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Comparative Analysis of Different Assumptions for the Design of Single-Contaminant Water Networks

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One common assumption used in the design of water/wastewater systems for single components is to fix the process outlet concentrations of the pollutant to its maximum allowed value. This converts the problem from one with nonlinear constraints into one with linear constraints. For problems minimizing freshwater consumption in single-contaminant systems, this assumption has been proven to lead to global optimality (Savelski and Bagajewicz, 2000). In this article, we investigate the effect of using this assumption in cases where it may not lead to global optimal solutions, namely when the number of connections is minimized and when the cost is minimized. We therefore show that the use of nonlinear models helps in dealing with degenerate solutions featuring the same freshwater consumption.

Keywords Water minimization; Water/wastewater process systems

Introduction

The water/wastewater allocation problem has been widely formulated as a freshwater intake minimization problem. In addition, although there are several graphical/conceptual and algorithmic methods that can be used, the problem has been efficiently addressed using mathematical programming, which is what we focus on in this article. Minimization of freshwater consumption can be achieved using reuse/recycle structures with the eventual addition of intermediate regeneration processes (Wang and Smith, 1994; Kuo and Smith, 1997; Feng et al., 2007; Ng et al., 2007a,b; Alva-Argaez et al., 2007).

The biggest challenge for the mathematical procedures is the presence of nonlinearities. Aside from stochastic approaches (genetic algorithms; Xu et al., 2003; Prakotpol and Srinophakun, 2004), which do not guarantee global optimality, many mathematical programming approaches using linear programming (LP), nonlinear programming (NLP), mixed integer linear programming (MILP), and mixed integer nonlinear programming (MINLP) were developed for this problem (Takama et al., 1980; El-Halwagi and Manousiouthakis, 1990; Galan and Grossmann, 1998; Alva-Argaez et al., 1998; Bagajewicz et al., 2000; Bagajewicz and Savelski, 2001; Karuppiah and Grossman, 2006).

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For single-contaminant cases in which water-using units are handled as mass exchangers, many methodologies are based on the optimality conditions determined by Savelski and Bagajewicz (2000). One of these necessary optimality conditions states that the outlet concentrations in each process are at their maximum value. The other one is a condition of monotonicity in the outlet concentrations, which is useful when using algorithmic methods (Savelski and Bagajewicz, 2001). This last condition is not relevant for mathematical programming approaches, although it can be used as an aid to exclude connections that do not comply with monotonicity and thus accelerate computations. Both conditions are summarized in the appendix in more detail.

Using the maximum concentration condition allows transforming nonlinear models into linear ones. However, we will see that the optimality conditions presented by Savelski and Bagajewicz (2000) are valid only when the objective function is freshwater consumption minimization and no structural constraints, like forbidden connections and/or combination of connections, exist. This was also pointed out by Doyle and Smith (1997), who focused on the multiple-contaminant case.

In this article we study the effects of using these particular conditions on problems involving costs and/or structural constraints. The original MINLP and the particular MILP models are presented and compared. The results prove that the necessary optimality conditions (every process at its maximum outlet pollutant concentration) cannot be used to optimize costs or freshwater when structural constraints exist. Additionally, we show that connections between units based on the monotonicity conditions should not be pre-excluded in these cases.

We first review the problem statement, then present the linear and nonlinear models, and, finally, show examples.

Problem Statement

Given a set of water-using units, a freshwater source, a wastewater discharge sink, and an available regeneration process (with a fixed outlet concentration), the optimum solution of different objectives is sought. Additionally, self-recycle in water-using units is excluded, which is also an assumption used by several previous studies. Even if added, it does not show up in optimal structures. The superstructure used to build these models is presented in Figure 1.

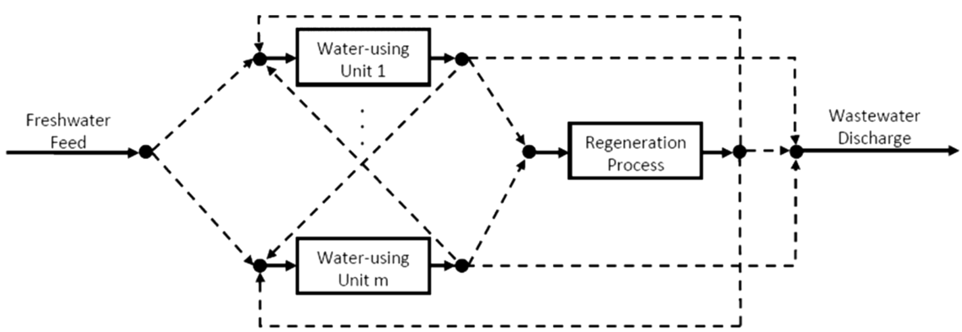

Figure 1. Superstructure used in the models.

Nonlinear Model

The corresponding nonlinear model to solve the water/wastewater allocation problem (WAP) previously defined is given by the following set of equations:

Balance of water on the units:

$$FW_{m^*} + FNU_{m^*} + \sum_{m \neq m^*} FUU_{m,m^*} = FUN_{m^*} + FS_{m^*} + \sum_{m \neq m^*} FUU_{m^*,m} \quad \forall m^* \tag{1}$$

where FW_{m^*} is the freshwater consumption of unit m^*, FNU_{m^*} is the flow rate from the regeneration process to unit m^*, FUU_{m,m^*} is the flow rate from unit m to unit m^*, FUN_{m^*} is the flow rate from unit m^* to the regeneration process, and FS_{m^*} is the flow rate from unit m^* to the discharge.

Balance of water on the regeneration process (without loss of generality, we assume only one is needed):

$$\sum_{m} FUN_m = FNS + \sum_{m} FNU_m \tag{2}$$

where FNS is the water discharge to end-of-pipe treatment from the regeneration process (we assume that the regeneration process has outlet concentrations larger than the disposal limits). Thus, the mixture of all the streams sent to wastewater disposal has to be further treated by the end-of-pipe treatment.

Balance of the contaminant on the units:

$$\begin{aligned} & FW_{m^*} C^{ws} + FNU_{m^*} C^n + \sum_{m \neq m^*} FUU_{m,m^*} C_m^{out} + \Delta m_{m^*} \\ & \quad = \left(FUN_{m^*} + FS_{m^*} + \sum_{m \neq m^*} FUU_{m^*,m} \right) C_{m^*}^{out} \quad \forall m^* \end{aligned} \tag{3}$$

where C^{ws} is the contaminant concentration of freshwater ws, C^n is the outlet contaminant concentration of the regeneration process (which is a predefined parameter), $C_{m^*}^{out}$ is the outlet concentration of unit m^*, and Δm_{m^*} is the contaminant mass load of unit m^*.

Limit of inlet concentration on the units:

$$\begin{aligned} & FW_{m^*} C^{ws} + FNU_{m^*} C^n + \sum_{m \neq m^*} FUU_{m,m^*} C_m^{out} \\ & \quad \leq \left(FW_{m^*} + FNU_{m^*} + \sum_{m \neq m^*} FUU_{m,m^*} \right) C_{m^*}^{\max,in} \quad \forall m^* \end{aligned} \tag{4}$$

where $C_{m^*}^{\max,in}$ is the inlet maximum contaminant concentration for unit m^*.

