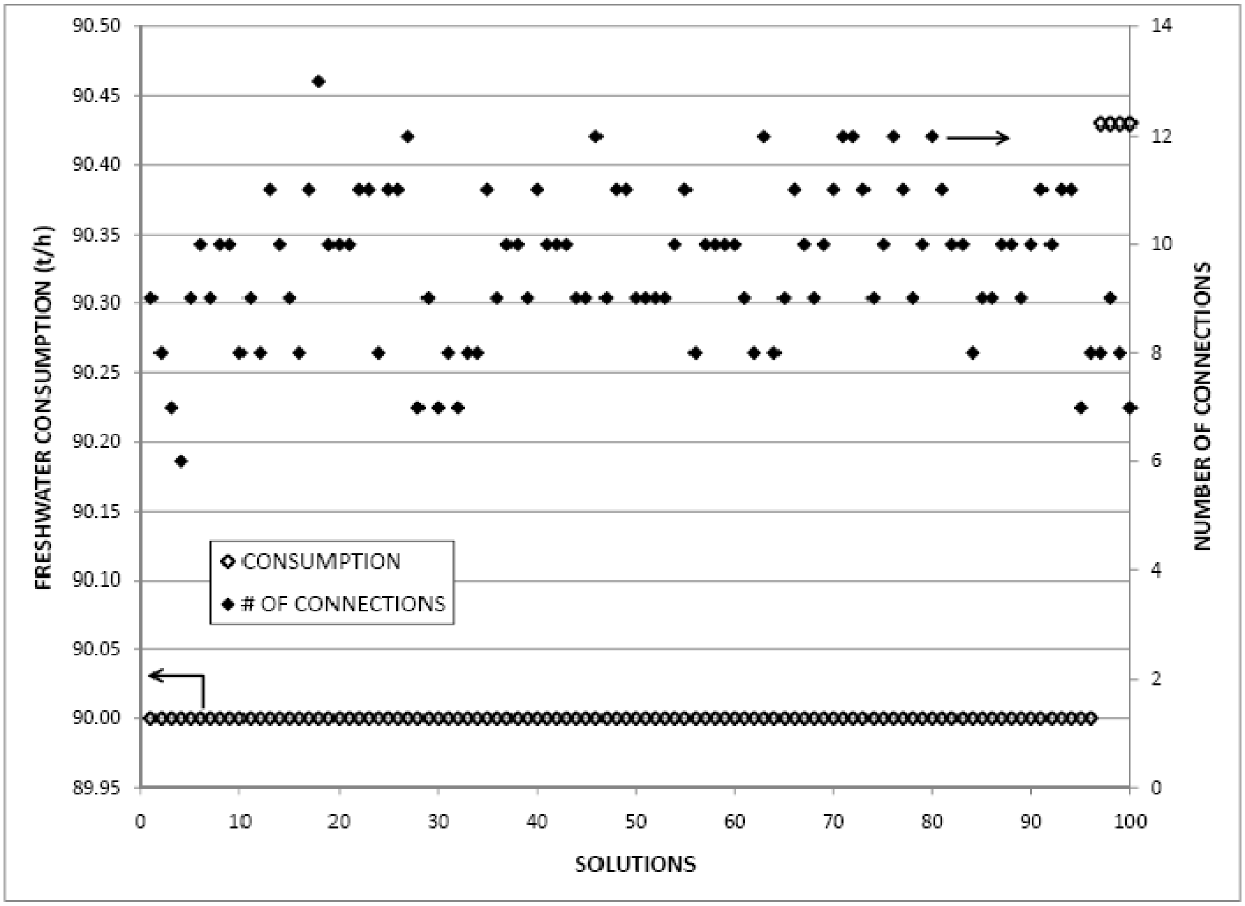

Figure 1 – Hundred first solutions for minimum freshwater consumption of the water-using subsystem single contaminant example from Wang and Smith (1994).

To determine what the right network is, one needs to add cost. This can be done by

- Making an assessment of the cost of each network after they are found, a strategy that may work well if the number of networks is small.
- Solving the problem again, fixing the flowrate to its minimum and minimizing capital cost, or cost of regeneration, or both.

We note that only in the case where the effluent from the end-of-pipe treatment is not recycled and totally disposed of, the cost of regeneration is proportional to the cost of freshwater and therefore treatment costs cannot be used as an economical objective (see Faria and Bagajewicz, 2009a).

We point out here the core of our claim, that pinch-technology-based methods as well as other graphical and algorithmic procedures are in principle incapable of performing the above proposed sorting and therefore they fail to provide proper insights beyond identifying the value of minimum consumption, something that mathematical programming can also easily determine.

Example 2

This is the case of *water-using subsystem* optimization presented by Wang and Smith (1994), which involves two water-using units and two contaminants and minimizes freshwater consumption. Table 2 presents the limiting data of this problem. The minimum freshwater consumption of this network without reuse is 63.33 ton/h.

Table 2 – Limiting data of example 1.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	4	0	100
	B	2	25	75
2	A	5.6	80	240
	B	2.1	30	90

As no regeneration process is used in this example, only two cases are analyzed:

- No recycle of the end-of-pipe treatment (optimization of *water-using subsystem*);
- The effluent stream from the end-of-pipe treatment can be reused by the water-using units (*total water system*).

We discussed the advantages and disadvantages of these systems earlier (Faria and Bagajewicz, 2009b). For the end-of-pipe treatment, it is assumed that an outlet concentration of 10 ppm for both contaminants, which are in agreement with the maximum allowed to disposal.

For the first case (no recycle of end-of-pipe treatment allowed) the minimum freshwater consumption can be reduced to 54 t/h, which is approximately 15% less than the current consumption obtained when no water reuse is considered. When alternative solutions are investigated, it indicates the existence of a unique solution (no-degeneracy) at 54 t/h, that is, no degeneracy. The next possible solution identified when the first is excluded features 63.33 t/h, which is the network without reuse and is not degenerate either.

If for some reason (cost for example, as it was explored in Faria and Bagajewicz, 2009a) one would want to explore higher consumptions, 3 possible networks consuming 66.67 ton/h are found. Note that if one wants to minimize number of connection, the optimum network is network 5, which is a network in series and has the largest consumption. All these networks are presented in Table 3.

Next, we analyze the case in which the recycle of the effluent stream from the end-of-pipe treatment is allowed. In such case, the minimum freshwater consumption can be further reduced to 40 ton/h freshwater consumption network. This is 26% lower than the previous case (and 36.8% lower than the consumption without reuse).

Eleven feasible alternative networks were found in this case, in which the first three solutions obtained consume 40 t/h of freshwater and the next three 41 t/h. The eleven feasible solutions are summarized in Figure 2. The 3 solutions at minimum consumption and the subsequent 3 slightly higher are presented in Table 4. Quite clearly, in this case, the networks use a very small flowrate in some connections and for this reason will not be even considered. Others, like network 3, exhibit independent cycles, which are usually avoided.

Table 3 – Alternative network configurations for the *water-using subsystem* of the multiple contaminants example from Wang and Smith (1994).

