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Design of water utilization systems in process plants with a single contaminant

Mariano Savelski [1], Miguel Bagajewicz *

University of Oklahoma, CEMS, 100 E. Boyd St., EC, T-335, Norman, OK 73019, USA

Abstract

This paper illustrates necessary conditions of optimality for single component water-using networks in process plants. These necessary conditions correspond to the optimal water allocation planning (WAP) problem that considers wastewater reuse on the basis of a single contaminant and where the objective is to minimize the total water intake. The conditions under which degenerate solutions are possible are also identified. Examples are discussed. A method that can be implemented by hand is also provided.

1. Introduction

The chemical and petrochemical industry makes an intensive usage of water. As a result, wastewater streams containing several contaminants (phenols, sulfides, ammonia, benzene, oil, etc.) create an environmental pollution problem. Water cleanup has been the object of several retrofit programs in industry, and several legislations exist that regulate and establish goals for these efforts (e.g. Clean Water Act in the USA).

For decades, the primary concern has always focused on end-of-pipe wastewater treatment. When pollutants are selectively removed during the process, the wastewater can be reused and/or recycled. 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 concept of reusing water started to be investigated systematically in the 1980s. This problem has received the name of Water/Wastewater Allocation Planning (WAP) problem. The search for optimal wastewater reuse solutions was addressed by industry itself more than 20 years ago [1–3]. Two major systematic strategies were developed: the use of superstructures coupled with mathematical programming and a graphic targeting procedure coupled with loop breaking.

Takama et al. [4] used mathematical programming to solve a refinery example. A superstructure of all water using operations and cleanup processes was set up and an optimization was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. Wang and Smith [5] presented a method based on targeting and a design procedure based on heuristics similar to those used in heat exchanger network design. The targeting part of this procedure is in reality an application of mass exchange technology [6, 7]. Since mixing of lean streams was not introduced in the original work of El-Halwagi and Manousiouthakis [6] or the few immediate follow-up papers, Wang and Smith [5] resorted to an ad-hoc design procedure based on the identified target. Despite these special approaches, the problem should be regarded as a mass exchanger network problem and not a separate area of research. Nevertheless, one cannot minimize the visionary work of Professor Umeda [4]. Olesen and Polley [8] recognized the difficulties of the design procedure proposed by Wang and Smith [5] and introduced a simplified design procedure for single contaminant. However, this approach cannot handle more than four or five operations as stated by the authors, mostly because it is based on a special ad-hoc inspection procedure. Kuo and Smith [9] proposed another graphical design method that slightly improves the matching techniques used by Wang and Smith [5] but left some unresolved issues that make its application somewhat uncertain even for a single contaminant.

On the other hand, superstructure models present serious numerical difficulties. Due to the nonlinear nature of the constraints the straight use of NLP packages to

* Corresponding author. Tel.: +1-405-325-5458; fax: +1-405-325-5813.

E-mail address: bagajewicz@ou.edu (M. Bagajewicz).

[1] Present address: Rowan University, Chemical Engineering Department, 328 Henry M. Rowan Hall, Glassboro, NJ 08028, USA.

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Nomenclature

C	concentration of contaminant (ppm)
f	component flowrate (g/h)
F	water flowrate (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

solve the problem often renders infeasible solutions. Doyle and Smith [10] proposed an iterative procedure to solve this bilinearly constrained problem. Alva-Argaez et al. [11] continued this line of work and proposed solving a two-phase procedure for the solution of a non-convex MINLP. Even after the problem has been successfully solved there is no guarantee about the optimality of the optimum. Finally, Huang et al. [12] also present a mathematical programming solution of the combined problem of water allocation and treatment.

In this paper, we present necessary conditions of optimality for the single-contaminant WAP problem. These conditions are used as part of a design procedure (WaterSave) for the WAP problem. The complete proof of the necessary conditions of optimality can be found elsewhere [13]. The globally optimal nature of the design procedure we present in this paper is substantiated by Savelski and Bagajewicz [14]. Finally, the necessary conditions of optimality have been used to discuss an MILP approach to solve the problem [15] and the combined water allocation and heat recovery problem [16,17]. In this paper, we only present a method to solve the single component problem using a method that can be applied by hand. This procedure can be used efficiently for single component problems such as the water management in the pulp and paper industry, the washing procedures in the semiconductor industry, and as long as the concentration of the contaminant is low, for any washing process even based on solvents other than water.

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.

Limits on inlet and an 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. Before we discuss our necessary conditions of optimality, some definitions that will be useful later are presented.

2.1. Definitions

The following types of water-using sets and processes can be defined:

- *Fresh Water User Processes* (FWU): these are processes that require fresh water. They may also be consumers of wastewater.
- *Wastewater User Processes* (WWU): these are processes that are fed solely by wastewater.
- *Head Processes* (H): this is a special case of a FWU that utilizes only fresh water.
- *Intermediate Wastewater User Processes* (I): these are processes that are fed by wastewater from other processes and feed other processes with the wastewater they produce.
- *Terminal Wastewater User Processes* (T): these are processes that are fed by wastewater from other processes, but they discharge their wastewater to treatment.
- *Set of Precursors of a Process j* (P_j): this is the set of all processes that send wastewater to process j.
- *Set of Receivers of Process j* (R_j): this is the set of all processes where wastewater from process j is sent.