Limit of outlet concentration on the units:

$$C_{m^*}^{out} \leq C_{m^*}^{\max,out} \quad \forall m^* \tag{5}$$

Binary variables are added to identify the existence of connections and to be used in cost objective functions:

$$FW_m \leq U\ YW_m \qquad \forall m \tag{6}$$

$$FUN_m \leq UYUN_m \qquad \forall m \tag{7}$$

$$FNU_m \leq UYNU_m \qquad \forall m \tag{8}$$

$$FUU_{m^*,m} \leq UYUU_{m^*,m} \qquad \forall m^*, m \tag{9}$$

$$FNS \leq UYNS \tag{10}$$

$$FS_m \leq UYS_m \qquad \forall m \tag{11}$$

In these equations, YW_m, $YUU_{m^*,m}$, YUN_m, YNS, YNU_m, and YS_m are binary variables used to determine the existence of flow rates going from the freshwater source to the units, from one unit to another unit, from a unit to the regeneration process, from the regeneration process to a unit, from the regeneration process to the discharge and from a unit to the discharge, respectively. U is the maximum value (upper bound) of flow rate allowed in the connections.

Objective Functions

Because it is known that the water allocation problem generally presents degenerate solutions (different sets of decision variables giving the same objective values) when freshwater is minimized (Bagajewicz and Savelski, 2001), it is possible to further use some economic objectives to sort the best solution among these degenerate ones. Some of the possible objective functions are presented below.

Minimum number of connections:

$$Min\left(\sum_m \left(YWU_m + YS_m + YUN_m + YNU_m + \sum_{m^* \neq m} YUU_{m,m^*}\right) + YNS\right) \tag{12}$$

Minimum capital cost:

$$Min\Bigg(RegCost_n + \sum_m \left(\begin{array}{c} YWU_m ICWU_m + YS_m ICS_m + \sum_{m^* \neq m} (YUU_{m,m^*} ICUU_{m,m^*}) \\ + YUN_m ICUN_m + YNU_m ICNU_m \end{array}\right) + YNSICNS\Bigg) \tag{13}$$

where $ICWU_m$, ICS_m, $ICUU_{m,\ m^*}$, $ICUN_m$, $ICNU_m$, and $ICNS$ are the investment cost with connections. The cost of the regeneration unit *RegCost* can be either a function of the treated flow rate (which can be linear or nonlinear) or a constant value. The equations used to calculate the capital investment of the regeneration process are presented in each example.

In addition, we will also explore the use of the maximum outlet concentrations assumption when total annualized cost is minimized:

Minimum annualized cost:

$$Min\left(\alpha\sum_m FWU_m + \beta\sum_m FUN_m + af\left(\begin{array}{c} RegCost_n + \sum_m \left(\begin{array}{c} YWU_m ICWU_m + YS_m ICS_m + \\ \sum_{m^*\neq m}(YUU_{m,m^*} ICUU_{m,m^*}) \\ + YUN_m ICUN_m + YNU_m ICNU_m \end{array}\right) \\ + YNS\ ICNS \end{array}\right)\right) \tag{14}$$

where α is the freshwater cost, β is the operating cost of the regeneration process, and *af* is the annual discount factor.

Linear Models

Savelski and Bagajewicz (2000) proved that when minimum freshwater is sought, then, there is an optimum solution in which the outlet concentration of each water-using unit reaches its maximum value. As a result, Equations (3) and (4) can be rewritten as follows (Bagajewicz and Savelski, 2001):

$$\begin{aligned} & FW_{m^*} C^{ws} + FNU_{m^*} C^{n} + \sum_{m\neq m^*} FUU_{m,m^*} C_m^{out,\max} + \Delta m_{m^*} \\ & \quad = \left(FUN_{m^*} + FS_{m^*} + \sum_{m\neq m^*} FUU_{m^*,m}\right) C_{m^*}^{out,\max} \quad \forall m^* \end{aligned} \tag{15}$$

$$\begin{aligned} & FW_{m^*} C^{ws} + FNU_{m^*} C^{n} + \sum_{m\neq m^*} FUU_{m,m^*} C_m^{out,\max} \\ & \quad \leq \left(FW_{m^*} + FNU_{n,m^*} + \sum_{m\neq m^*} FUU_{m,m^*}\right) C_{m^*}^{\max,in} \quad \forall m^* \end{aligned} \tag{16}$$

We now discuss the use of this assumption solving examples using different objective functions and/or structural constraints. The examples were implemented in GAMS (Brooke et al., 1998). The linear model is solved using GAMS/CPLEX and the nonlinear model using GAMS/DICOPT.

Example 1

We start with an example involving a small-scale problem using the one posed by Wang and Smith (1994) with four water-using units. The configuration of the network without reuse (which we call a conventional network) and its respective limiting data are presented in Figure 2.

The minimization of freshwater consumption using both models, linear and nonlinear, renders the same minimum of freshwater usage (90 ton/h). However, there are

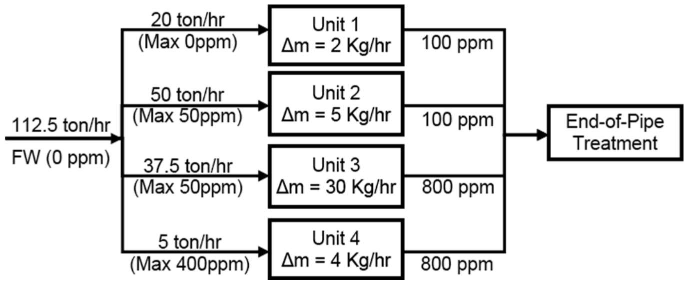

Figure 2. Network configuration without reuse and its limiting data.

degenerate solutions in which the maximum outlet concentration is reached and others in which the outlet concentration is lower than the maximum.

Minimizing the Number of Connections among Degenerate Solutions

Both models were used to analyze the validity of the maximum outlet concentration condition when the minimum number of connections is used as the objective. In both cases, the freshwater consumption is set to be 90 ton/h, which is the minimum that can be calculated using the water pinch and several other different methodologies.

The number of connections of the solution obtained by the linear model is eight (Figure 3) while the nonlinear model renders six connections (Figure 4). Note that the nonlinear model also has a simpler structure.

Because the outlet concentration is fixed in the linear model, every unit that requires an inlet concentration lower than the minimum outlet concentration among the units has to be supplied by freshwater. In this example one can see that this happens for Units 2 and 3. Their maximum allowed inlet concentration is 50 ppm, and the minimum outlet concentration among all the units is 100 ppm. Thus, there is no other option for these units than to be totally or partially supplied by freshwater. In other words, these two connections must exist when the maximum outlet concentration condition is used. Conversely, the nonlinear model can lower the outlet concentration of one (or more) unit(s) and remove the need for dilution. Indeed, Figure 4 shows that Unit 1 does not reach its maximum concentration and thus feeds Unit 3 without dilution. This issue can become significant when the physical distance between the freshwater source and the units is a concern (layout and/or cost issues).

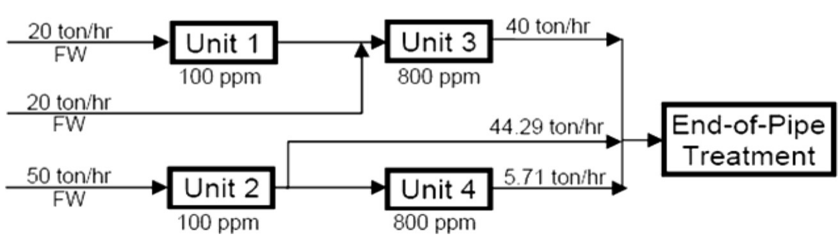

Figure 3. Solution with minimum number of connections: linear model.