		Unit 1	**Unit 2**	**EOP**
Network 1 54 ton/h	Freshwater	40	14 t/h	-
	Unit 1	-	21 t/h	19 t/h
	Unit 2	-	-	35 t/h
Network 2 63.33 ton/h	Freshwater	40 t/h	23.33 t/h	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	23.33 t/h
Network 3 66.67 ton/h	Freshwater	57.143 t/h	9.524 t/h	-
	Unit 1	-	57.143 t/h	-
	Unit 2	-	-	66.667 t/h
Network 4 66.67 ton/h	Freshwater	66.667 t/h	-	-
	Unit 1	-	44.094 t/h	22.572 t/h
	Unit 2	-	-	44.094 t/h
Network 5 66.67 ton/h	Freshwater	66.667 t/h	-	-
	Unit 1	-	66.667 t/h	-
	Unit 2	-	-	66.667 t/h

- A minimum flowrate of 1 t/h was used.

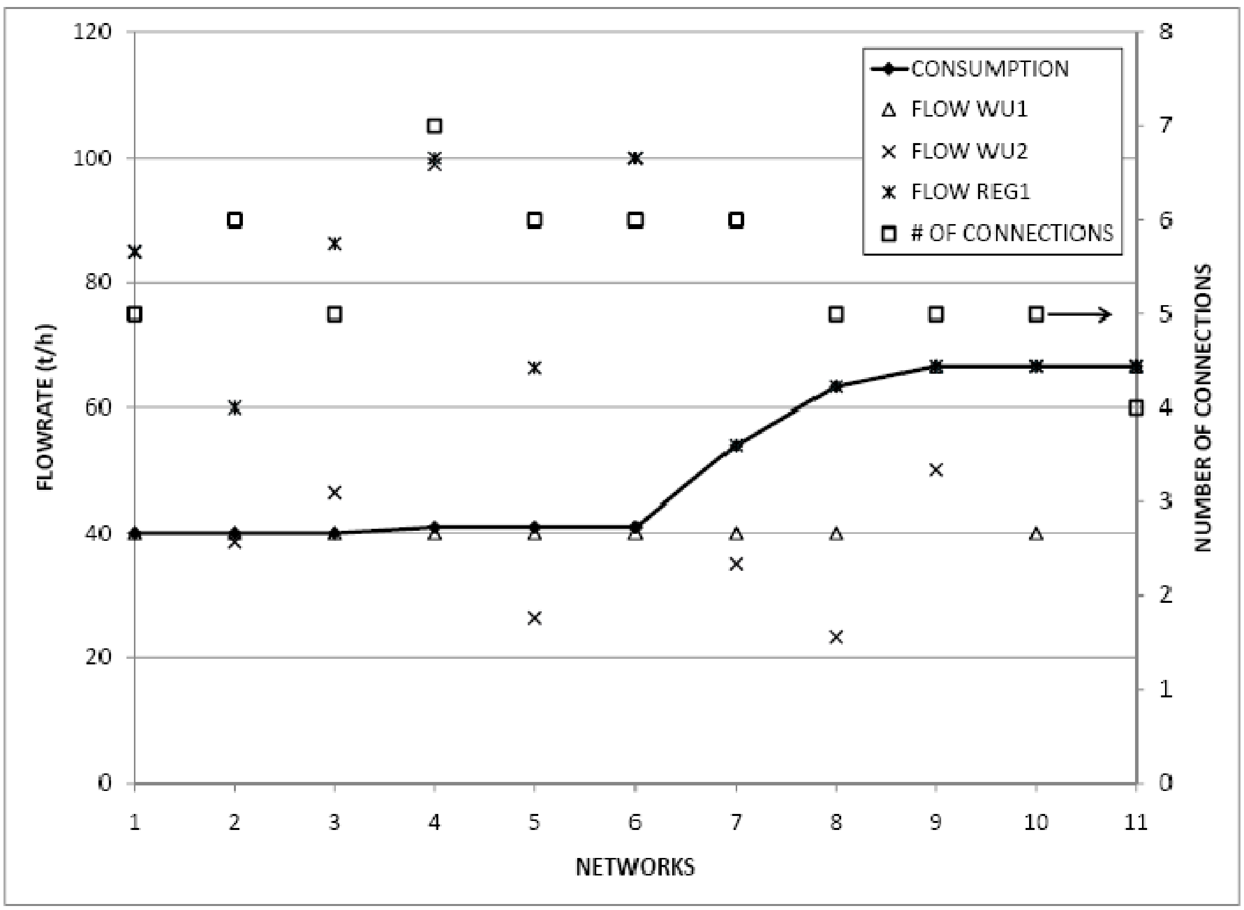

Figure 2 – Feasible networks for the *total water system* of the multiple contaminants from Wang and Smith (1994).

Table 4 – Alternative solutions at minimum consumptions for the *total water system* of the multiple contaminants from Wang and Smith (1994).

		Unit 1	Unit 2	EOP
Network 1 40 t/h	Freshwater	40 t/h	-	-
	Unit 1	-	40 t/h	-
	Unit 2	-	-	85 t/h
	EOP	-	45 t/h	-
Network 2 40 t/h	Freshwater	40 t/h	-	-
	Unit 1	-	18.56 t/h	21.44 t/h
	Unit 2	-	-	38.56 t/h
	EOP	-	20 t/h	-
Network 3 40 t/h	Freshwater	40 t/h	-	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	46.33 t/h
	EOP	-	46.33 t/h	-
Network 4 41 t/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	39 t/h	1 t/h
	Unit 2	-	-	99 t/h
	EOP	-	59 t/h	-
Network 5 41 t/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	26.418 t/h
	EOP	-	25.418 t/h	-
Network 6 41 t/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	40 t/h	40 t/h
	Unit 2	-	-	100 t/h
	EOP	-	59 t/h	-

*A minimum flowrate of 1 ton/h was used.

The fact that pinch technology or other graphical and algorithmic procedures are not designed to look for cost, take into account forbidden connections, and have difficulties handling multicomponent cases, is known. Therefore, unless these methods become able to consider forbidden combination of connections, the above exercise cannot be made using methods other than mathematical programming. When costs are considered, the statement also applies as we shall see below.

We now present examples with much larger degeneracy and discuss the issue of costs.

Example 3

Putra and Amminudin (2008) analyzed a larger refinery problem, which was originally presented by Kuo and Smith (1998) and later also investigated by Gunaratman et al. (2005) and Alva-Argaez et al. (2007). This is a *total water system problem* that has five water-using units, three regeneration processes and considers three contaminants. Putra and Amminudin (2008) showed four alternative solutions for this problem and compared them with the results previously obtained by others. Guanaratman et al. (2005) and Alva-Argaez et al. (2007) solved for total annualized cost, including piping cost. Tables 5 to 7 show the data used in this example. The discharge limits of this system are 20 ppm for HC, 5 ppm for H_2S and 100 ppm for suspended solids (SS). The freshwater cost is $0.2/t and the system operates 8600 hours per year. A 10% rate of discount is assumed. We used a minimum flowrate through the connection of 5 t/h and a maximum through the connection and processes of 200 t/h.

