PERGAMON

Chemical Engineering Science 56 (2001) 1897–1911

Chemical Engineering Science

www.elsevier.nl/locate/ces

Algorithmic procedure to design water utilization systems featuring a single contaminant in process plants

Mariano J. Savelski[1], Miguel J. Bagajewicz*

School of Chemical Engineering and Materials Science, University of Oklahoma, Norman, OK, USA

Received 9 July 1999; received in revised form 1 May 2000; accepted 15 May 2000

Abstract

This paper introduces a non-iterative algorithmic procedure to design water utilization networks in refineries and process plants. The procedure is based on necessary and sufficient conditions of optimality that allow the construction of a global optimal solution without the need or a targeting procedure. In addition, the steps of this procedure are such that it can be implemented by hand and have no limitations on the problem size.

Keywords: Water management; Wasterwater reuse

1. Introduction

Several industrial processes require water for their daily operation. Stripping, liquid–liquid extraction and washing operations are among the many processes present in refineries and chemical plants where water is intensively utilized. After utilizing the water, these processes deliver wastewater, which may contain several contaminants. Therefore, wastewater treatment constitutes a primary concern in most industrial sites. In turn, wastewater treatment has always focused on end-of-pipe solutions, which has been seen as the sole remedy to meet imposed discharge limits. Scarcity of water and stricter regulations on industrial effluents has created a different view on water usage. The possibility of selectively reuse wastewater within battery limits has become an option worth exploring. Wastewater reuse and/or recycle can be performed with or without intermediate treatment. This produces a direct impact in the overall amount of fresh makeup water usage as well as in the amount of wastewater that reaches final treatment.

The search for optimal wastewater reuse solutions was addressed by industry itself more than 20 years ago (Carnes, Ford, & Brady, 1973; Skylov, & Stenzel, 1974; Hospondarec & Thompson, 1974; Mishra, Fan, & Erickson, 1975). The concept of reusingwater started to be investigated systematically in the 1980s.

Takama, Kuriyama, Shiroko, and Umeda (1980) used mathematical programming to solve a refinery example problem. A superstructure of all water using operations and cleanup processes was set up and an optimization was then carried out to simplify the structure of the system by removing irrelevant and uneconomical connections. The authors transformed the model into a series of problems without inequality constraints by using a penalty function and finally solving it using the complex method.

Wang and Smith (1994) presented a graphical method based on targeting. The basic concept underlying the methodology is mass exchanger network (MEN) technology, which was in turn first proposed by El-Halwagi and Manousiouthakis (1989) and was later applied to the removal of phenol from refinery wastewater (El-Halwagi & Manousiouthakis, 1990). Departing from the classical representation and solution procedures of mass exchanger network technology, Wang and Smith (1994) proposed a methodology to determine optimal reuse solutions. They also explored options of regenerating wastewater even when the pollutant level has not reached end-of-pipe conditions, or has not been reused throughout the entire process. The authors approached the water allocation problem using targeting graphical representations and heuristic techniques for the design of the realizing network.

* Corresponding author. Tel.: + 1-405-325-5418; fax: + 1-405-325-5813.

E-mail addresses: savelski@rowan.edu (M.J. Savelski), bagajewicz@ou.edu (M.J. Bagajewicz).

[1] Present address: Rowan University, Chemical Engineering, 201 Mullica Hill Road, Glassboro, NJ 08028, USA.

0009-2509/01/$ - see front matter
PII: S0009-2509(00)00405-X

Kuo and Smith (1995) approached the problem in combination with the distribution of wastewater to clean-up operations and used graphical representations and superstructures of alternative designs. Alva-Argáez, Kokossis, and Smith (1998a,b) as well as Huang et al. (1999) presented a solution approach for multicomponent systems based on mathematical programming. They modeled the problem as a nonconvex MINLP and then solved it using a two-phase strategy. As stated by the authors, this approach does not guarantee global optimality. In addition, Alva-Argáez, Vallianatos, and Kokossis (1999) used certain simplifying assumptions to propose a transshipment model. Finally, Savelski, Rivas, and Bagajewicz (1999) presented a method that guarantees global optimality for the solution of the multicomponent problem.

All the above work constitutes important attempts to solve the single and multiple contaminant water/wastewater distribution problems. However, with the exception of the method of Savelski et al. (1999), these methods have either numerical or implementation problems that prevent them from being robust. In this work, we propose an algorithmic design procedure that targets the single-contaminant water allocation problem while providing at the same time a realizing network. The new approach is based on previously developed necessary conditions of optimality (Savelski & Bagajewicz, 1999a, 2000). The paper is restricted to problems with single contaminants. Despite this limitation, there are industrial cases where the method is applicable. The pulp and paper industry uses massive amounts of water and there the concern is on suspended solids only. The painting industry as well as the steel and semiconductor industries also care about total levels of a single contaminant.

The paper is organized as follows: A few definitions and necessary conditions of optimality are reviewed first. Next, certain conditions of maximum reuse of wastewater will be presented. These conditions are later used as a basis of the design procedure. Once this design procedure is presented, a proof of optimality is given. Finally, examples are worked out.

2. Problem statement

Given a set of water-using/water-disposing processes, it is desired to determine a network of interconnections of water streams among the processes so that the overall fresh water consumption is minimized while the processes receive water of adequate quality. This is what is referred to as the water/wastewater allocation planning (WAP) problem. A more stringent version of this problem was presented by Takama et al. (1980) and later used by Wang and Smith (1994). In this version, limits on inlet and outlet concentration of pollutant are imposed a priori on each process and a fixed load of contaminants is used. These inlet and outlet concentrations limits account for corrosion, fouling, maximum solubility, etc.

3. Necessary conditions of optimality

The necessary conditions of optimality are presented in a sequence of theorems. The proofs can be found in Savelski and Bagajewicz (2000). The terminology used was also introduced in the aforementioned paper. We briefly restate the theorems.

Theorem 1. *Necessary condition of concentration monotonicity.*

If a solution to the WAP is optimal, then at every partial wastewater provider (PWP), the outlet concentrations are not lower than the concentration of the combined wastewater stream coming from all the precursors. In other words, given a process j that satisfies the definition of PWP, that is $F_{j,\text{out}} > 0$, then $C_{j,\text{out}} \geqslant C_{P_j,j}$, where $C_{P_j,j}$ is the concentration of the combined wastewater of all the precursors.

Fig. 1 presents the set of interconnections of interest, omitting others that are not relevant to this case.

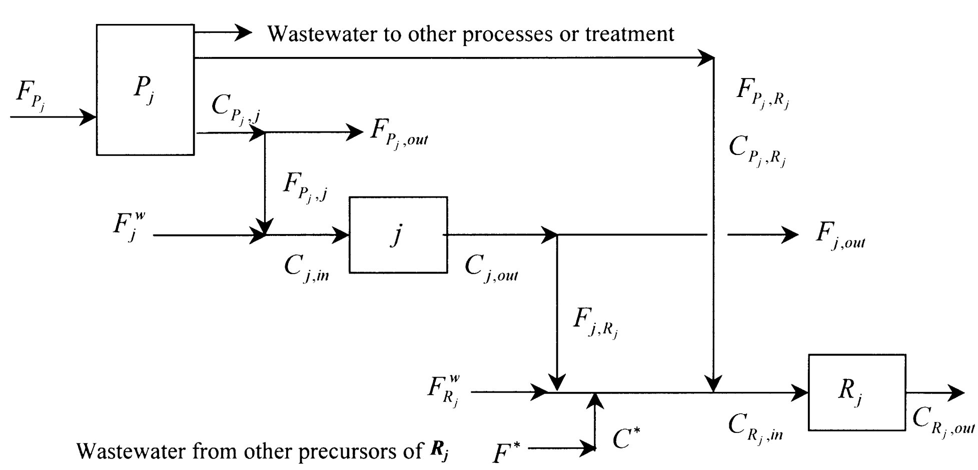

Fig. 1 . Typical water interconnections.

Theorem 2. *Necessary condition of maximum outlet concentration.*

If a solution of the WAP problem is optimal then all FWU processes have reached their maximum possible outlet concentration. Degenerate solutions with lower outlet concentrations but the same overall freshwater consumption may exist. However, these degenerate solutions are such that the flowrate through the process is larger. Thus, they are not preferred. Nevertheless, after the design is obtained, these degenerate solutions can be explored with ease, as they do not alter the connection pattern.

These theorems are accompanied by a set of corollaries (Savelski & Bagajewicz, 2000), which are not essential for this paper.

4. Conditions of maximum reuse

We now derive a series of rules to calculate the amount of wastewater that a process can receive from its precursors in such a way that the amount of fresh water is minimized.