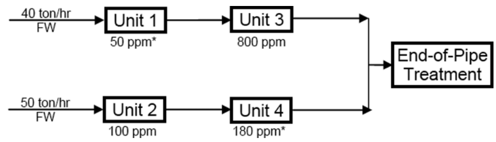

Figure 4. Solution with minimum number of connections: nonlinear model. *: concentrations lower than the maximum.

Minimizing the Cost of Connections among Degenerate Solutions

The cost of connections is now minimized, maintaining the freshwater consumption at the minimum of 90 ton/h. We set all costs to zero except the costs of connections between freshwater source and Units 2 and 3 ($10,000 each). As expected, the linear model reached a minimum cost of $20,000. This is the same solution found when the number of connection was minimized (Figure 3). The nonlinear model, in turn, shows a network with no costs, that is, both connections that had a cost were avoided. Figure 5 shows this solution. Note that Unit 1 reaches an outlet concentration (lower than its maximum and the one found in Figure 4) that allows the absence of connections between freshwater and Units 2 and 3.

Feasible Flow Rate Ranges Feeding Water-Using Units

We show now that the nonlinear model has a greater flexibility to vary flow rates in the water-using units, which can have an impact on costs. To do that, the feasible regions are investigated.

In the case of Unit 1 (Figure 6), only one inlet concentration is possible (0 ppm). Then, a graph directly relating outlet concentration and flow rate is presented. The contaminant balance for the units (Equation (3)) shows that the outlet concentration decreases when the flow rate through the unit increases. When the linear model is used, there is only one feasible flow rate for Unit 1 (20 ton/h). Otherwise, the model with free outlet concentration can have a variety of flow rates, which will reduce the outlet concentration.

Figure 7 shows the outlet concentration as a function of the inlet concentration at different flow rates of Unit 2. The inlet concentration of Unit 2 was varied from zero to its maximum allowed inlet concentration. Note that the feasible solutions for the linear model are limited by a maximum flow rate (100 ton/h). This does not happen when the outlet concentration is free (nonlinear model). Moreover, in the linear

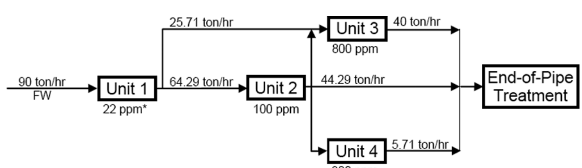

Figure 5. Solution with minimum cost of connections: nonlinear model. *: concentrations lower than the maximum.

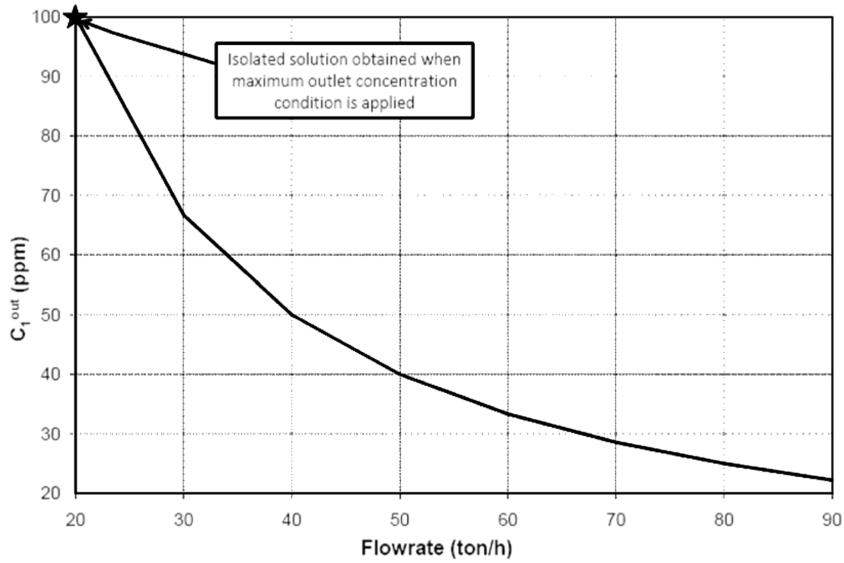

Figure 6. Feasible flow rates through Unit 1.

case each feasible flow rate has a unique inlet concentration, which does not happen in the nonlinear case. Indeed, the flexibility of the model when maximum outlet concentration condition is not applied can be observed by the larger feasible region (shadow region). Similar behavior is found for Units 3 and 4.

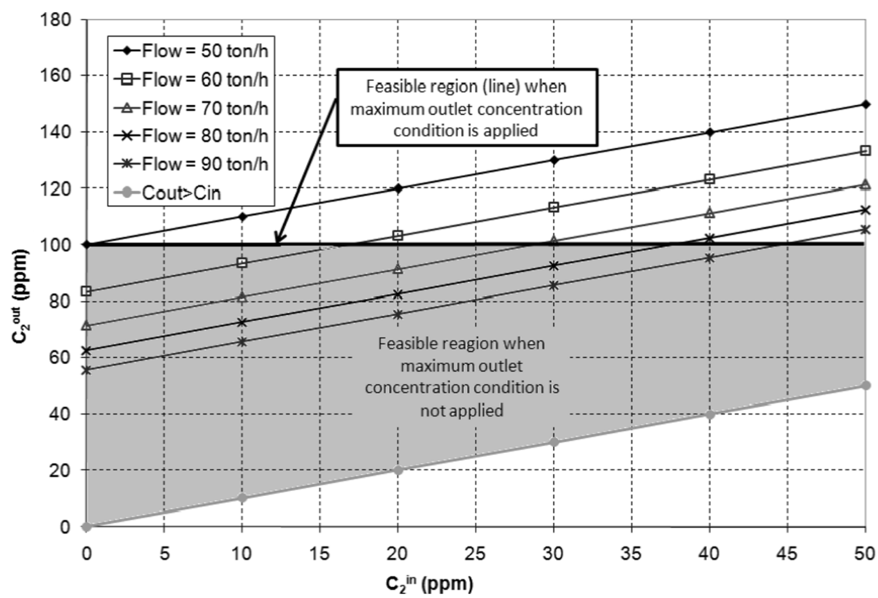

Figure 7. Feasible flow rates through Unit 2.

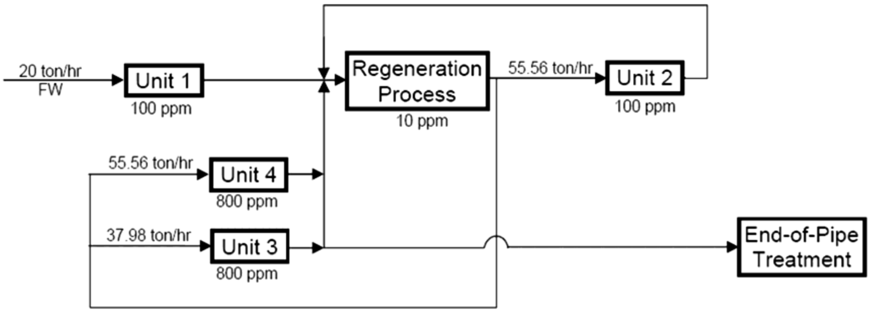

Figure 8. Optimal solution for example 2: both models.