Finally, the following definitions will help in the presentation of the necessary conditions.

- *Partial Wastewater Providers* (PWP): this is a process whose wastewater is partially reused by other processes, that is, a portion of its wastewater is sent directly to treatment.
- *Total Wastewater Providers* (TWP): this is a process whose wastewater is fully reused by other processes.

3. Necessary conditions of optimality

The necessary conditions of optimality are presented in a sequence of theorems. The proofs are given by Savelski and Bagajewicz [13].

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 $F_{j,\text{out}} \geqslant 0$, then $C_{j,\text{out}} \geqslant C_{\text{P}_j,j}$, where $C_{\text{P}_j,j}$ is the concentration of the combined wastewater of all the precursors. Fig. 1 presents the set of interconnections of interest, omitting other existing that are not of relevant to this case.

Corollary 1. *If for a given process j a solution is optimal and $C_{P_j,j} = C_{j,out}$, (monotonicity is not strictly satisfied, only weakly) then the solution is degenerated in the sense that any wastewater send to process j from its precursors does not alter the total water intake. In other words, the system's water intake is indifferent to such wastewater allocation.*

Corollary 2. *If a process is a TWP there exists at least one possible optimal solution that satisfies monotonicity.*

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 Partial Provider Head Process is equal to its maximum.

Corollary 1. *If a Head Process h is optimal and is a Total Wastewater Provider (i.e. $F_{h,out} = 0$), then any solution having $C_{h,out} \in \left[C_{R_h,in}, C_{h,out}^{\max}\right]$ is also optimal with the same fresh water intake.*

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.

Corollary 1. *If an Intermediate Process j is a Total Wastewater Provider, then any solution having $C_{j,out} \in \left[C_{R_j,in}, C_{j,out}^{\max}\right]$ is also optimal with the same fresh water intake.*

Corollary 2. *If $C_{P_j,j} \geqslant C_{j,in}^{\max}$, it is also a necessary condition of optimality that the Intermediate Process j reaches its inlet maximum concentration.*

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 Fresh Water user Process reaches its possible maximum.

Savelski and Bagajewicz [13] provide the proof of these necessary conditions.

4. Algorithmic design method

Based on the aforementioned optimality conditions a design method is proposed. A brief description of the new method follows:

- Step 1: Order the processes from the lowest to the highest maximum possible outlet concentration.
- Step 2: Provide fresh water to the first process of the list such that its maximum possible outlet concentration is reached. Repeat the procedure for all fresh water users.
- Step 3: Maximize the reusable wastewater from Step 2.
  — If the process is a freshwater user, use as much water of the least concentration possible. Dilute

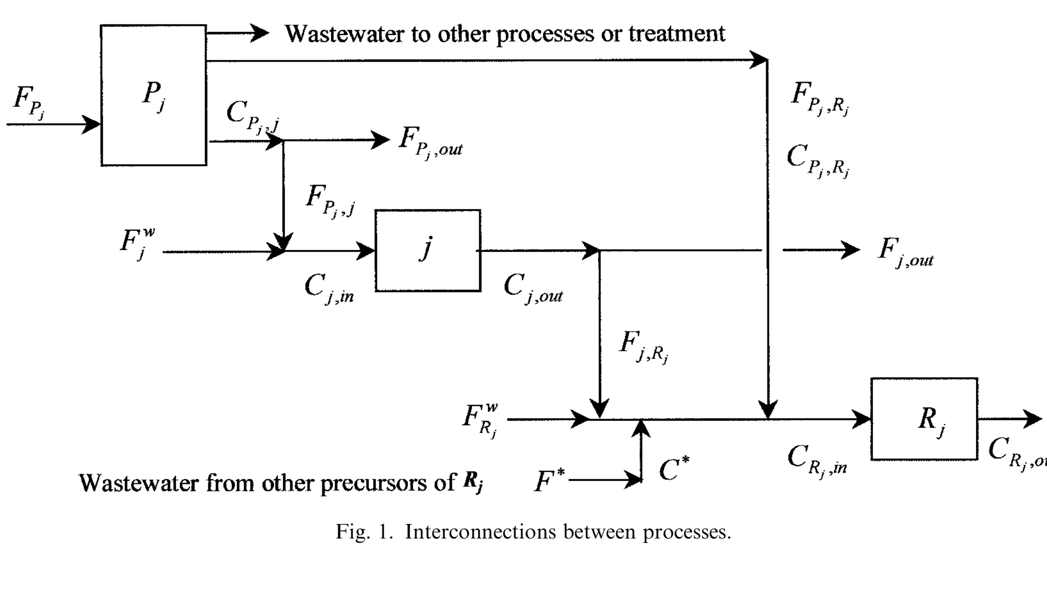

Fig. 1. Interconnections between processes.

with fresh water so that the maximum inlet concentration is not surpassed. Always assume the maximum outlet concentration is reached. This provides the balance equations to calculate the flowrates to use, that is

$$F_{1,n} = F_1, F_{2,n} = F_2, ..., = F_{s,n} \leqslant F_s, F_{s+1,n} = 0, \ldots, F_{n-1,n} = 0 \quad (1)$$

where the $F_{s,n}$ is obtained by setting the inlet concentration to process n to its maximum value. In the extreme case, all wastewater from all processes are sent to process n and the inlet concentration is lower than the maximum.