Table 5 – Water using units limiting data of example 3.

Water units	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
(U1) Steam stripping	HC	0.75	0	15
	H_2S	20	0	400
	SS	1.75	0	35
(U2) HDS-1	HC	3.4	20	120
	H_2S	414.8	300	12500
	SS	4.59	45	180
(U3) Desalter	HC	5.6	120	220
	H_2S	1.4	20	45
	SS	520.8	200	9500
(U4) VDU	HC	0.16	0	20
	H_2S	0.48	0	60
	SS	0.16	0	20
(U5) HDS-2	HC	0.8	50	150
	H_2S	60.8	400	8000
	SS	0.48	60	120

Table 6 – Regeneration processes data of example 3.

Regeneration Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
(R1) Steam stripping	HC	0	1	16,800
	H_2S	99.9		
	SS	0		
(R2) Biological treatment	HC	70	0.0067	12,600
	H_2S	90		
	SS	98		
(R3) API separator	HC	95	0	4,800
	H_2S	0		
	SS	50		

Table 7 – Distances for example 3.

$d_{i,j}$	WU 1	WU 2	WU 3	WU 4	WU 5	RG 1	RG 2	RG 3	Discharge
FW	30	25	70	50	90	200	500	600	2000
WU 1	0	30	80	150	400	90	150	200	1200
WU 2	30	0	60	100	165	100	150	150	1000
WU 3	80	60	0	50	75	120	90	350	800
WU 4	150	100	50	0	150	250	170	400	650
WU 5	400	165	75	150	0	300	120	200	300
RG 1	90	100	120	250	300	0	125	80	250
RG 2	150	150	90	170	120	125	0	35	100
RG 3	200	150	350	400	200	80	35	0	100

Using the distances of Table 7 and assuming a velocity of 1 m/s, the piping costs are given by:

$$FIJC_{i,j} = 124.6\ d_{i,j} \qquad \forall i \in \{W, U, R\},\ j \in \{W, U, R, S\} \qquad (31)$$

$$VIJC_{i,j} = 1.001\ d_{i,j} \qquad \forall i \in \{W, U, R\},\ j \in \{W, U, R, S\} \qquad (32)$$

The best known solution minimizing TAC is $616,824 (Alva-Argaez et al., 2007).

In our procedure, we identified the minimum consumption (58 t/h) by solving the problem without costs. We also solved for minimum total annual cost (without fixing the freshwater flowrate) to global optimality using Baron and specifying 1% tolerance. The run took 7 hrs, 5 minutes and rendered a network featuring a minimum total annual cost of $574,155, which happens to feature the previously identified minimum consumption of 58 t/h.

To analyze the degeneracy of this problem at the minimum consumption, we fix the consumption at its minimum (58 t/h) and look for feasibe solutions up to 100 solutions. We do this by using a minimum cost objective function, and a 99% gap for the global method (Faria and Bagajewicz, 2008, 2009c). This is different from what was done in Example 1 and 2. Here we are having the explicit purpose of saving computational time. Indeed, if one runs minimizing freshwater and forbids previously foud networks, the computational time is higher. In addition, we can identify lower costs networks earlier. Finally, one could try to run only once in order to identify the network with lowest cost. Such a run takes much longer than our alternative (7 hours vs. 1 hour and 40 minutes to find 100 feasible networks). We claim that the minimum cost network that one would identify if one runs to 0% gap features a set of connections that is eventually identified later, as long as all degenerate solutions are explored and one does not stop earlier. That said, we obtain the same connections, but not necessarily the same flows.

We reiterate that we are not guaranteeing that we obtain the global solution featuring minimum cost. We are simply obtaining alternative networks featuring the same freshwater consumption.

The results for the netwoks identified are presented in Figure 3. We present them in a increasing cost order of total annualized cost, which is not necessarily the order they are found. We also add operating cost, annualized capital cost and number of connections for completeness. The overall running time of our methodology is 201 CPUs to identify the minimum freshwater consumption, and 2525 CPUsto find the hundred degenerate solutions. We point out that the first 20 are fast and then, because of the network exclusion constraints, the running time per run increases for some of them.

Note that the lowest TAC found among these 100 solutions is $572,767, which is lower than the one found by BARON using 1% global optimality tolerance. It is worth pointing out that this best solution found among the 100 options was the 5th network, which took 76 CPUs. The flows through the water-using units and regeneration processes corresponding to these solutions are presented in Figures 4 and 5 respectively.

We note that this procedure does not guarantee global optimality of costs, even though we can see it identifies good solutions when we compare to the ONLY solution one can find using BARON.

Additionally, if one wants to look at different criteria (always operating at minimum consumption), one can chose the network with minimum TAC, or minimum operating cost, minimum capital cost or smaller complexity (here identified as the number of connections). Table 8 compares these options (the bold numbers are the ones corresponding to the minimum value of the optimization). Note that the network with minimum TAC has also the minimum operating cost. However, among the 100 found solutions there are other 14 networks that have the same operating costs. Figures 6 to 8 show the three networks presented in Table 8.