Example 2

In example 2, we allow the addition of a regeneration process in the problem studied in example 1. The regeneration process added has a fixed outlet concentration of 10 ppm. Both models reach the same minimum flow rate (20 ton/h) and the same network structure when minimum freshwater is used as an objective. The solution is shown in Figure 8. The required connections between freshwater source and Units 2 and 3 are no longer needed. This is because now there is an option of using water coming from the regeneration process, which has an outlet concentration (10 ppm) lower than the maximum allowed inlet concentration in Units 2 and 3 (50 ppm).

We now investigate how to obtain economically advantageous degenerate solutions. Thus, the freshwater flow rate is fixed at 20 ton/h.

Minimizing the Number of Connections among Degenerate Solutions

The linear model shows a minimum of eight connections (Figure 9), while the non-linear model requires only seven connections (Figure 10). Interestingly, both solutions present isolated zero discharge cycles, which is not always convenient due to control/flexibility reasons (the load in the units might vary and there is no freshwater to add to respond to the changes) and the need to prevent the accumulation of compounds that are not removed in the regeneration processes. In fact, this is not a situation that is often seen in industry, and, while feasible, there are many

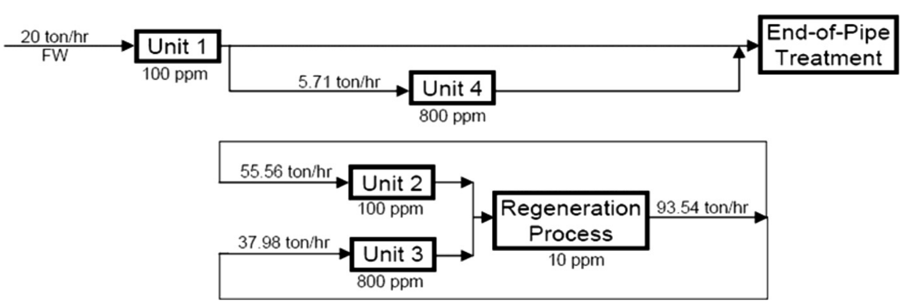

Figure 9. Minimum number of connections for example 2: linear model.

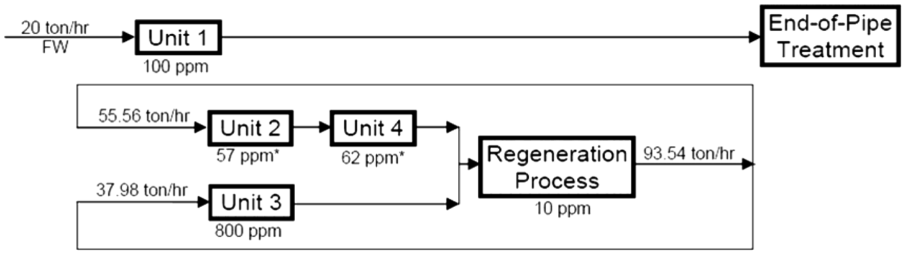

Figure 10. Minimum number of connections for example 2: nonlinear model. *: concentrations lower than the maximum.

impediments to implement them. It is not unthinkable that in the future, the pressure to reduce water consumption will increase and these impediments will be sorted out.

Elimination of Closed Cycles

To avoid closed cycles, forbidden connections constraints are added to the models. The following constraint forbids a closed cycle between one unit and the regeneration process:

$$YUN_m + YNU_m \leq 1 \quad \forall m \tag{17}$$

Note that the idea here is not to forbid the recycles involving a unit and a regeneration process, but to avoid the isolated cycles. The suggested constraint cannot guarantee the nonexistence of these cycles since one involving two units and the regeneration process still can exist. However, it reduces the possibility of the existence of these cycles. If this constraint does not work for this example, a new one can be added. In the above solution, this constraint would forbid the loop between the regeneration process and Unit 3. Now, only isolated loops involving the regeneration and two units can show up. In such a case constraints similar to (17) can be written. We omit going into more detail on this matter as this is not the central issue of this study.

The minimum freshwater consumption is solved first. As a result, the linear model does not give the same minimum freshwater consumption as the nonlinear model. The first one gives 40 ton/h of freshwater usage, while the nonlinear model renders 20 ton/h of freshwater usage. These networks are shown in Figures 11 and 12.

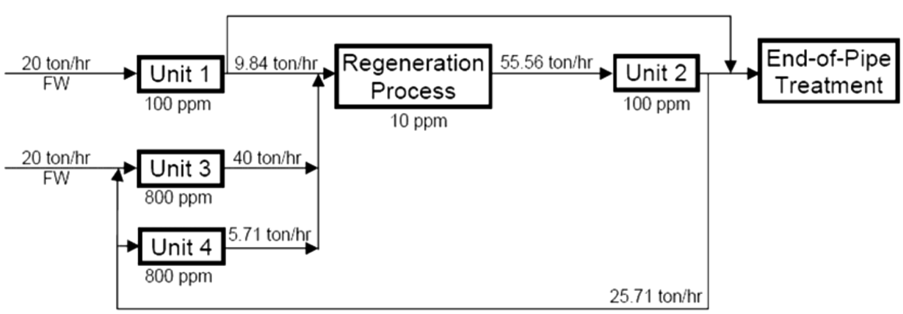

Figure 11. Minimum freshwater usage for example 2, forbidding cycles: linear model.

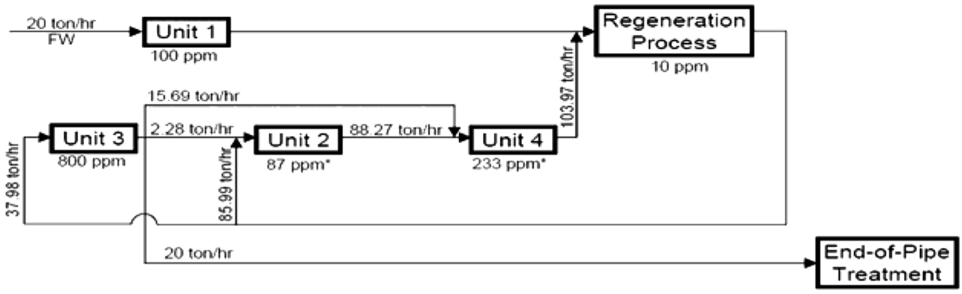

Figure 12. Minimum freshwater use for example 2, forbidding cycles: nonlinear model. *: concentrations lower than the maximum.

These results show that the maximum outlet concentration assumption does not fail only when other objective functions (cost or number of connections) are used, but also when minimum freshwater usage is aimed at under structural constraints.

Minimizing the Number of Connections among Degenerate Solutions with Forbidden Cyclic Connections

The linear model solution finds the network presented in Figure 11, which was obtained by eliminating cycles. This network has ten connections and does not have disconnected zero discharge cycles. Figure 13 shows the solution of minimizing the number of connections using the nonlinear model with forbidden cycles between the regeneration process and units. The found solution has eight connections and no isolated cycles.

Note that the nonlinear model renders a smaller number of connections (eight compared to ten in the network found using the linear model) but a larger regeneration capacity (90.56 ton/h compared to 55.56 ton/h in the network found using the linear model). We now look at cost.