Consider a set of $(n-1)$ precursors of process n (Fig. 2). We assume that process n has a maximum outlet concentration that is larger than that of all its precursors (monotonicity). In Fig. 2, all possible connections from the precursors of process n are indicated. We now proceed to determine the optimal policy of water allocation, such that the fresh water usage of process n is minimum. Next, for the case when the fresh water usage is zero, we develop an allocation policy for wastewater users. Later, we will prove that the use of these policies guarantees optimality.

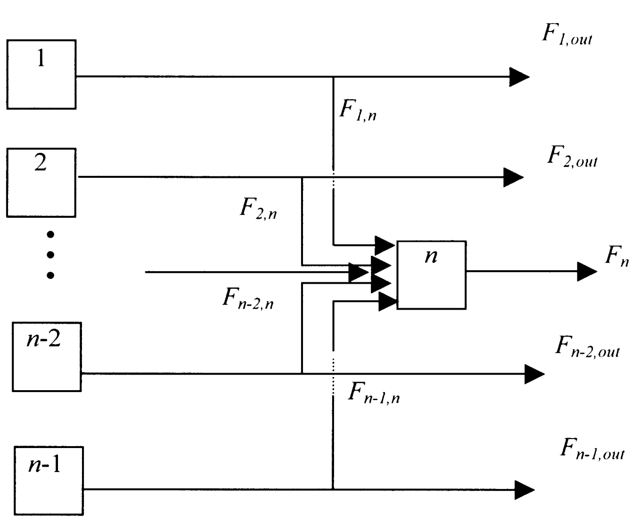

Fig. 2. Precursors of process n.

4.1. Maximum reuse for fresh water users

Without loss of generality, assume that the outlet concentrations of all these processes are ordered monotonically.

$$C_{1,\mathrm{out}}^{\max} \leqslant C_{2,\mathrm{out}}^{\max} \leqslant \cdots \leqslant C_{n-1,\mathrm{out}}^{\max} \leqslant C_{n,\mathrm{out}}^{\max}. \tag{1}$$

The last inequality is a reflection of the necessary condition of monotonicity. Consider now the following optimization problem:

$$\begin{aligned} \text{Min} \quad & F_n^w \\ \text{s.t.} \quad & F_{i,n} \leqslant F_i, \\ & C_{n,\mathrm{in}} \leqslant C_{n,\mathrm{in}}^{\max}, \\ & C_{n,\mathrm{out}} \leqslant C_{n,\mathrm{out}}^{\max}, \\ & F_{i,n} \geqslant 0, \end{aligned} \tag{2}$$

which aims at the best reuse policy, the one that minimizes fresh water usage. We now convert this problem into a linear problem.

Note first that by Theorem 2 of the necessary conditions the outlet concentration is at its maximum value ($C_{n,\mathrm{out}} = C_{n,\mathrm{out}}^{\max}$). Thus, in an optimal structure a component mass balance over process n is

$$\sum_{i=1}^{n-1} F_{i,n} C_{i,\mathrm{out}}^{\max} + L_n = \left(F_n^w + \sum_{i=1}^{n-1} F_{i,n}\right) C_{n,\mathrm{out}}^{\max}, \tag{3}$$

where L_n is the load of process n. This is a linear relation that can be rewritten as follows:

$$F_n^w = K_n - \sum_{i=1}^{n-1} F_{i,n} \alpha_{i,n}, \tag{4}$$

where

$$\alpha_{i,n} = \left(1 - \frac{C_{i,\mathrm{out}}^{\max}}{C_{n,\mathrm{out}}^{\max}}\right) \quad \text{and} \quad K_n = \frac{L_n}{C_{n,\mathrm{out}}^{\max}}.$$

Consider now the component mass balance at the inlet of process n.

$$\left(\sum_{i=1}^{n-1} F_{i,n} + F_n^w\right) C_{n,\mathrm{in}} = \sum_{i=1}^{n-1} F_{i,n} C_{i,\mathrm{out}}^{\max}. \tag{5}$$

Replacing Eqs. (4) into (5) and rearranging, one obtains

$$C_{n,\mathrm{in}} = \frac{\sum_{i=1}^{n-1} F_{i,n} C_{i,\mathrm{out}}^{\max}}{K_n + \sum_{i=1}^{n-1} F_{i,n}(1-\alpha_{i,n})}. \tag{6}$$

Therefore, replacing Eq. (6) in $C_{n,\mathrm{in}} \leqslant C_{n,\mathrm{in}}^{\max}$ one obtains

$$\sum_{i=1}^{n-1} F_{i,n} r_{i,n} \leqslant T_n, \tag{7}$$

where

$$r_{i,n} = C_{i,\mathrm{out}}^{\max} - C_{n,\mathrm{in}}^{\max}(1-\alpha_{i,n}), \tag{8}$$

$$T_n = K_n C_{n,\mathrm{in}}^{\max}. \tag{9}$$

We now replace Eqs. (7) and (4) into Eq. (2) to obtain

$$\begin{aligned} \text{Max} \quad & \textstyle\sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} \\ \text{s.t.} \quad & F_{i,n} \leqslant F_i, \\ & \sum_{i=1}^{n-1} F_{i,n} r_{i,n} \leqslant T_n, \\ & \sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} \leqslant K_n, \\ & F_{i,n} \geqslant 0, \end{aligned} \tag{10}$$

which is a linear program. The last constraint ensures that $F_n^w \geqslant 0$. We will now show that the solution of Eq. (10) can be obtained analytically.

First note that Eq. (8) can be rewritten as follows:

$$r_{i,n} = C_{i,\mathrm{out}}^{\max} - C_{n,\mathrm{in}}^{\max}(1-\alpha_{i,n}) = C_{i,\mathrm{out}}^{\max} - C_{n,\mathrm{in}}^{\max}\left(\frac{C_{i,\mathrm{out}}^{\max}}{C_{n,\mathrm{out}}^{\max}}\right) = C_{i,\mathrm{out}}^{\max}\left(1 - \frac{C_{n,\mathrm{in}}^{\max}}{C_{n,\mathrm{out}}^{\max}}\right), \tag{11}$$

from which we can conclude that,

$$r_{i,n} \geqslant 0, \quad \forall i = 1,\ldots,(n-1). \tag{12}$$

In addition, because of Eq. (1), we have

$$r_{1,n} \leqslant r_{2,n} \leqslant \cdots \leqslant r_{i,n-1}, \tag{13}$$

$$\alpha_{1,n} \geqslant \alpha_{2,n} \geqslant \cdots \geqslant \alpha_{i,n-1}. \tag{14}$$

We now analyze the possible solutions of this optimization problem. Consider the following two cases: (a) The inlet concentration of process n does not reach its maximum, and (b) otherwise. Since this analysis is for fresh water users, in both cases, the fresh water usage is positive, that is, Eq. (2) has a strictly positive solution.

(a) $C_{n,\mathrm{in}} < C_{n,\mathrm{in}}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} < T_n$. In this case, it is easy to prove that the solution of Eq. (10) must be $F_{i,n} = F_i$, $\forall i$. Indeed, if $F_{i,n} < F_i$ for any i, then $F_{i,n}$ can be increased without violating the constraints of Eq. (10), thus increasing the objective function.

(b) $C_{n,\mathrm{in}} = C_{n,\mathrm{in}}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} = T_n$. In this case, the solution has the following form:

$$\begin{aligned} & F_{1,n} = F_1, \\ & F_{2,n} = F_2, \\ & \vdots \\ & F_{s,n} \leqslant F_s, \\ & F_{s+1,n} = 0 \\ & \vdots \\ & F_{n-1,n} = 0 \end{aligned} \tag{15}$$

with

$$F_{s,n} = \frac{K_n C_{n,\mathrm{in}}^{\max}}{C_{s,\mathrm{out}}^{\max} - (1-\alpha_{s,n}) C_{n,\mathrm{in}}^{\max}} \quad \text{if } s = 1,$$

$$F_{s,n} = \frac{K_n C_{n,\mathrm{in}}^{\max} - \sum_{i=1}^{s-1} F_i [C_{i,\mathrm{out}}^{\max} - (1-\alpha_{i,n}) C_{n,\mathrm{in}}^{\max}]}{C_{s,\mathrm{out}}^{\max} - (1-\alpha_{s,n}) C_{n,\mathrm{in}}^{\max}} \quad \text{for } s > 1, \tag{16}$$

which is obtained from Eq. (6) assuming that $C_{n,\mathrm{in}} = C_{n,\mathrm{in}}^{\max}$. Processes 1 through $s-1$ are total wastewater providers of process n, whereas process s is a partial wastewater provider of process n. A formal procedure to determine s will be presented later.