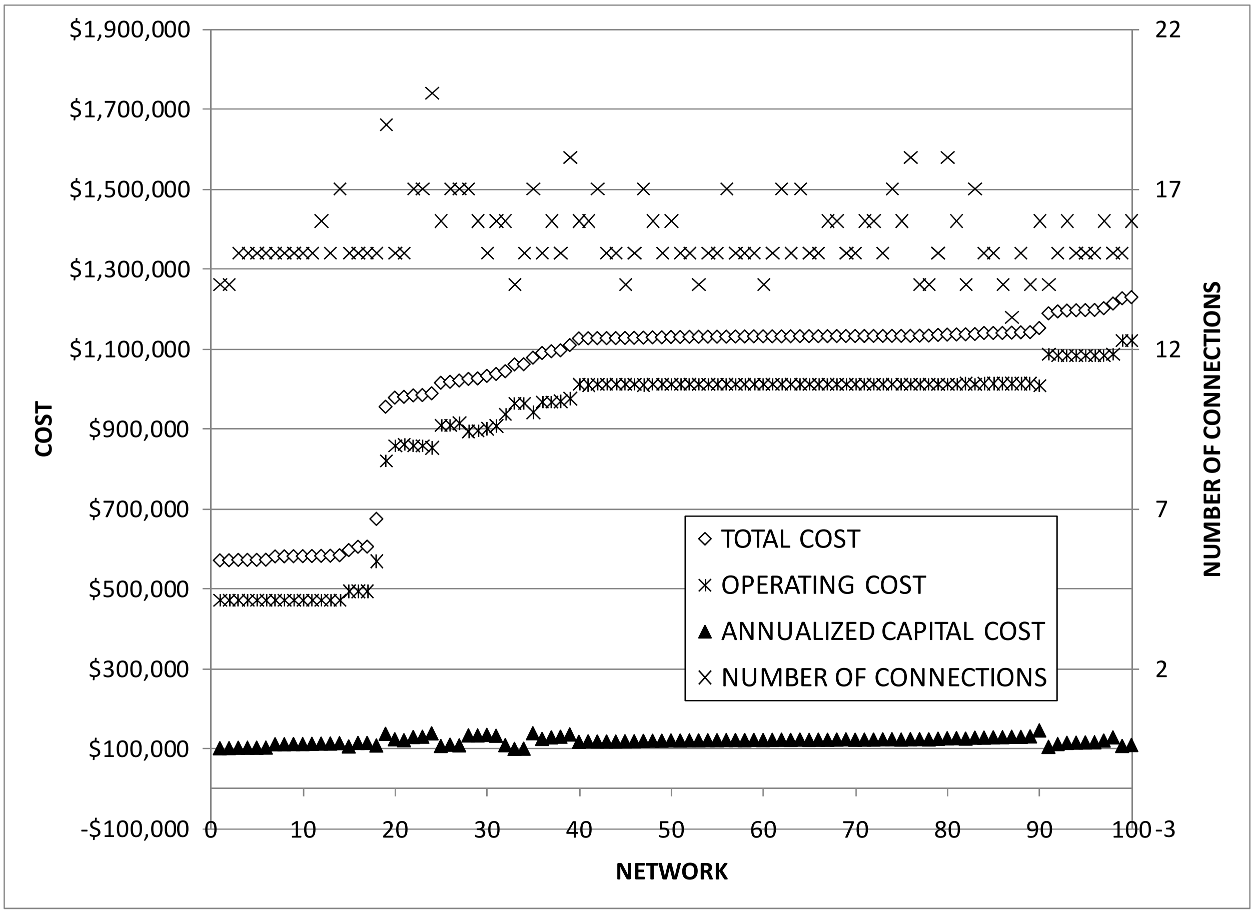

Figure 3 – Hundred minimum consumption (58 t/h) alternative network configurations of refinery example from Kuo and Smith (1998).

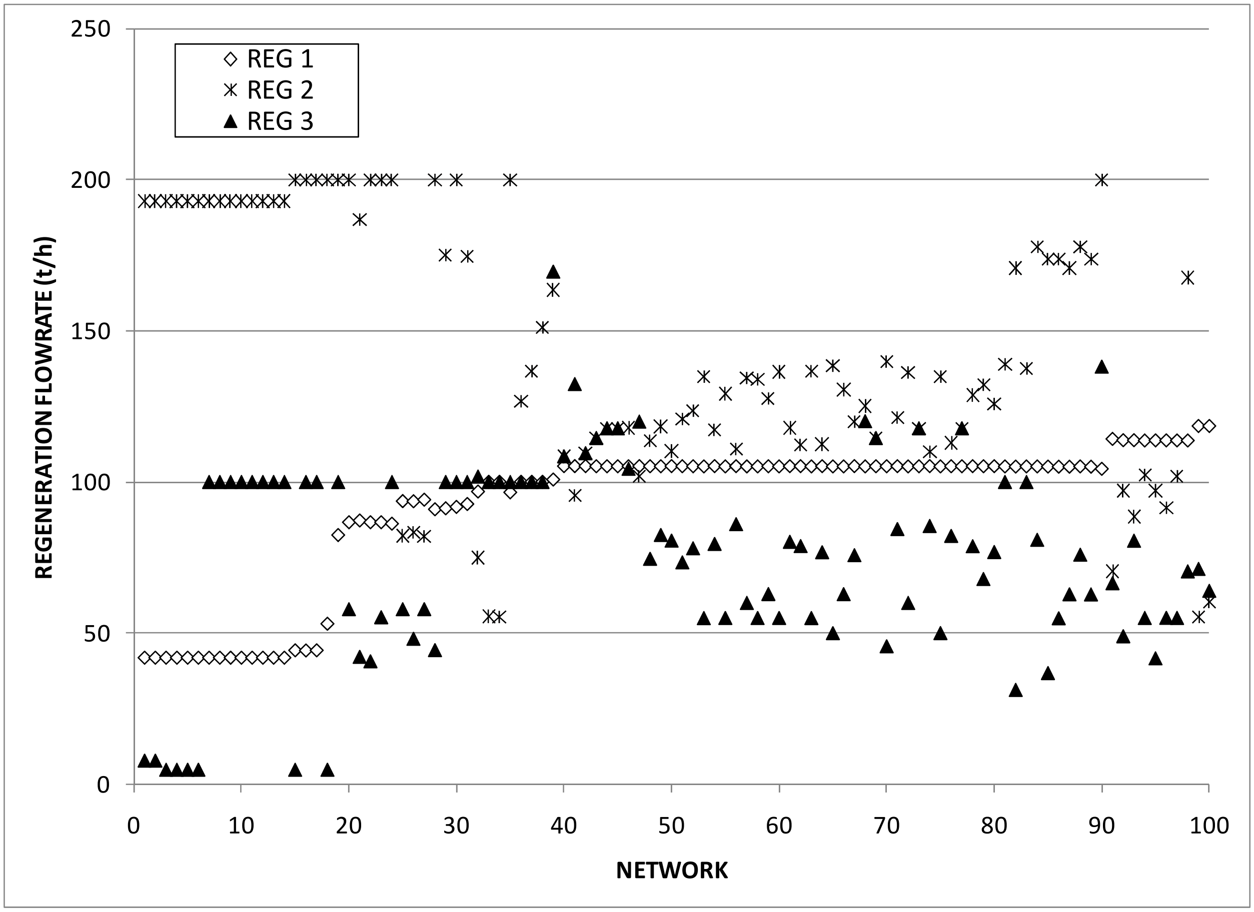

Figure 4 – Water-using unit flowrates - Hundred alternative network configurations at minimum consumption (58 t/h) for the refinery example from Kuo and Smith (1998).

Table 8 – Networks with best criteria.

Criteria	TAC ($/year)	Operating cost ($/year)	Capital cost ($)	Number of connections
TAC	**572,767**	472,073	1,006,944	14
Operating cost	572,767	**472,073**	1,006,944	14
Capital cost	1,062,126	962,963	**991,626**	14
Number of connections	1,141,479	1,012,617	1,288,623	**13**