Minimizing Capital Cost among Degenerate Solutions with Forbidden Connections

In this example the cost of the regeneration process is given by:

$$RegCost = 16,800\, RegCap^{0.7} \tag{18}$$

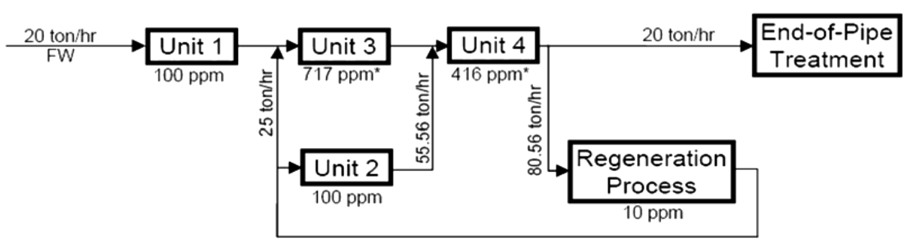

Figure 13. Minimum number of connections, forbidding disconnected closed cycles: nonlinear model. *: concentrations lower than the maximum.

Table I. Capital costs of the connections

	Unit 1	Unit 2	Unit 3	Unit 4	Reg.	End-of-pipe treatment
FW	\$30,000	\$45,000	\$25,000	\$60,000		
Unit 1	—	\$150,000	\$110,000	\$45,000	\$145,000	\$15,000
Unit 2	\$50,000	—	\$134,000	\$40,000	\$37,000	\$30,000
Unit 3	\$180,000	\$35,000	—	\$42,000	\$91,000	\$20,000
Unit 4	\$163,000	\$130,000	\$90,000	—	\$132,000	\$34,000
Reg.	\$33,000	\$130,000	\$50,000	\$98,000	—	\$45,000

where *RegCap* is the capacity of the regeneration process, which is in turn given by:

$$RegCap = \sum_{m} FUN_m \tag{19}$$

The capital costs of connections between the regeneration process and units, among units, and between units and the end-of-pipe treatment are presented in Table I. Both models (with forbidden connections) were applied over their range of reuse. Note that because the capital cost of the regeneration process is nonlinear, both models need to be solved using a nonlinear solver. The difference here is that in one case all outlet concentrations are fixed to be the maximum value. The solutions are presented in Figure 14.

The solutions show that the use of maximum outlet concentration condition generates networks with higher capital costs for every freshwater flow rate inside

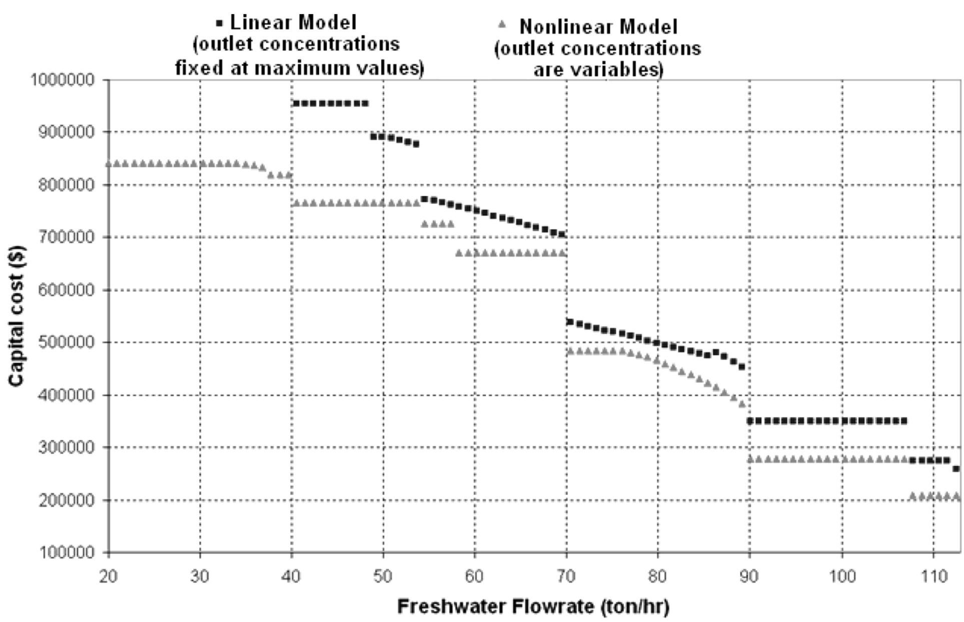

Figure 14. Comparison of capital cost of networks of example 2 that operate at different freshwater consumption values, forbidding disconnected closed cycles.

its feasible range. Also, the linear model with forbidden connections cannot reach the same minimum freshwater consumption reached by the nonlinear model.

An interesting observation here is that the nonlinear model is able to generate a network with a capital cost lower than the conventional one (network without reuse as in Figure 2), which is the minimum capital cost solution for the linear model. In both cases, the minimum capital cost corresponds to the network with the maximum flow rate (112.5 ton/h). For this maximum flow rate, the capital cost of the network generated by the linear model is $259,000 and the one obtained by the nonlinear model is $209,000. Additionally, it is worth noting the network generated by the nonlinear model can operate with lower freshwater consumption. That is, the last six freshwater consumption points generated by the nonlinear model (Figure 14) represent the same network. The optimum network at the last freshwater consumption point (112.5 ton/h) for the linear model corresponds to the one presented in Figure 2 (no reuse). This network cannot operate at a freshwater consumption lower than 112.5 ton/h. However, using a variable outlet concentration allows finding an optimum network at the same freshwater consumption that is not only cheaper but also can operate at lower flow rates. This is possible only because the outlet concentrations are not set to their maximum value. This network is presented in Figure 15.

Example 3

Example 3 presents the analysis of a larger scale network presented by Bagajewicz and Savelski (2001). This network has ten water-using units, and the corresponding limiting data are presented in Table II. The freshwater usage of the analyzed network was minimized, and both models achieved 165.94 ton/h as expected (Figure 16). This represents the same solution presented by Savelski and Bagajewicz (2000). The degenerate solutions are analyzed next.

Since this example was previously solved by Bagajewicz and Savelski (2001) applying the maximum outlet concentration conditions, both results are compared and discussed. It is worth noting that if the maximum outlet concentration condition is applied, one could already detect that processes 1 to 5 and 8 to 9 would need freshwater since their maximum inlet concentration is lower than the minimum outlet concentration of all processes. Using the nonlinear model (outlet concentration as a variable), this conclusion cannot be made, and, consequently, the feasible region is not reduced (as shown in the previous example, Figures 6 and 7).

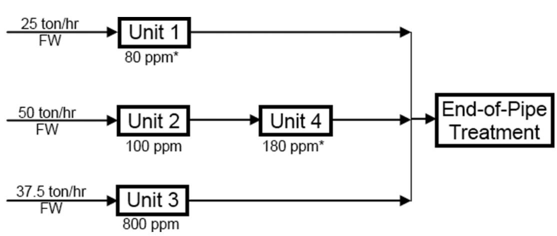

Figure 15. Network with the lowest capital cost generated by the nonlinear model. *: concentrations lower than the maximum.