Proof. Consider a feasible perturbation of Eq. (15). We will show that such perturbation leads to an increase in fresh water intake. Assume $F_{k,n} = F_k - \delta_k$ for some $k < s$. Rewrite the second constraint of Eq. (10) as follows:

$$(F_k - \delta_k) r_{k,n} + \sum_{i=1, i\neq k}^{s-1} F_i r_{i,n} + F_{s,n} r_{s,n} + F_{t,n} r_{t,n} = T_n, \tag{17}$$

where we have assumed that some flowrate $F_{t,n} (t > s)$ is not zero. From Eq. (17), we obtain the following relationship between $F_{t,n}$ and δ_k:

$$F_{t,n} = \frac{T_n - (F_k - \delta_k) r_{k,n} - \sum_{i=1, i\neq k}^{s-1} F_i r_{i,n} - F_{s,n} r_{s,n}}{r_{t,n}}. \tag{18}$$

In turn, the change in objective function is

$$\Delta of = -\delta_k \alpha_{k,n} + F_{t,n}\alpha_{t,n}. \tag{19}$$

Thus, substituting Eq. (18) into Eq. (19) and rearranging

$$\Delta of = \delta_k \left(\frac{r_{k,n}}{r_{t,n}} \alpha_{t,n} - \alpha_{k,n} \right). \tag{20}$$

Using Eqs. (12)–(14) one can find that Eq. (20) is negative except when all outlet concentrations in Eq. (1) are equal. In such case, Eq. (20) is zero. In such case, it does not make a difference what wastewater is used. This concludes the proof. □

4.2. Maximum reuse for wastewater users

Without loss of generality, we assume the monotonicity given by Eq. (1). If a WWU has more than one candidate precursor then there may exist infinitely many feasible solutions to the water assignment problem of such a process. When all precursors have concentrations lower than the maximum inlet concentration of process

n ($c^{\max}_{j,\text{out}} \leqslant c^{\max}_{n,\text{in}}\ \forall j$), all linear combinations of wastewater flowrates from the precursors of n can be formed. These linear combinations are only constrained by a component mass balance and the maximum outlet concentration necessary condition. When some precursors have outlet concentrations higher than the maximum inlet concentration of process n ($C^{\max}_{j,\text{out}} \leqslant C^{\max}_{n,\text{in}}\ j = 1,\dots,k$ and $C^{\max}_{j,\text{out}} > C^{\max}_{n,\text{in}}\ j \geqslant k+1,\dots,n-1$), then, linear combinations of available wastewaters of concentration higher and lower than $C^{\max}_{n,\text{in}}$ can be formed. The precursors with $C_{i,\text{out}} \leqslant C^{\max}_{n,\text{in}}$ can be seen as pseudo-fresh water sources each one with a certain cost associated, the better the quality the higher the cost. The precursors with $C_{i,\text{out}} > C^{\max}_{n,\text{in}}$ can then be considered as the actual reusable wastewater sources. Thus, the first k wastewaters can be considered as "good-quality" precursors because they can be used to dilute the rest, which could not otherwise be used. If the WWU under consideration were the last process to be analyzed, then the assignment of water would not really affect the total water intake. However, when some receivers downstream of process n are FWUs, the quality of the wastewater available needs to be preserved so that these other fresh water receivers downstream receive the cleanest wastewater possible. As we shall see later, this heuristic can be proven to be always true. Thus, the problem of assigning water to a WWU is analogous to that of the FWU.

To preserve the cleanest pseudo-fresh waters, we set up the following optimization problem:

$$\begin{aligned} \text{Min} \quad & \textstyle\sum_{i=1}^{k} \mu_{i,n} F_{i,n} \\ \text{s.t.} \quad & C_{n,\text{in}} \leqslant C^{\max}_{n,\text{in}}, \\ & C_{n,\text{out}} \leqslant C^{\max}_{n,\text{out}}, \\ & 0 \leqslant F_{i,n} \leqslant F_i, \quad \forall i \in \mathbf{P}_n, \end{aligned} \tag{21}$$

where $\mu_{i,n} = (C^{\max}_{n,\text{in}} - C^{\max}_{i,\text{out}})$, a positive number except when ($C^{\max}_{n,\text{in}} = C^{\max}_{i,\text{out}}$). This objective function aims at minimizing the consumption of water of the lowest concentration that is preserving the best-quality wastewater for possible downstream FWUs. We will now convert problem (21) into a linear problem as it was done with Eq. (2).

By Theorem 2 of the necessary conditions of optimality, the outlet concentration is at its maximum value ($C_{n,\text{out}} = C^{\max}_{n,\text{out}}$). Thus, using a component mass balance over process n, and since $F^w_n = 0$, we have that Eq. (4) becomes

$$\sum_{i=1}^{n-1} F_{i,n} \alpha_{i,n} = K_n. \tag{22}$$

Now, the component mass at the inlet of process n is given by Eq. (7).

We now replace Eqs. (7) and (22) into Eq. (21) to obtain

$$\begin{aligned} \text{Min} \quad & \sum_{i=1}^{k} \mu_{i,n} F_{i,n} \\ \text{s.t.} \quad & \sum_{i=1}^{n-1} F_{i,n} r_{i,n} \leqslant T_n, \\ & \sum_{i=1}^{n-1} F_{i,n} \alpha_{i,n} = K_n, \\ & 0 \leqslant F_{i,n} \leqslant F_i, \quad \forall i \in \mathbf{P}_n, \end{aligned} \tag{23}$$

which is a linear problem.

We now analyze the two aforementioned cases.

Case I: All precursors are pseudo-fresh water sources. $C^{\max}_{n-1,\text{out}} < C^{\max}_{n,\text{in}}$.

In this case, we use the dirtiest water first and, if it is not enough, we continue using water of the next highest concentration until all requirements are fulfilled. The following set of formulas corresponds to the maximum reuse allocation:

$$\begin{aligned} & F_{j,n} = 0 \quad \forall j < p, \\ & F_{j,n} = F_j \quad \forall j > p, \end{aligned} \tag{24}$$

$$\begin{aligned} & F_{p,n} = \frac{L_n}{C^{\max}_{n,\text{out}} - C^{\max}_{p,\text{out}}} \quad \text{if } p = 1, \\ & F_{p,n} = \frac{L_n - \sum_{i=p+1}^{n-1} F_i (C^{\max}_{n,\text{out}} - C^{\max}_{i,\text{out}})}{C^{\max}_{n,\text{out}} - C^{\max}_{p,\text{out}}} \quad \text{if } p > 1. \end{aligned} \tag{25}$$

An algorithm procedure will be presented later to establish the partial wastewater provider p. The proof to show that this policy preserves the cleanest wastewater possible is straightforward.

Case II: Only some precursors are pseudo-fresh water sources; i.e.

$$\begin{aligned} & C^{\max}_{i,\text{out}} \leqslant C^{\max}_{n,\text{in}} \quad \forall i \leqslant k, \\ & C^{\max}_{i,\text{out}} > C^{\max}_{n,\text{in}} \quad \forall i > k. \end{aligned} \tag{26}$$

We now prove that the optimal solution of Eq. (23) is given a combination of the dirtiest set of pseudo-fresh water precursors possible and the cleanest set of wastewater available. The former policy is driven directly by the objective function of Eq. (23). The latter is indirectly driven by the same objective function. Indeed, as less polluted water is used, the usage of pseudo-fresh water is smaller. Fig. 3 illustrate one such generic combination.

Consider the following two cases: (a) The inlet concentration of process n does not reach its maximum, and (b) otherwise.

(a) $C_{n,\text{in}} < C^{\max}_{n,\text{in}}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} < T_n$. In this case, the solution of Eq. (23) is given by a complete use of wastewater and a partial use of pseudo-fresh waters, that is: $F_{i,n} = F_i$ $\forall i \in [k+1, n-1]$, $F_{j,n} = F_j\ \forall j \in [s+1, k]$ and $F_{j,s} < F_s$ for some s. The identification of the partial wastewater provider s will be presented later. The proof is simple: If

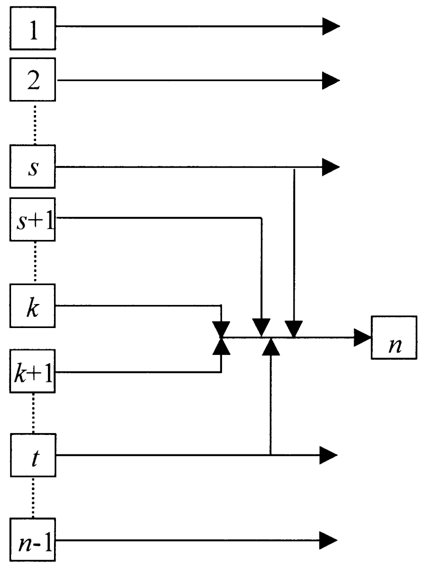

Fig. 3. Wastewater user.

the allocation of a wastewater is not total, that is, $F_{t,n} < F_t$ ($t > k$), then $F_{t,n}$ can be increased because the inlet concentration of process n has not reached its maximum. As a result, one or more of the pseudo-fresh waters $F_{j,n}$ ($j \leqslant k$) has to be decreased to maintain the component balance ($\sum_i F_{i,n}\alpha_{i,n} = K_n$). It is easy to see that these two changes lead to a decrease of the objective function.