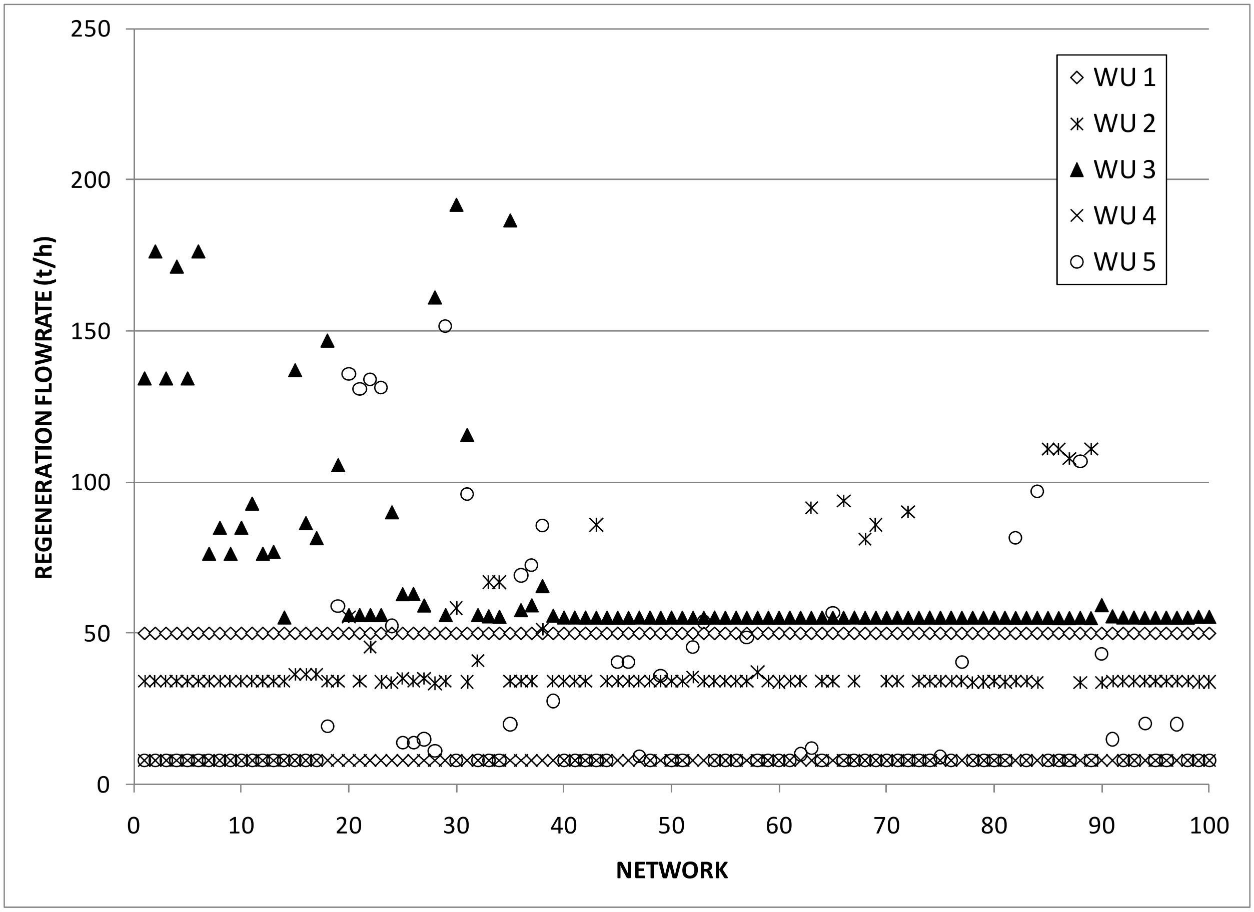

Figure 5 – Regeneration processes flowrates - Hundred alternative network configurations at minimum consumption (58 t/h) for the refinery example from Kuo and Smith (1998).

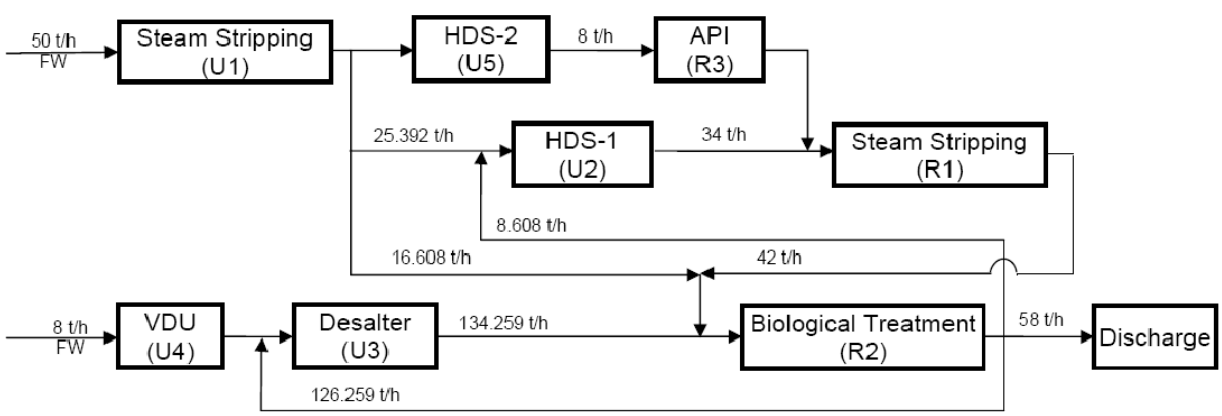

Figure 6 – Network with minimum TAC (and minimum operating cost).

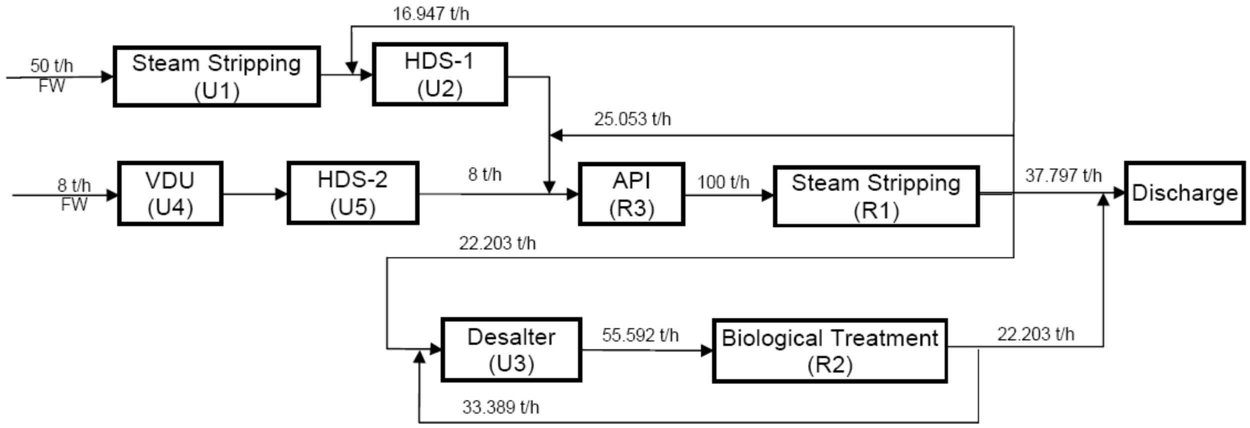

Figure 7 – Network with minimum capital cost.