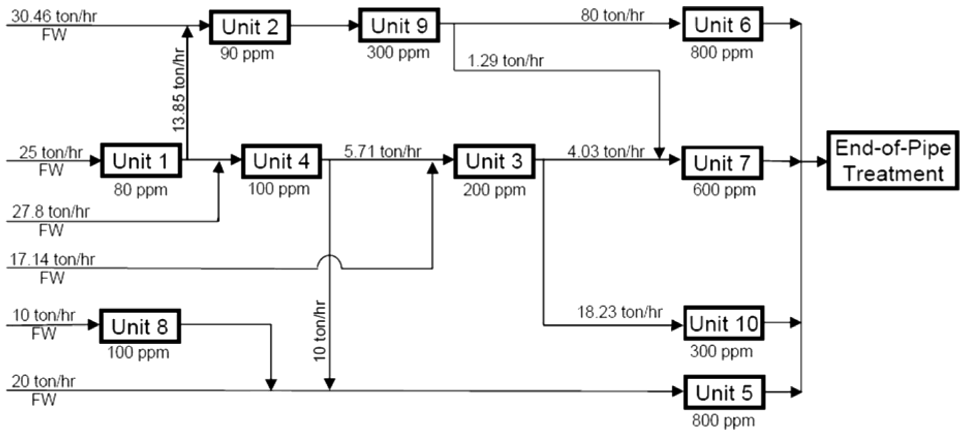

Figure 16. Minimum freshwater consumption: solution from both linear and nonlinear models.

The freshwater usage of the analyzed network was minimized, and both models achieved 165.94 ton/h as expected (Figure 16). This represents the same solution presented by Savelski and Bagajewicz (2000). The degenerate solutions are analyzed next.

Minimizing the Number of Connections among Degenerate Solutions

We first analyze the minimum number of connections of the network that features the minimum freshwater consumption. In other words, we look for degenerate solutions. Both models were run, and the networks presented in Figures 17 and 18 were found using the linear and nonlinear models respectively. The minimum number of connections found by the linear model is 22. Conversely, the nonlinear model is able to reduce this number to 21. Note that in the nonlinear model (Figure 18) Units 1, 2, 6, 7, and 10 do not reach their maximum outlet concentration.

Table II. Limiting data for example 3

Process number	Mass load of contaminant (kg/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum freshwater flow rate (ton/h)
1	2.00	25	80	25.00
2	2.88	25	90	32.00
3	4.00	25	200	20.00
4	3.00	50	100	30.00
5	30.00	50	800	37.50
6	5.00	400	800	6.25
7	2.00	400	600	3.33
8	1.00	0	100	10.00
9	20.00	50	300	66.67
10	6.50	150	300	21.67

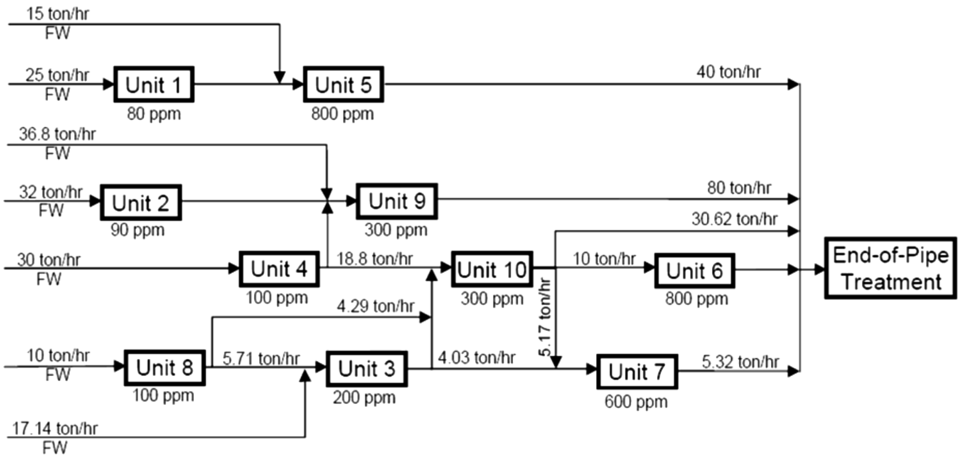

Figure 17. Solution with minimum number of connections: linear model.

Minimizing Cost of Connections Among Degenerate Solutions

The minimum cost of connections was also analyzed. The cost data proposed by Bagajewicz and Savelski (2001) are presented in Table III. They pre-excluded some of the connections (the ones without costs associated) using the monotonicity condition proved by Savelski and Bagajewicz (2000). However, this condition may not be valid for the cases when one lets the outlet concentrations vary. In fact, the solution for the minimum number of connections previously shown (Figure 18) has connections that were excluded by the monotonicity conditions. To evaluate the validity of this condition on the minimization of costs and forbidden connections, the problem is solved first considering this pre-exclusion and then not considering it. The authors also excluded the costs between freshwater source and units, claiming that connection from the freshwater source cannot be different from

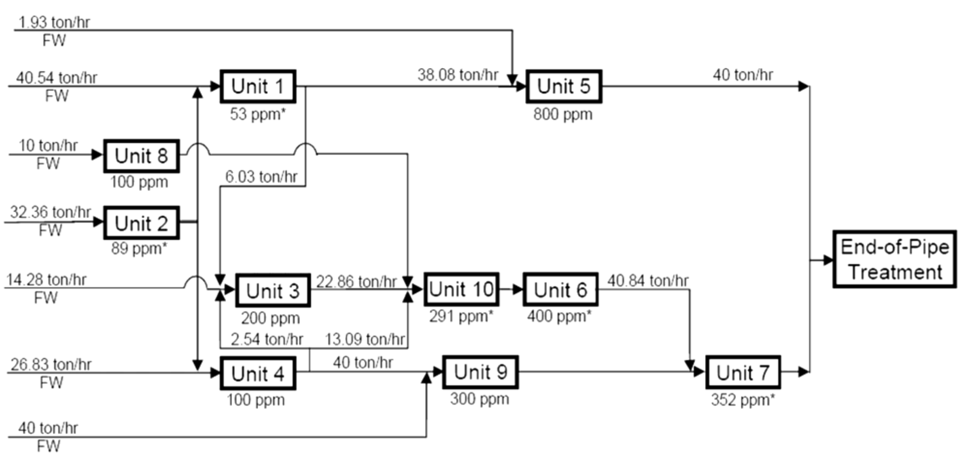

Figure 18. Solution with minimum number of connections: nonlinear model. *: concentrations lower than the maximum.

Table III. Cost of connections for example 3 ($ per year)

Process	1	2	3	4	5	6	7	8	9	10	WWT
1	—	2.42	2.98	3.17	3.54	3.54	3.54	—	2.98	2.79	5.42
2	—	—	2.79	2.98	3.54	3.54	3.54	—	3.17	2.98	5.42
3	—	—	—	—	2.98	3.17	3.54	—	3.54	3.54	4.67
4	—	—	2.42	—	2.79	2.98	3.54	—	3.54	3.54	4.67
5	—	—	—	—	—	—	—	—	—	—	3.92
6	—	—	—	—	—	—	—	—	—	—	3.92
7	—	—	—	—	2.98	2.79	—	—	—	—	3.92
8	—	—	3.54	—	3.17	2.98	2.42	—	2.79	2.98	3.92
9	—	—	—	—	3.54	3.54	2.98	—	—	—	4.67
10	—	—	—	—	3.54	3.54	3.17	—	—	—	4.67

the ones gotten before (minimization of freshwater). However, as discussed in example 1, these connections are always required only when the linear model is used. The nonlinear model may not render some of these connections.