(b) $C_{n,\text{in}} = C_{n,\text{in}}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} = T_n$. In this scheme, pseudo-fresh waters from process s ($s < k$) to process k are used to dilute wastewaters from process ($k+1$) to process t ($t > k$). Once the partial wastewater providers s and t are identified, the following flowrates are obtained.

$$F_{j,n} = F_j, \quad \forall j = (s+1),\ldots,(t-1),$$

$$F_{s,n} < F_s,$$

$$F_{t,n} < F_t, \tag{27}$$

where $F_{s,n}$ and $F_{t,n}$ can be obtained from the following set of equations:

$$F_{s,n} r_{s,n} + F_{t,n} r_{t,n} = T_n - \sum_{p=s+1}^{t-1} F_p r_{p,n},$$

$$F_{s,n} \alpha_{s,n} + F_{t,n} \alpha_{t,n} = K_n - \sum_{p=s+1}^{t-1} F_p \alpha_{p,n}, \tag{28}$$

We now prove that Eqs. (27) and (28) give the optimal solutions of Eq. (26).

Consider a feasible perturbation of Eq. (27). We will show that such perturbation leads to an increase in the value of the objective function. Assume we increase the flowrate of a process j ($j < k$), thus decreasing the flowrate of a process p ($p > k$). Therefore, we can write the perturbation of Eq. (27) as follows:

$$\bar{F}_{j,n} = F_{j,n} + \delta_j, \quad j \leqslant s,$$

$$\bar{F}_{p,n} = F_{p,n} - \delta_p, \quad s < p \leqslant k,$$

$$\bar{F}_{i,n} = F_{i,n}, \quad \forall i \neq p, \forall i \neq j,$$

$$\delta_j, \delta_p > 0. \tag{29}$$

The change in the objective function is given by

$$\Delta of = \mu_j \delta_j - \mu_p \delta_p. \tag{30}$$

Replacing Eq. (29) in the second equation of Eq. (28) and rearranging, we obtain

$$\frac{\delta_p}{\delta_j} = \frac{\alpha_{j,n}}{\alpha_{p,n}}. \tag{31}$$

Replacing Eq. (31) into Eq. (30), one obtains

$$\Delta of = \delta_j \left(\mu_{j,n} - \frac{\alpha_{j,n}}{\alpha_{p,n}} \mu_{p,n} \right). \tag{32}$$

Using the definitions of α, μ and doing some algebraic manipulations, we obtain

$$\Delta of = \delta_j \left(\frac{(C_{p,\text{out}}^{\max} - C_{j,\text{out}}^{\max})(C_{n,\text{out}}^{\max} - C_{n,\text{in}}^{\max})}{(C_{n,\text{out}}^{\max} - C_{p,\text{out}}^{\max})} \right). \tag{33}$$

One can easily verify that Eq. (33) is strictly positive unless $C_{p,\text{out}} = C_{j,\text{out}}$ in which case it is zero. □

We now present the maximum reuse algorithm, which systematically implements of the above presented wastewater allocation process. Consider the following definition first:

Definition. A maximum reuse structure is a flowsheet that satisfies the property that all inlet wastewater flows to any unit are obtained using the maximum reuse algorithm.

5. Maximum reuse algorithm

Given wastewater available from $n-1$ processes the maximum reuse allocation of wastewater to process n is given by the application of the algorithm below. The algorithm is based on the assumption that process n is a WWU. If no precursor has a concentration lower than the maximum inlet concentration of process n or a contradiction is found, then it is solved as a FWU.

Algorithm

1. Assume process n is a WWU. Then, there are two alternatives. Either all the pseudo-fresh water precursors have concentrations lower than the maximum inlet concentration of process n (Case I) or only some of its precursors satisfy this inequality (Case II).
2. *Case I*: Assume $p = n - 1$. Calculate $F_{p,n}$ using Eqs. (24) and (25). If the value of $F_{p,n}$ calculated is larger than F_p, then make $F_{p,n} = F_p$ update p ($p = p - 1$)

and repeat the procedure. If the water from all precursors is exhausted and the water requirements are still unfulfilled, then process n is not a WWU but a FWU. In such case, go to 6. Otherwise, stop.

3. *Case II*: Assume the partial wastewater providers to be $s = k$ and $t = k + 1$. Apply Eqs. (27) and (28).
4. If, $F_{k,n} \leqslant F_k$ and $F_{k+1,n} \leqslant F_{k+1}$ then stop. Otherwise, go to 5.
5. If either flowrate results larger than its corresponding available flowrate, then this implies that all the available wastewater from the precursor must be used and that another set of precursors is needed. Therefore, if $F_{s,n} > F_s$, make $F_{s,n} = F_s$ update s ($s = s - 1$), and/or if $F_{t,n} > F_t$ make $F_{t,n} = F_t$ update t ($t = t + 1$) and return to 3. If all pseudo-fresh water precursors are exhausted and the water requirements are still unfulfilled, then process n is not a WWU but a FWU. In such case, go to 6.
6. The process has been determined to be a FWU. Assume the partial wastewater provider to be $s = 1$. Calculate $F_{1,n}, \ldots, F_{s,n}$ and F_n^w using Eqs. (15), (16) and (4). If $F_{s,n} > F_s$, then make $F_{s,n} = F_s$, update s ($s = s + 1$) and repeat the process. Otherwise, if $F_{s,n} \leqslant F_s$ stop.

6. Design procedure

The following design procedure is proposed:

1. Feed fresh water to all the processes that have zero inlet maximum concentration (head processes). To calculate the required flowrate use the following:

$$F_h^w = \frac{L_h}{C_{h,\text{out}}^{\max}} \tag{34}$$

   If no process has zero inlet maximum concentration take the process with the lowest maximum outlet concentration.
2. Order the rest of processes in increasing order of maximum outlet concentration.
3. Take the first process of the list and apply the maximum reuse algorithm. Exclude from the list of sources those that violate monotonicity.
4. Keep applying the maximum reuse rule in this fashion for all the rest of the processes.

The above procedure satisfies all necessary conditions of optimum (monotonicity in the outlet concentrations and outlet concentrations at their maximum values). We now prove that the maximum reuse algorithm leads to an optimal structure.

6.1. Proof of optimality

Theorem. *The maximum reuse structure is optimal.*

Proof. The proof is by mathematical induction. By construction, it is true for two processes. Now we assume it is true for $n - 1$ processes and we will prove it is true for n processes. Consider first a structure with $n - 1$ processes. By the optimality condition of monotonicity we know that process n is not a precursor of any of the $n - 1$ first processes. Consider first an overall balance on a structure that contains all n processes.

$$W = \sum_{i=1}^{n-1} F_i^w + F_n^w = \sum_{i=1}^{n-1} F_{i,\text{out}} + F_n, \tag{35}$$

$$L = \sum_{i=1}^{n} L_i = \sum_{i=1}^{n-1} F_{i,\text{out}} C_{i,\text{out}}^{\max} + F_n C_{n,\text{out}}^{\max}. \tag{36}$$

Eliminating F_n, one obtains

$$W = Z_n + \sum_{i=1}^{n-1} F_{i,\text{out}} \alpha_{i,n}, \tag{37}$$

where $Z_n = L_n / C_{n,\text{out}}^{\max}$. The optimal water allocation policy for the system with n units is either

(a) a system where the water allocation for the first $n - 1$ units is a maximum reuse structure, or

(b) the water allocation in the first $n - 1$ processes is such that the fresh water consumption of these first $n - 1$ processes is larger than the optimum assumed for these $n - 1$ processes, but leads to an overall smaller fresh water consumption.

We now explore the two options.

(a) In this case, the theorem is readily proved, as the only water allocation policy that will minimize F_n^w is the one obtained applying the maximum reuse algorithm to process n.

(b) Assume that the fresh water consumption of process s is increased,

$$\bar{F}_s^w = F_s^w + \delta_s^w. \tag{38}$$

However, if the overall structure is to be optimal, the concentration at the outlet of process s should be maintained at its maximum. To achieve this, a smaller amount of wastewater from its precursors has to be used. Thus, the only effect of the perturbation is to lower the inlet concentration $C_{s,\text{in}}$ and to decrease the flowrate through process s (F_s). However, in a maximum reuse structure there is at the most only one precursor (k) that has wastewater sending to process s for which $F_{k,s} < F_k$. The rest are either $F_{j,s} = F_j$ or zero.

Therefore, to achieve the maximum concentration in process s the following feasible perturbation must accompany Eq. (38).

$$\bar{F}_{k,s} = F_{k,s} - \delta_k. \tag{39}$$

Accordingly,

$$\bar{F}_{k,\text{out}} = F_{k,\text{out}} + \delta_k \tag{40}$$

for some precursor k of process s. Fig. 4 illustrates the section of the flowsheet under study.