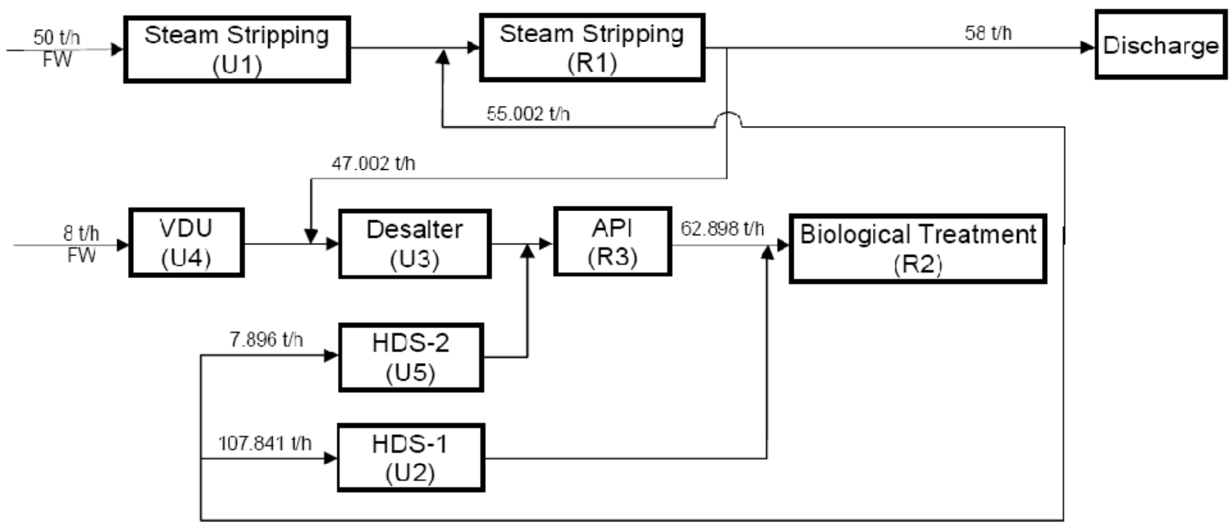

Figure 8 – Network with minimum number of connections.

The results presented so far do not considered structural constraints or practical considerations other than the ones given by the input data. Putra and Amminudin (2008) discuss some of these issues. Their concerns were regarding the following two practical issues:

1. The API separator should be placed in the upstream of biological treatment due to increase in performance (higher inlet concentration) and to guarantee that oil is not sent to the biological treatment;
2. Regeneration recycling shouldn't be allowed to avoid accumulation of certain contaminants. In other words, the regeneration process cannot send treated water back to the units that sent wastewater to it.

Applying these criteria, they eliminate 2 of the 4 alternative solutions found by their procedure. In our case, we apply our procedure including these practical issues. To consider the first one, we just added a maximum inlet concentration of 66 ppm of HC to the biological treatment. This value corresponds to the maximum value above which the biological treatment is not able to bring the concentration down to the HC environmental limit (20 ppm). For the second issue, we add a constraint to forbid all direct recycles, reuse recycling and regeneration recycling. This constraint is the following:

$$YIJ_{i,j} + YJI_{j,i} \leq 1 \quad \forall (i,j) \in \{(u,u^*),(u,r),(r,u),(r,r^*)\} \tag{33}$$

The minimum freshwater consumption obtained using this modified problem is also 58 t/h. As before, we fix the consumption and find the first 100 alternative solutions. The costs are presented in Figure 9 and the minimum TAC found among the 100 solution is $592,573. This optimum network is presented in Figure 10.

We notice that incorporating this constraint forced the network to avoid a direct recycle to the same regeneration process, but it found a recycle through another unit. In reality additional constraints could be added to avoid recycles to any units through as many processes as one wants. Instead of trying to forbid recycles, because of the fear that some contaminants/impurities/inerts may accumulate, a better modeling answer is to add strict inlet limitations to all units, including regeneration processes, even if the compounds that are picked up in the water units are not subject to removal.

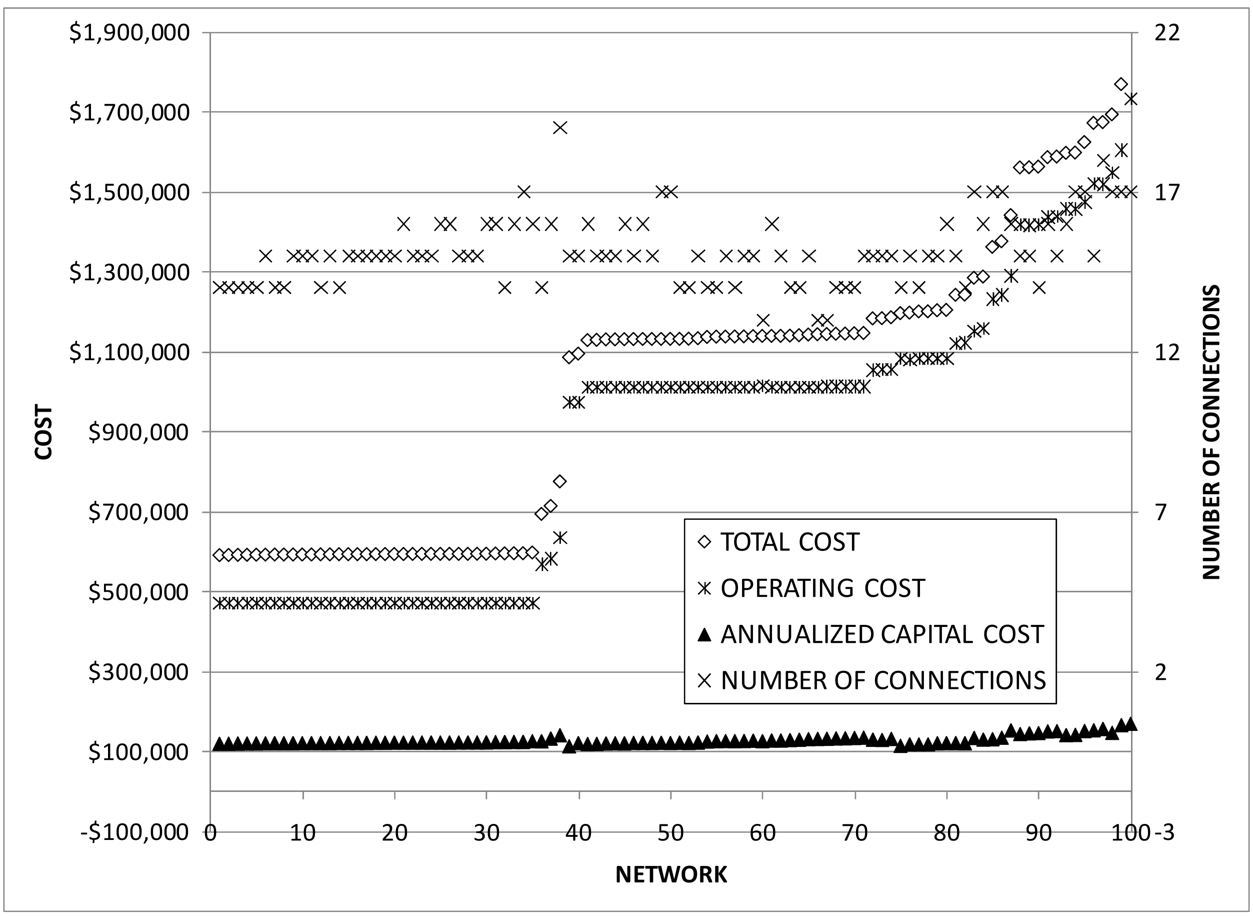

Figure 9 – Hundred minimum consumption (58 t/h) alternative network configurations of refinery example from Kuo and Smith (1998) including the practical issues pointed out by Putra and Amminudin (2008).