First we present the solutions obtained when the exclusion of some connections (by the monotonicity condition) is applied. The minimization of capital cost at the minimum flow rate (165.94 ton/h) using the linear model gives a cost with connections of $53.16, where 22 connections are needed. This is the same solution found by Bagajewicz and Savelski (2001). The corresponding network is presented in Figure 19. For the nonlinear model, the minimum cost is $39.72, which is 25% lower. Note that the outlet concentrations of Units 1, 2, 6, 7, and 10 did not reach their maximum outlet concentration. The network that represents the found solution, together with the outlet concentrations of the units, is presented in Figure 20. This solution has also 21 connections, which is the minimum obtained when the number of connections is minimized. Even when some of the connections are excluded by the monotonicity condition, the nonlinear model is capable of reaching 21 connections.

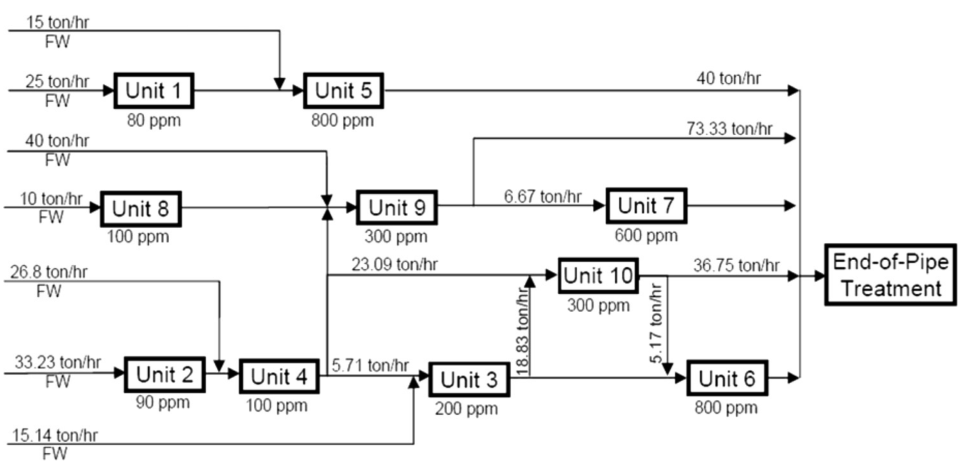

Figure 19. Solution with minimum connections cost considering predefined connections: linear model.

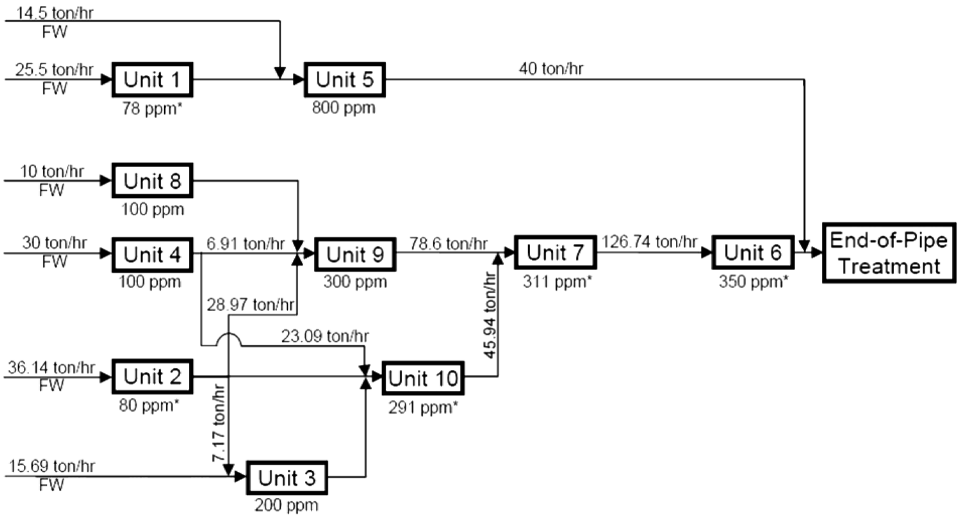

Figure 20. Minimum connections cost considering pre-excluded connections: nonlinear model. *: concentrations lower than the maximum.

We now analyze the minimum connection costs when all the possible combinations of connections are allowed. To guarantee we are analyzing only the possibility of existence and not the decision due to cost, the cost of these previously excluded connections (the connections without the costs of Table III) are set to zero. The solution obtained using the linear and nonlinear models are presented in Figures 21 and 22 respectively. Interestingly, the linear model could now reach a

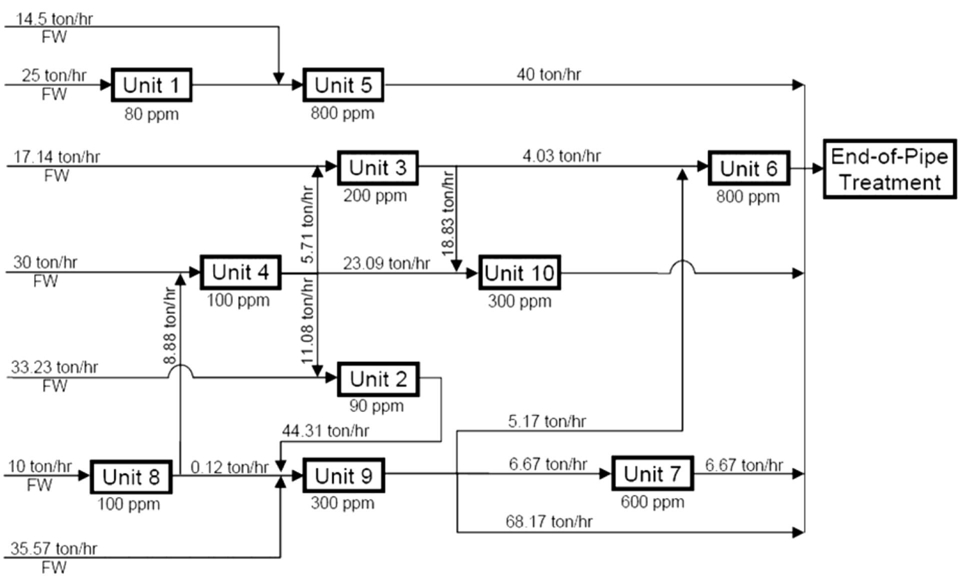

Figure 21. Solution with minimum connections cost considering all possible connections: linear model.

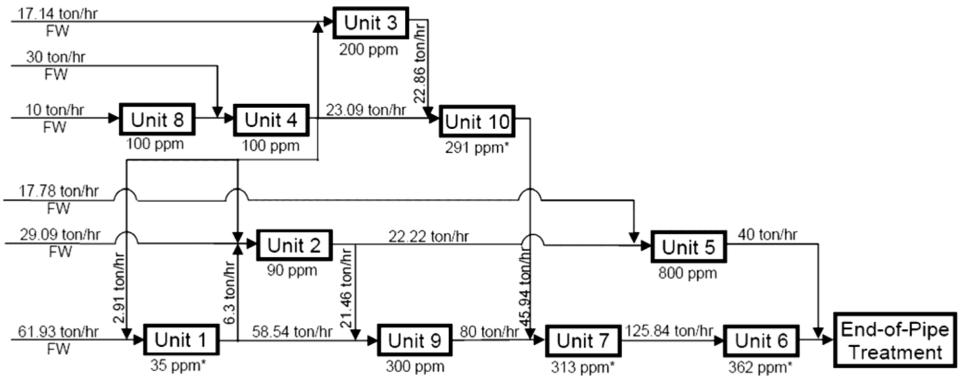

Figure 22. Solution with minimum connections cost considering all possible connections: nonlinear model. *: concentrations lower than the maximum.

lower cost of connections ($49.80) than when some connections were excluded by the monotonicity condition. This solution shows a connection from Unit 8 to Unit 4 that was excluded in the previous case and it substitutes the connection from Unit 2 to Unit 4 in the previous case. The nonlinear model also reaches a lower cost ($38.40) and Units 1, 6, 7, and 10 do not reach their maximum concentration.