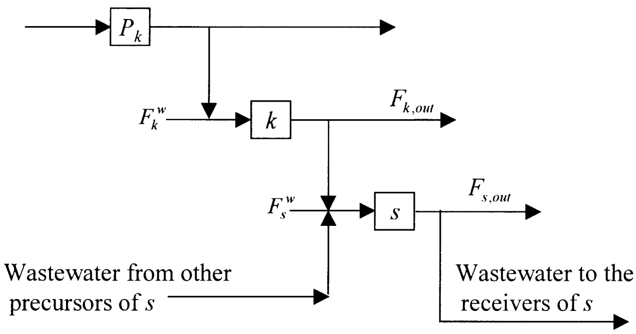

Fig. 4. Maximum reuse structure.

We notice again that the perturbation of these two processes (s and k) is feasible only if the precursor has wastewater that has not been reused ($F_{k,\mathrm{out}} > 0$). The other possibility is to reduce the total water flowrate of process k. If process k is a head process, the fresh water intake is already at it minimum, so the perturbation is also infeasible. Otherwise, to reduce the total flowrate through process k, the fresh water intake of some precursor of this process has to be also reduced. This stems from the fact that a reduction of F_k^w (if there is any) would violate the maximum concentration at its outlet. As shown above, this needs to be accompanied by an increase in fresh water intake which leads to the same situation over and over, until one finds a head process or a precursor for which some of its wastewater is not reused. We call this, a chain of precursors. Therefore, the perturbation of fresh water intake is infeasible if no process in the chain of precursors has wastewater that is not being reused.

Notice that

$$\delta_k = \frac{\delta_s^w}{\alpha_{k,s}}, \tag{41}$$

which can be obtained using a component balance over process s. Thus,

$$\bar{F}_s = F_s - \delta_k + \delta_s^w = F_s - \delta_s^w\left(\frac{1-\alpha_{k,s}}{\alpha_{k,s}}\right), \tag{42}$$

which confirms that F_s also decreases. It also shows that the perturbation is feasible if and only if $F_{s,\mathrm{out}} \geqslant \delta_s^w((1-\alpha_{k,s})/\alpha_{k,s})$.

Because of this perturbation, $F_{s,\mathrm{out}}$ decreases, and the rest of the structure downstream remains unaltered. This statement stems from the fact that a perturbation of $F_{s,r}$, process r being a receiver of process s, leads to an increase in F_r^w, perturbation we do not want to make because it leads to the same analysis for process r, is the one we are making for process s.

Thus, the change in fresh water intake is given by

$$\Delta W = \bar{W} - W = \sum_{i=1}^{n-1} \alpha_{i,n}(\bar{F}_{i,\mathrm{out}} - F_{i,\mathrm{out}}) = \alpha_{k,n}\delta_k + \alpha_{s,n}(\delta_s^w - \delta_k). \tag{43}$$

Replacing Eq. (41) into Eq. (43) and applying the definition of α, one obtains

$$\Delta W = \delta_s^w, \tag{44}$$

which is positive by definition. This concludes the proof that a perturbation in one FWU leads to an overall increase in water consumption.

Consider now that $F_{k,\mathrm{out}} = 0$, and therefore there is a chain of precursors $D = \{k_1, k_2, \ldots, k_t\}$ such that the wastewater of some process k_1 is not completely reused that is $F_{k_1,\mathrm{out}} > 0$ (Fig. 5).

For this chain, we have

$$\bar{F}_{k_i}^w = F_{k_i}^w + \delta_{k_i}^w, \quad k_i = k_2, k_3, \ldots, k_t. \tag{45}$$

In addition, since $F_{k_i,\mathrm{out}} = 0$, then

$$\bar{F}_{k_i,k_{i+1}} = \bar{F}_{k_i}, \quad k_i = k_2, \ldots, k_t \tag{46}$$

and

$$\bar{F}_{k_i} = F_{k_i} - \delta_{k_i}, \quad k_i = k_2, k_3, \ldots, k_t. \tag{47}$$

Relation Eq. (41) holds for δ_{k_i-1}, that is

$$\delta_{k_i-1} = \frac{\delta_{k_i}^w}{\alpha_{k_i-1,k_i}}. \tag{48}$$

Now, similarly to Eq. (42), the process through process k_i is

$$\bar{F}_{k_i} = F_{k_i} - \delta_{k_i-1} + \delta_{k_i}^w = F_{k_i} - \delta_{k_i}^w\left(\frac{1-\alpha_{k_i-1,k_i}}{\alpha_{k_i-1,k_i}}\right). \tag{49}$$

Using Eqs. (47)–(49)

$$\delta_{k_i} = \delta_{k_i-1}(1-\alpha_{k_i-1,k_i}). \tag{50}$$

Applying Eq. (50) recursively and using Eq. (41), one obtains

$$\delta_{k_i} = \frac{\delta_{k_t}}{\prod_{m=k_i}^{k_t-1}(1-\alpha_{m,m+1})} = \frac{\delta_s^w}{\alpha_{k_t,s}\prod_{m=k_i}^{k_t-1}(1-\alpha_{m,m+1})}, \tag{51}$$

which is positive. Thus, using Eq. (37)

$$\Delta W = \delta_{k_1}\alpha_{k_1,n} + \Delta F_s \alpha_{s,n}. \tag{52}$$

Then, form Eq. (42)

$$\Delta W = \delta_{k_1}\alpha_{k_1,n} - \delta_s^w\left(\frac{1-\alpha_{k_t,s}}{\alpha_{k_t,s}}\right)\alpha_{s,n}. \tag{53}$$

Using Eq. (51) and the fact that $\alpha_{k_1,n} > \alpha_{s,n}$, one obtains

$$\Delta W = \delta_{k_1}\left[\alpha_{k_1,n} - (1-\alpha_{k_t,s})\alpha_{s,n}\prod_{m=k_1}^{k_t-1}(1-\alpha_{m,m+1})\right] \geqslant \delta_{k_1}\alpha_{s,n}\left[1-(1-\alpha_{k_t,s})\prod_{m=k_1}^{k_t-1}(1-\alpha_{m,m+1})\right]. \tag{54}$$

The last term is positive.

Consequently, we have shown that any feasible perturbation of the proposed fresh water intake of the

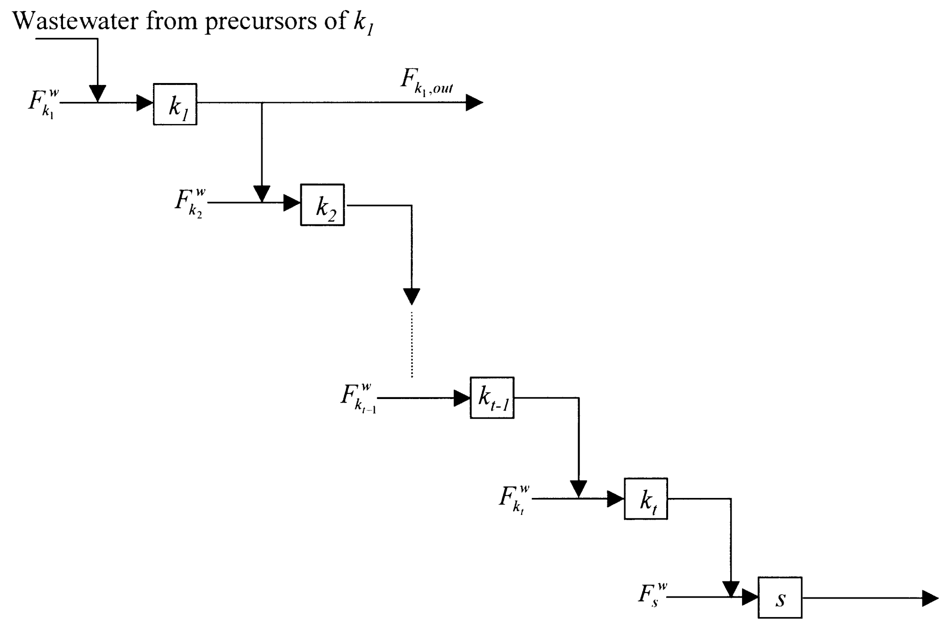

Fig. 5. Processes chain.

optimum given by a maximum reused structure leads to an increase of overall fresh water intake.

To finalize the proof, we now show that the reuse structure of WWUs is optimal.

Consider, without loss of generality, that process $(n-1)$ is a WWU. Assume also, that process n is a FWU. Otherwise, if process n is a WWU, then any allocation policy does not alter the overall water usage.

Consider a perturbation of the wastewater allocation to process $(n-1)$. We will show that the perturbation leads to an increase of the fresh water usage of process n. Fig. 6 illustrates one generic result of the maximum reuse rule applied to process n.