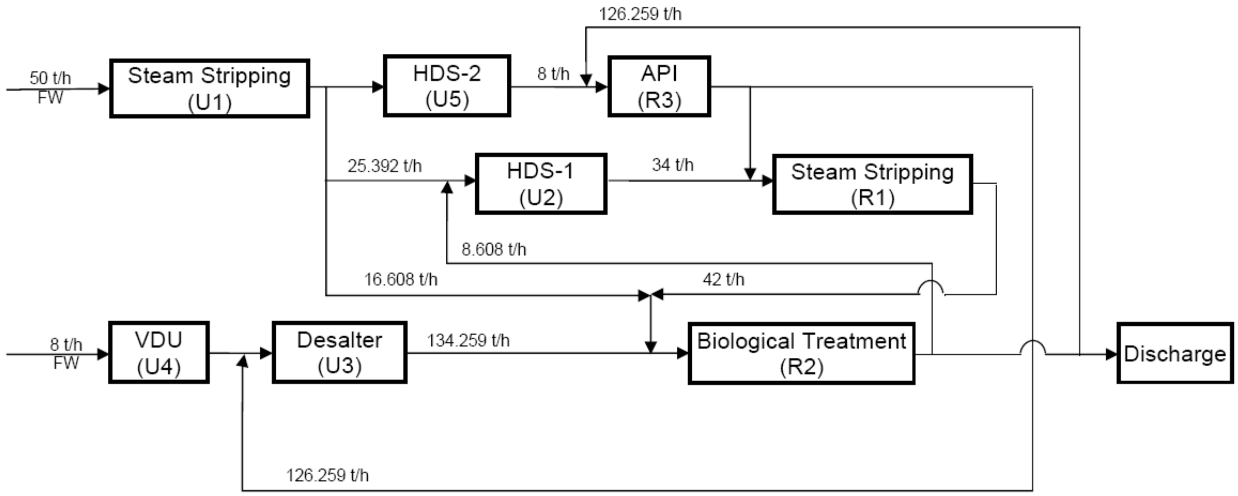

Figure 10 – Network with minimum TAC of Example 3 considering practical issues.

Example 4

In this example we want to find the first 50 solutions minimizing TAC without fixing the freshwater consumption at its minimum. For this example we use the *total water system* presented as example 4 by Karuppiah and Grossmann (2006). The data for this example is presented in Tables 9 and 10. Additionally, the discharge limit of all the contaminants is 10 ppm.

Table 9 – Water using units limiting data of example 4.

Process	Contaminant	Mass Load (kg/h)	$C^{in,max}$ (ppm)	F^{max} (t/h)
1	A	1	0	40
	B	1.5	0	
	C	1	0	
2	A	1	50	50
	B	1	50	
	C	1	50	
3	A	1	50	50
	B	1	50	
	C	1	50	
4	A	2	50	50
	B	2	50	
	C	2	50	
5	A	1	25	25
	B	1	25	
	C	0	25	

Table 10 – Regeneration processes data of example 4.

Process	Contaminant	Removal ratio (%)	OPN_r	CCR_r
1	A	95	1	16,800
	B	0		
	C	0		
2	A	0	0.04	9,500
	B	0		
	C	95		
3	A	0	0.0067	12,600
	B	95		
	C	0		

Karuppiah and Grossmann (2006a) solved the problem as an NLP problem. However, setting aside the fact that the NLP model for this problem renders a solution with unpractical small flowrates, to consistently forbid networks we need to impose a minimum allowed flowrate through the connection so the connection only exists if there is a flowrate different than zero. Thus, our problem becomes an MINLP.

The optimum solution (within 1% tolerance) of this MINLP problem was given by Faria and Bagajewicz (2009d) and it features a cost of $1,033,859.85 when the minimum flowrate through connections is set as 1 t/h in 73.79 CPU sec. In turn, Baron found a minimum TAC of $1,036,384 in 287 s using a 1% tolerance. The lowest TAC found using our proposed procedure is $1,033,832, which is also slightly lower than both 1% tolerance global solution found by Faria and Bagajewicz (2009d) and Baron. The reason for this is that the network with TAC of $1,033,832 is not the first network found with 1% tolerance. In reality it is found in after forbidden the 4 first networks found using 1% tolerance. At this exact cost there are other 7 alternatives and the 50th largest TAC is $1,035,288. Note that this high degeneracy in TAC can be attributed to the absence of connection costs. In this problem the only variables that account for the TAC are the freshwater consumption and flowrates through regeneration processes.

Figures 6 and 7 show the costs and regeneration flowrates for the 50 lowest TAC solution obtained for this problem. Because this procedure was done to find the global solutions every time a network is forbidden, it takes much longer than the previous one (20 hrs). However, when we run this problem with 99% gap with the purpose of only finding feasible networks, we are able to identify 500 networks in 12 hours and 30 min, the first 50 alternative networks found in 25 minutes.