Minimizing Total Annualized Cost

We now minimize the total annual cost using the objective function presented in Equation (14). It is assumed the freshwater cost (α) is $0.3/ton and the annual discount factor (*af*) is 0.1 (over 10 years).

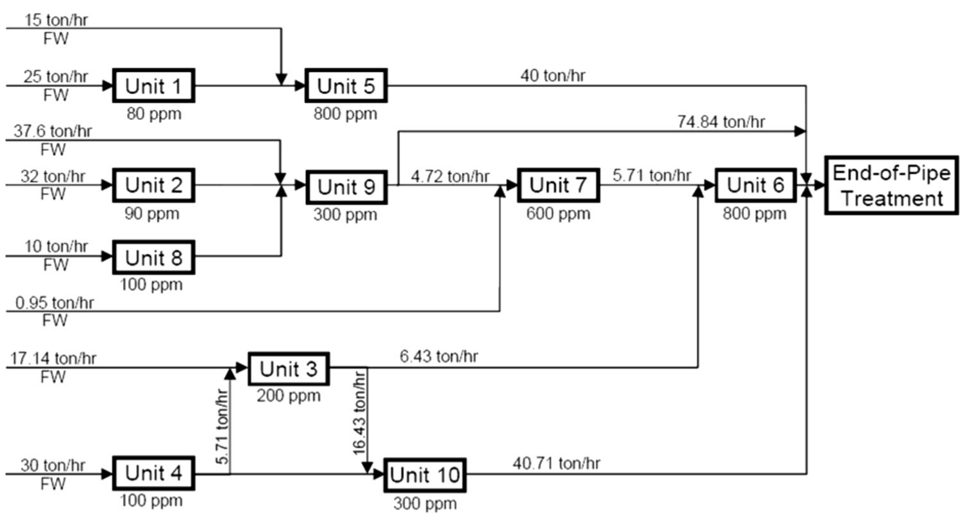

Figure 23. Solution with minimum total cost considering all possible connections: linear model.

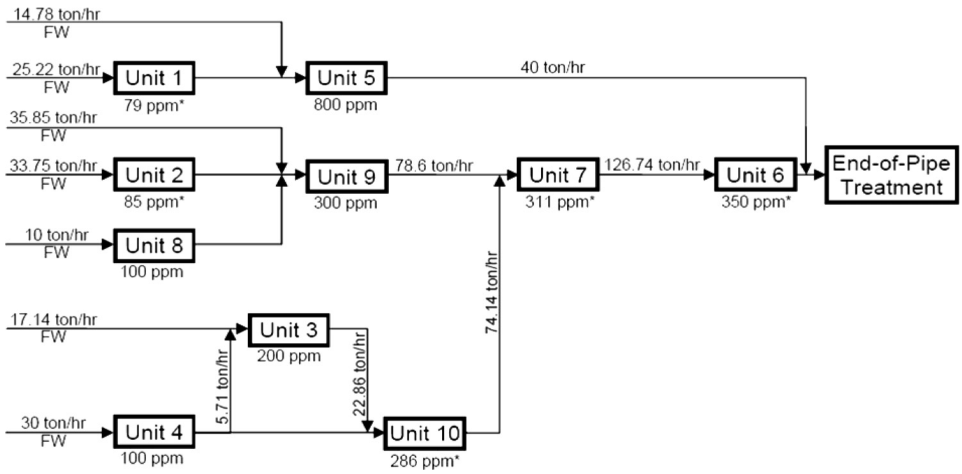

Figure 24. Solution with minimum total cost considering all possible connections: nonlinear model. *: concentrations lower than the maximum.

The linear model gives a minimum total annual cost of $54.82 at 167.70 ton/h. This solution consumes slightly more freshwater than the minimum possible. This network is presented in Figure 23.

The minimum annual cost obtained using the nonlinear model is $53.60 for a network that consumes 166.74 tons of freshwater per hour. The found network is presented in Figure 24. Once again, Units 1, 2, 6, 7, and 10 do not reach their maximum outlet concentration.

Conclusions

A comparative analysis of results obtained using the water allocation original MINLP model and a model that applies particular conditions to design single-contaminant water networks was made. The comparison is based on the application of the optimality conditions (maximum outlet concentration and monotonicity conditions) to minimize objective functions other than minimum freshwater. The influence of structural constraints was also analyzed. Results show that in both cases these conditions should not be used.

Nomenclature

Subscripts

M	mass exchanger units
N	treatment processes
S	wastewater discharge
W	water sources

Parameters

$C^{max,in}$	maximum inlet
$C^{max,out}$	maximum outlet concentration
C^{n}	concentration of the treatment process

C^{ws}	concentration of the water source
IC	investment costs
Δm	mass load
U	maximum value (upper bound) of flow rate allowed through connections
α	cost of freshwater

Variables

C^{out}	outlet concentration
FNS	flow rate from the regeneration process to the discharge
FNU_{m^*}	flow rate from the regeneration process to unit m^*
FS_{m^*}	flow rate from unit m^* to the discharge
FUN_{m^*}	flow rate from unit m^* to the regeneration process
FUU_{m,m^*}	flow rate from unit m to unit m^*
FW_{m^*}	freshwater consumption of unit m^*
Y	connections (binary variable)
YW_m	Binary variable to determine the existence of connection between freshwater source and units
$YUU_{m,m}$	Binary variable to determine the existence of connection between units
YUN_m	Binary variable to determine the existence of connection between units and regeneration process
YNU_m	Binary variable to determine the existence of connection between regeneration process and units
YNS	Binary variable to determine the existence of connection between regeneration process and discharge
YS_m	Binary variable to determine the existence of connection between units and discharge

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Appendix: Summary of the Optimality Conditions (Savelski and Bagajewicz, 2000)

Definitions:

Head processes: Water-using units that receive only freshwater.

Intermediate processes: Water-using units that receive water previously used by other water-using unit(s) and also send their used water to other water-using unit(s).

Terminal processes: Water-using units that receive water previously used by other water-using unit(s) and also send their used water only to treatment.

Partial wastewater provider: Water-using units that send part of their used water to other water-using unit(s) and another part to treatment.

Theorem 1 (necessary condition of concentration monotonicity): *If a solution to the WAP is optimal, then at every partial wastewater provider, the outlet concentrations are not lower than the concentration of the combined wastewater stream coming from all the precursors.*

Theorem 2 (necessary condition of maximum concentration for head processes): *If a solution of the WAP problem is optimal, then the outlet concentration of a head process is equal to its maximum, or an equivalent solution with the same overall freshwater consumption exists in which the concentration is at its maximum.*

Theorem 3 (necessary condition of maximum concentration for intermediate processes): *If the solution of the WAP problem is optimal then the outlet concentration* *of an intermediate process reaches its maximum, or an equivalent solution with the same overall freshwater consumption exists where the concentration is at its maximum.*

Theorem 4 (necessary condition of maximum concentration for terminal processes): *If the solution of the WAP problem is optimal then the outlet concentration of a terminal freshwater user process reaches its possible maximum, or an equivalent solution with the same overall freshwater consumption exists.*