According to the maximum reuse rule, $F_{m,n-1} < F_m$, $F_{i,n-1} = F_i \;\; \forall i \;\; [m+1,\dots,\; p-1]$, $F_{p,n-1} < F_p$ and $F_{j,n-1} = 0 \;\; \forall j \in [p+1,\dots,n-2]$. Consider now that a feasible perturbation is introduced:

$$\bar{F}_{p,n} = F_{p,n} - \delta_p,$$

$$\bar{F}_{p+1,n} = \delta_{p+1},$$

$$\delta > 0. \tag{55}$$

We will first prove that increasing the flowrate of a wastewater precursor of higher concentration (δ_{p+1}) leads to an increase in the flowrate of a pseudo-fresh water precursor. That is $\delta_m > 0$.

Writing Eq. (28) before and after the perturbation and subtracting, one obtains

$$\delta_m r_{m,n-1} - \delta_p r_{p,n-1} + \delta_{p+1} r_{p+1,n-1} = 0, \tag{56}$$

$$\delta_m \alpha_{m,n-1} - \delta_p \alpha_{p,n-1} + \delta_{p+1} \alpha_{p+1,n-1} = 0. \tag{57}$$

Solving for δ_m as a function of δ_{p+1}, we get

$$\delta_m = \delta_{p+1} \frac{(\alpha_{p+1,n-1} r_{p,n-1} - \alpha_{p,n-1} r_{p+1,n-1})}{(\alpha_{p,n-1} r_{m,n-1} - \alpha_{m,n} r_{p,n-1})}. \tag{58}$$

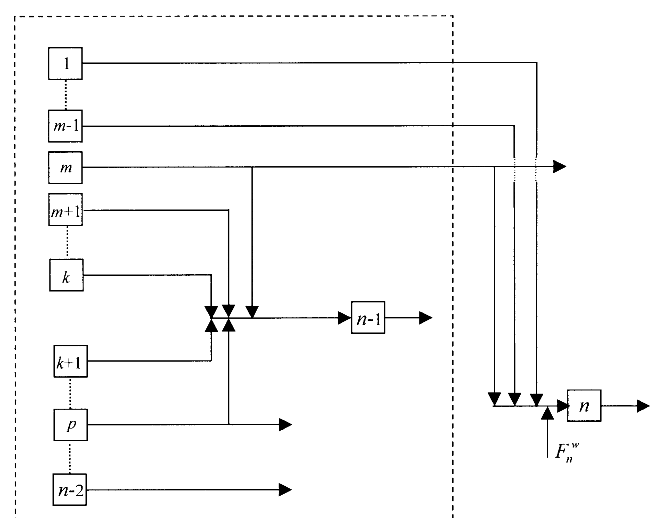

Fig. 6. Maximum reuse genetic structure for a wwu.

Using the definition of α and r, one obtains

$$\delta_m = \delta_{p+1} \frac{(C^{\max}_{p+1,\text{out}} - C^{\max}_{p,\text{out}})}{(C^{\max}_{p,\text{out}} - C^{\max}_{m,\text{out}})}. \tag{59}$$

Therefore, by virtue of the monotonicity of the outlet concentrations of the precursors, $\delta_m > 0$. By substituting in Eq. (56), one can verify that $\delta_p > 0$.

By construction, the above perturbations would not alter the total fresh water intake of the network system that includes process $n-1$. However, if process n is a FWU and consumes wastewater from process m, then a reduction of available wastewater of low concentration will in itself increase F^w_n. This is straightforward from Eqs. (15), (16) and (4). □

Remark. The above proof only shows that the algorithmic procedure provides one optimal solution. There are, however, many other solutions of the same overall fresh water consumption that can be constructed (Savelski & Bagajewicz, 1999b). This result stems from the fact that the maximum reuse policy is a sufficient condition of optimum, not a necessary one. For example, in the optimality proof we showed that departing from the maximum reuse policy for WWUs does not always lead to an increase in fresh water usage.

7. Examples

We now show some examples from the literature where the network obtained using the algorithmic procedure is compared to the reported one.

Example 1. This example is taken from Wang and Smith (1994). The system involves four processes and their corresponding data is given in Table 1.

We now show how the new design methodology is applied to this problem.

Step 1: Identify head processes

Process 1 is the only process with maximum inlet concentration equal to zero. Using Eq. (34), one obtains

$$F_1^w = \frac{L_1}{C_{1,\text{out}}^{\max}} = \frac{2000\ \text{g/h}}{100\ \text{ppm}} = 20.0\ \text{ton/h}.$$

Step 2: Maximum outlet concentration ordering.

There are three processes left to order. That is

Process number	$C_{\text{out}}^{\max}$
2	100
3	800
4	800

Since processes 3 and 4 has the same outlet maximum concentration, either one could be listed first.

Table 1
Example from Wang and Smith (1994)

Process number	Mass load of contaminant (kg/h)	$C_{\text{in}}^{\max}$ (ppm)	$C_{\text{out}}^{\max}$ (ppm)
1	2.0	0	100
2	5.0	50	100
3	30.0	50	800
4	4.0	400	800

Step 3: Apply the maximum reuse rules

3.1. We take the first process of the list (process 2) and apply the rule. We realize that due to the necessary condition of monotonicity, there are no possible precursors for this process. Therefore, fresh water is fed to process 2.

Calculating the necessary fresh water intake, we obtain

$$F_2^w = 50.0\ \text{ton/h}.$$

3.2. We take process 3 and apply the rules. The maximum outlet concentration of this process allows us to supply it with wastewater from either process 1 or 2.

Using Eq. (16), we can write

$$F_{1,3} = \frac{K_3 C_{3,\text{in}}^{\max}}{C_{1,\text{out}}^{\max} - (1 - \alpha_{1,3}) C_{3,\text{in}}^{\max}} = \frac{37.5 \cdot 50}{100 - (1 - 0.875) \cdot 50} = 20.0\ \text{ton/h},$$

$F_{1,3} = 20.0 = F_1$. Consequently, we can fulfill process 3 water intake by using process 1 only. We now calculate the necessary fresh water intake using Eq. (4).

$$F_3^w = K_3 - F_{1,3}\alpha_{1,3} = 37.5 - 20.0 \cdot 0.875 = 20.0\ \text{ton/h}.$$

3.3. Finally, we consider process 4. This process has only one monotone precursor, which is process 2. Process 3 has wastewater of the same concentration as the maximum outlet process 4. Therefore, it cannot be used as a wastewater provider. The outlet concentration of process 2 is lower than the maximum inlet concentration of process 4, therefore the latter is a WWU candidate (Case I).

Using Eq. (25), one obtains

$$F_{2,4} = \frac{L_4}{(C_{4,\text{out}}^{\max} - C_{2,\text{out}}^{\max})} = \frac{4{,}000}{(800 - 100)} = 5.7143\ \text{ton}/h < F_2.$$

Since $F_{2,4} < F_2$, process 4 does not require any other water intake to fulfill its requirements. Consequently, it is a true WWU and the problem is solved.

Finally, we calculated the total fresh water intake that the network requires, that is

$$W = F_1^w + F_2^w + F_3^w = 20.0 + 50.0 + 20.0 = 90.0\ \text{ton/h}.$$

Both, the water consumption and the network design (Fig. 7) coincide with those reported by Wang and Smith (1994).

Table 2 summarizes all flowrates and final inlet and outlet concentrations of each process.

Example 2. This example is taken from Olesen and Polley (1997). The system involves six processes and their corresponding data are given in Table 3.

The minimum flowrate reported is 157.14 ton/h. Olesen and Polley (1997) obtained a realizing network by methods of inspection. Fig. 8 shows this network.

Table 4 summarizes the results of this example problem for the network obtained by Olesen and Polley (1997). The minimum fresh water consumption is met, so the solution is optimal but constitutes a degeneracy of the solution network depicted in Fig. 9. The flowsheet shown in Fig. 9, obtained using the maximum reuse algorithm, satisfies all the necessary conditions of optimality and meets the 157.143 ton/h minimum fresh water consumption.

Table 5 shows the results for the network depicted in Fig. 9. In this flowsheet all processes have reached maximum outlet concentration through maximum reuse. All

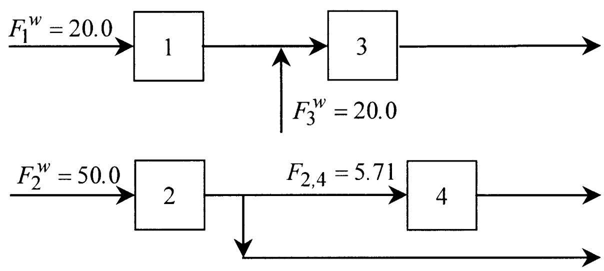

Fig. 7. Solution network for Example 1.