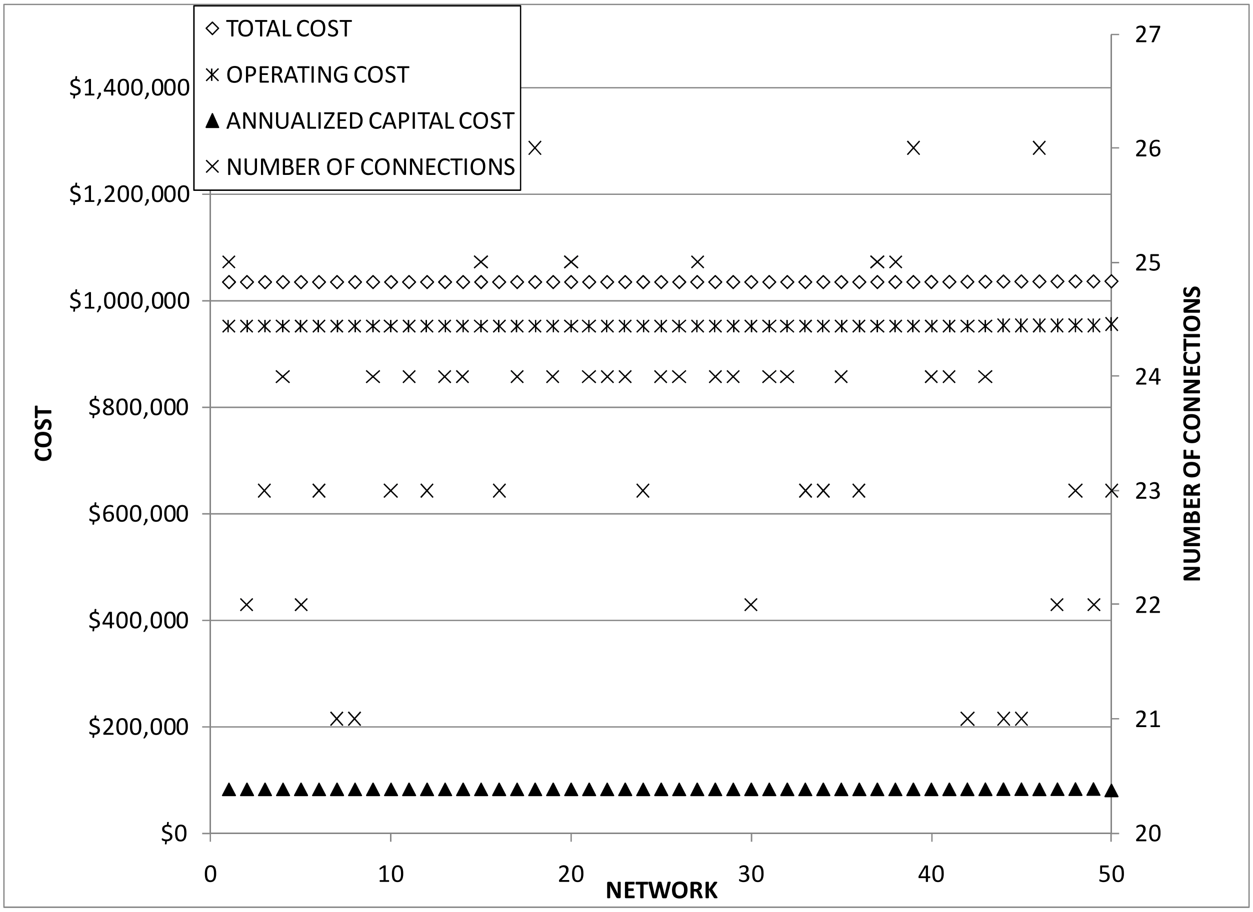

Figure 11 – Costs - Fifty alternative network configurations at minimum TAC for the modified example 4 from Karuppiah and Grossmann (2006).

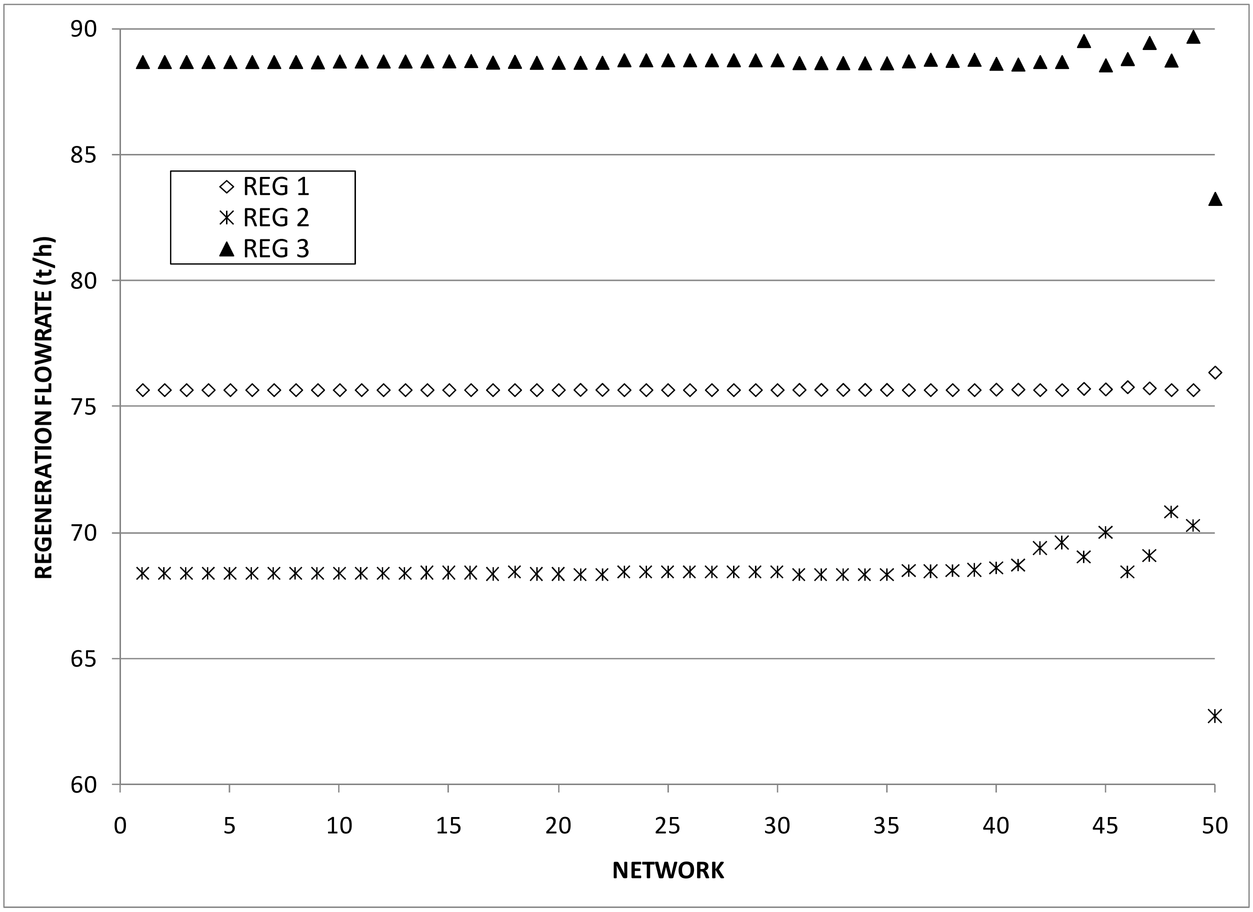

Figure 12 – Regeneration processes flowrates - Fifty alternative network configurations at minimum TAC for the modified example 4 from Karuppiah and Grossmann (2006).

Conclusions

In this article we pointed out the fact that minimum freshwater solutions of water management problems in process plants exhibits sometimes a large degeneracy. We argue that even for single contaminant cases, pinch-technology based methods as well as other algorithmic ones cannot provide the insights they claim they can provide and are unable to deal effectively with the identification of all the degenerate solutions, not even show whether the degeneracy is small or large. We show that degeneracy not only shows in minimum freshwater consumption problems, but also in cases where total cost is minimized. We argued that ONLY mathematical programming-based methods can perform this task and we presented a methodology to identify as many degenerate and suboptimal solutions as one desires.

Finally, we believe that the degeneracy should disappear with more detailed modeling. For example, once maximum inlet concentrations are imposed for regeneration processes, or their efficiencies are function of inlet conditions (concentration, flowrates, etc), some of the alternatives may not be feasible anymore. However, given the above results, we still expect suboptimal solutions close to the global optimum.

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