Table 2
Final solution to Example 1

Process number	Type of process	Fresh water intake (ton/h)	Wastewater reuse (ton/h)	C_{in} (ppm)	C_{out} (ppm)
1	H	20.0	0.0	0.0	100.0
2	H	50.0	0.0	0.0	100.0
3	T	20.0	$F_{1,3} = 20.0$	50.0	800.0
4	WWU	0.0	$F_{2,4} = 5.714$	100.0	800.0

Table 3
Example from Olesen and Polley (1997)

Process number	Mass load of contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	2.0	25	80
2	5.0	25	100
3	4.0	25	200
4	5.0	50	100
5	30.0	50	800
6	4.0	400	800

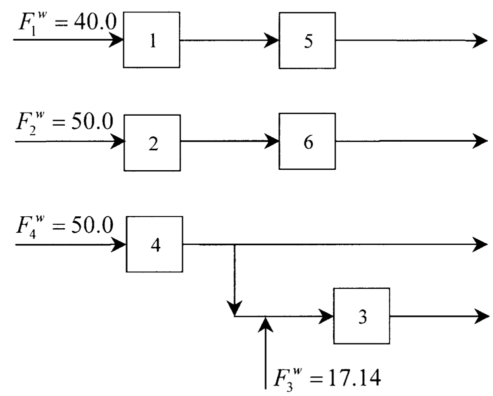

Fig. 8. Water network proposed by Olesen and Polley (1997).

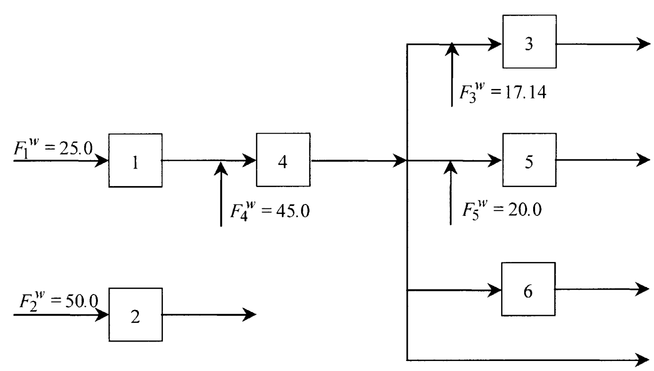

Fig. 9. Water network obtained using the maximum reuse algorithm in Example 2.

Table 4
Degenerate solution of Example 2

Process number	Fresh water intake (ton/h) (F_i^w)	Wastewater reuse (ton/h) ($F_{j,i}$)	Total flowrate (ton/h) (F_i)	C_{in} (ppm)	C_{out} (ppm)
1	40.0	0.0	40.0	0	50
2	50.0	0.0	50.0	0	100
3	17.143	$F_{4,3} = 5.714$	22.857	25	200
4	50.0	0.0	50.0	0	100
5	0.0	$F_{1,5} = 40.0$	40.0	50	800
6	0.0	$F_{2,6} = 50.0$	50.0	100.0	180.0
Total flowrate (ton/h)	157.143	95.714	252.857		

Table 5
Solution of Example 2

Process number	Fresh water intake (ton/h) (F_i^w)	Wastewater reuse (ton/h) ($F_{j,i}$)	Total flowrate (ton/h) (F_i)	C_{in} (ppm)	C_{out} (ppm)
1	25.0	0.0	25.0	0	80
2	50.0	0.0	50.0	0	100
3	17.143	$F_{4,3}$ = 5.714	22.857	25	200
4	45.0	$F_{1,4}$ = 25.0	70.0	28.57	100
5	20.0	$F_{4,5}$ = 20.0	40.0	50	800
6	0.0	$F_{4,6}$ = 5.714	5.714	100	800
Total flowrate (ton/h)	157.143	56.428	213.571		

Table 6
Data for Example 3

Process number	Mass load of contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Minimum fresh water flowrate without reuse (ton/h)
1	2.0	25	80	25.0
2	2.88	25	90	32.0
3	4.0	25	200	20.0
4	3.0	50	100	30.0
5	30.0	50	800	37.5
6	5.0	400	800	6.25
7	2.0	200	600	3.3333
8	1.0	0	100	10.0
9	20.0	50	300	66.6667
10	6.5	150	300	21.6667
	Total minimum flowrate (ton/h)		252.4167	

the necessary conditions of optimality are satisfied by the solution obtained using the maximum reuse algorithm.

It is important to point out that, even though degenerate solutions provide the same overall fresh water consumption, they feature larger flowrate through some processes. Comparing the fourth columns of Tables 4 and 5, the total flowrate through the degenerate solution is 18.4% larger than the total flowrate through the maximum reuse structure solution. This situation may lead to larger equipment.

Example 3. It comprises a system of 10 processes. This example is not taken from the literature. Table 6 shows the data for this example including all the minimum fresh water requirements of these processes without wastewater reuse.

Fig. 10 shows a solution network obtained using the algorithmic procedure. Table 7 shows all the resulting flowrates and final concentrations of the processes.

Table 7
Solution of Example 3

Process number	Type of process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum fresh water flowrate with reuse (ton/h)
1	H	0.0	0	80	25.0
2	I	$F_{1,2}$ = 13.8462	25	90	30.4615
3	I	$F_{2,3}$ = 6.3492	25	200	16.5079
4	I	$F_{1,4}$ = 11.1538 $F_{2,4}$ = 23.4188	50	100	25.4273
5	T	$F_{4,5}$ = 9.51428 $F_{8,5}$ = 10.0 $F_{9,5}$ = 0.16191	50	800	20.3238
6	WWU	$F_{9,6}$ = 16.6667	300	800	0.0
7	WWU	$F_{3,7}$ = 1.19047 $F_{4,7}$ = 1.90476 $F_{9,7}$ = 1.90476	200	600	0.0
8	H	0.0	0	100	10.0
9	T	$F_{2,9}$ = 14.5397 $F_{4,9}$ = 26.9143	50	300	38.5460
10	WWU	$F_{3,10}$ = 21.6667 $F_{4,10}$ = 21.6667	150	300	0.0
			Total minimum fresh water flowrate (ton/h)		166.2665

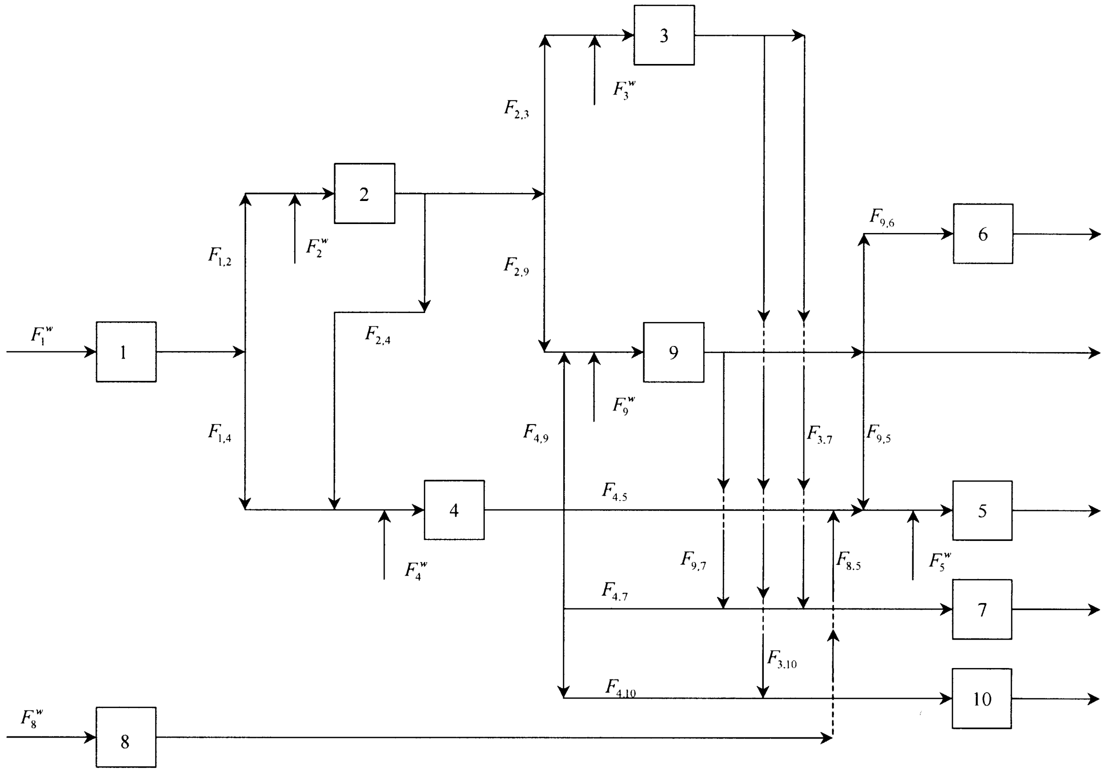

Fig. 10. Water network obtained for Example 3.

Table 8
Data for Example 4

Process number	Mass load of contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Minimum fresh water flowrate without reuse (ton/h)
1	1.0	0	80	12.5
2	2.0	0	100	20.0
3	2.0	0	120	16.6667
4	2.0	25	80	25.0
5	2.880	25	90	32.0
6	1.5	40	90	16.6667
7	3.0	50	100	30.0
8	4.0	75	120	33.3333
9	4.0	25	200	20.0
10	10.0	75	150	66.6667
11	8.0	120	200	40.0
12	1.8	200	300	6.0
13	20.0	75	300	66.6667
14	6.5	150	300	21.6667
15	2.0	200	600	3.3333
16	30.0	50	800	37.5
17	5.0	400	800	6.25
18	7.0	400	500	14.0
19	2.550	600	850	3.0
20	0.6	800	950	0.63158

Example 4. It presents a large-scale problem, which contains 20 processes. Table 8 shows the data for this example including all the minimum fresh water requirements of these processes without wastewater reuse. Fig. 11 shows the network system obtained using the algorithmic procedure. Tables 9A and 9B contain the network flowrates.

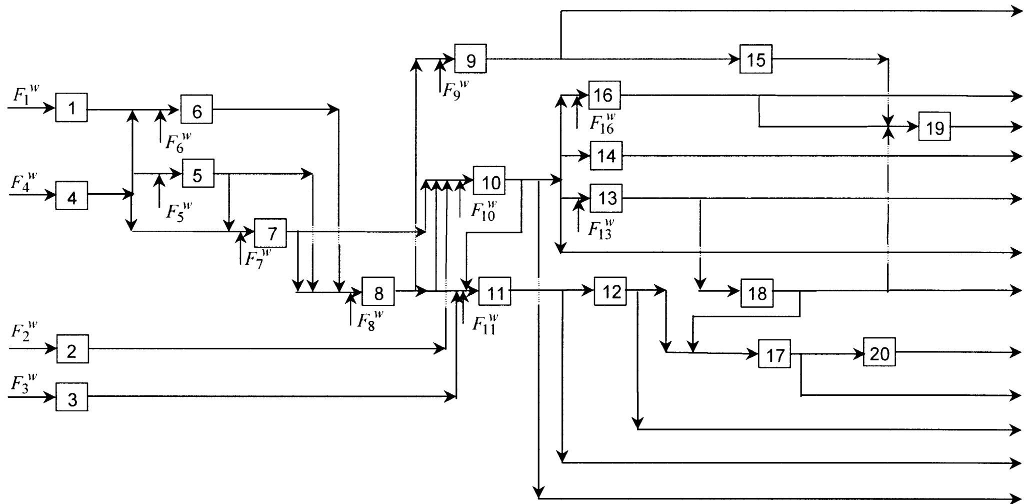

Fig. 11. Water network obtained using the maximum reuse algorithm in Example 4.

Table 9A
Processes 1–10 of Example 4

Process number	Type of process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum fresh water flowrate with reuse (ton/h)
1	H	0.0	0	80	12.5
2	H	0.0	0	100	20.0
3	H	0.0	0	120	16.667
4	H	0.0	0	80	25.0
5	I	$F_{4,5} = 13.846$	25	90	30.462
6	I	$F_{1,6} = 12.5$	40	90	15.0
		$F_{4,6} = 2.5$			
7	I	$F_{4,7} = 8.654$	50	100	25.705
		$F_{5,7} = 25.641$			
8	I	$F_{5,8} = 18.667$	75	120	17.356
		$F_{6,8} = 30.0$			
		$F_{7,8} = 22.867$			
9	I	$F_{8,9} = 4.762$	25	200	18.095
10	I	$F_{2,10} = 20.0$	75	150	40.478
		$F_{7,10} = 37.133$			
		$F_{8,10} = 35.722$			

Table 9B
Processes 11–20 of Example 4

Process number	Type of process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum fresh water flowrate with reuse (ton/h)
11	I	$F_{3,11} = 16.667$	120	200	6.986
		$F_{8,11} = 48.405$			
		$F_{10,11} = 27.943$			
12	I/WWU	$F_{11,12} = 18.0$	200	300	0.0
13	I	$F_{10,13} = 44.444$	75	300	44.444
14	T/WWU	$F_{10,14} = 43.333$	150	300	0.0
15	I/WWU	$F_{9,15} = 5.0$	200	600	0.0
16	I	$F_{10,16} = 13.333$	50	800	26.667
17	I/WWU	$F_{12,17} = 6.250$	400	800	0.0
		$F_{18,17} = 6.250$			
18	I/WWU	$F_{13,18} = 35.0$	300	500	0.0
19	T/WWU	$F_{15,19} = 5.0$	600	850	0.0
		$F_{16,19} = 1.733$			
		$F_{18,19} = 3.467$			
20	T/WWU	$F_{17,20} = 4.0$	800	950	0.0

The total fresh water that would be required if no reuse were done is 471.88158 ton/h. The minimum fresh water target found through the algorithmic procedure is 299.35873 ton/h, which means 36.6% water savings.

8. Conclusions

A new method to solve the water allocation problem in refineries and process plants has been presented. It has been shown through multiple examples that the procedure always provides the minimum fresh water target and a realizing network. The design can be performed totally by hand even for large-scale problems.

Notation

C	concentration of contaminant, ppm
F	water flowrate, ton/h
$\bar{F}$	water flowrate after a perturbation, ton/h

Subscripts

in	at inlet
out	at outlet
j	process j
P_j	precursors of j
R_j	receivers of j

Superscripts

min	minimum
max	maximum
*	additional sources
w	fresh water

Acknowledgements

This work was supported by EPA grant R825328-01-0.

References

Alva-Argáez, A., Kokossis, A. C., & Smith, R. (1998a). Automated design of industrial water networks. *A.I.Ch.E. Annual Meeting*, Miami, Paper 13f.

Alva-Argáez, A., Kokossis, A. C., & Smith, R. (1998b). Wastewater minimisation of industrial systems using and integrated approach. *Computers and Chemical Engineering*, *22*(Suppl.), S741–S744.

Alva-Argáez, A., Vallianatos, A., & Kokossis, A. C. (1999). A multicontaminant transshipment model for mass exchange networks and wastewater minimisation problems. *Computers and Chemical Engineering*, *23*, 1439–1453.

Carnes, B. A., Ford, D. L., & Brady, S. O. (1973). Treatment of refinery wastewaters for reuse. *National conference on complete water reuse*, Washington, DC.

El-Halwagi, M. M., & Manousiouthakis, V. (1989). Mass exchanger networks. *A.I.Ch.E. Journal*, *35*(8), 1233.

El-Halwagi, M. M., & Manousiouthakis, V. (1990). Automatic synthesis of mass exchanger networks with single component targets. *Chemical Engineering Science*, *45*(9), 2813.

Hospondarec, R. W., & Thompson, S. J. (1974). Oil-steam system for water reuse. *Proceeding of the Workshop*, *A.I.Ch.E.*, vol. 7.

Kuo, W. -C. J., & Smith, R. (1995). Designing for the interactions between water-use and effluent treatment. *Transactions of the Institute of Chemistry, Part A*, *76*, 287–301.

Mishra, P. N., Fan, L. T., & Erickson, L. E. (1975). Application of mathematical optimization techniques in computer aided design of wastewater treatment systems. *Water-1974 (II). A.I.Ch.E. Symposium Series*, vol. 71, p. 145.

Olesen, S. G., & Polley, G. T. (1997). A simple methodology for the design of water networks handling single contaminants. *Transactions of the Institution of Chemical Engineers, Part A*, *75*, 420–426.

Savelski, M. J., & Bagajewicz, M. J. (2000). On the optimality conditions of water utilization systems in process plants with single contaminants. *Chemical Engineering Science*. *55*(21), 5035–5048.

Savelski, M. J., & Bagajewicz, M. J. (1999a). A new algorithmic design procedure for the design of water utilization systems in refineries and process plants, *PRES'99*, Budapest, Hungary.

Savelski, M. J., & Bagajewicz, M. J. (1999b). On the use of linear models for the design of water utilization systems in refineries and process plants, Annual A.I.Ch.E. Meeting, Dallas, TX.

Savelski, M., Rivas, M., & Bagajewicz, M. (1999). A new approach to the design of water utilization systems with multiple contaminants in process plant. *Annual A.I.Ch.E. Meeting*, Dallas.

Skylov, V., Stenzel, R.A. (1974). Reuse of wastewaters-possibilities and problems, *Proceeding of the Workshop*, *A.I.Ch.E.*, vol. 7.

Takama, N., Kuriyama, T., Shiroko, K., Umeda, T. (1980). Optimal water allocation in a petroleum refinery. *Computers and Chemical Engineering*, *4*, 251–258.

Wang, Y. P., & Smith, R. (1994). Wastewater minimization. *Chemical Engineering Science*, *49*(7), 981.