— If the process is a wastewater user (no fresh water is needed), use as much water of concentration close to the maximum inlet concentration as possible. Thus, water of the closest higher concentration than the maximum inlet should be diluted with water with the closest lower concentration than the maximum inlet. Such pairs should be picked until the maximum outlet concentration is reached. Fig. 2 illustrates one such generic combination. In this scheme, pseudo-fresh waters from process s ($s < k$) to process k are used to dilute wastewater from process $(k+1)$ to process t ($t > k$). Once the partial wastewater providers s and t are identified, the following flowrates are obtained, the rest being zero.

$$F_{j,n} = F_j, \forall j = (s+1), \ldots, (t-1), F_{s,n} < Fs, F_{t,n} < F_t \quad (2)$$

The flowrates $F_{s,n}$ and $F_{t,n}$ can be obtained by requesting that the inlet and outlet concentrations be at its maximum.

- Step 4: Repeat Step 3 until all processes have been taken care of.

More details of this procedure are given by Savelski and Bagajewicz [14], who also provide a proof that this procedure provides a globally optimal solution. This method can be used to solve any single component problem by hand, even without the use of a calculator. Similar steps but using inlet concentrations to sort the processes have been used by Liu [18] as unproven heuristics.

5. Examples

We now show some examples form the literature and some additional ones solved using the WaterSave method. We also illustrate the degeneracy covered by the corollaries of the theorems.

5.1. Example 1

This example is taken from Wang and Smith [5]. The system involves four processes and their corresponding data is given in Table 1. The minimum flowrate reported is 90.0 ton/h and two realizing network are presented in Wang and Smith [5]. Each network was obtained using a different method. The first method maximizes the concentration driving forces and the second one minimizes the number of water sources. It can be observed that, even after breaking the loops, the final designs may be of no practical use. The first method for instance, proposed a splitting of process three. If process three were an indivisible unit, such as a desalter or a reflux drum, the network would have no real meaning. However, the second method provides, after several simplifications, a realistic realizing network. Fig. 3 shows the final network obtained using method two [5].

According to our definitions, processes 1, 2 and 3 are FWU processes while process 4 is a WWU process. Processes 1 and 2 are head processes and process 3 is a terminal process. There are no intermediate processes in this network. The application of the design procedure is

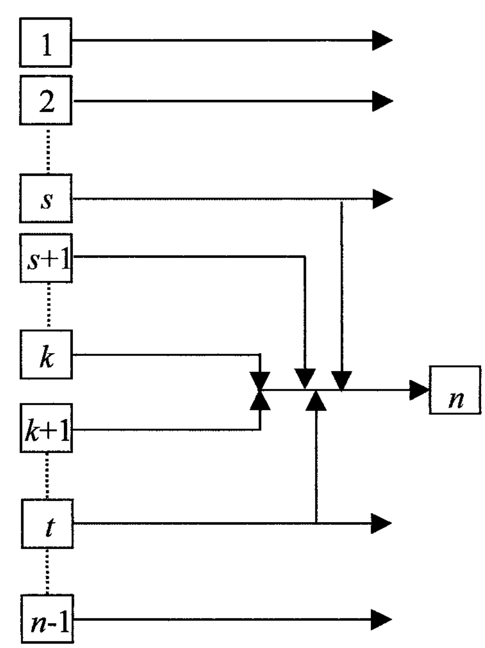

Fig. 2. Generic water allocation to a wastewater user.

Table 1
Example from Wang and Smith [5]

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

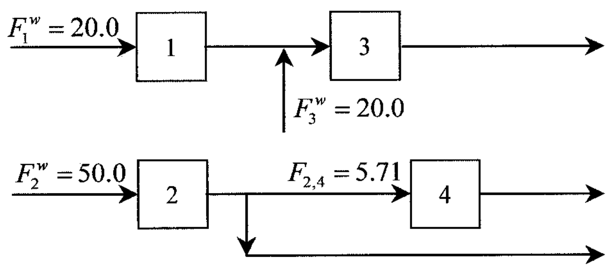

Fig. 3. Solution of Example 1 [5].

Table 2
Example from Olesen and Polley [8]

Process number	Mass load of contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	2.0	25	100
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

therefore straightforward. We allocate water to processes 1 and 2 directly. Next, wastewater from these processes can be sent to either process 3 or 4, alternatively (because they have the same outlet concentration). Finally, the usage of wastewater from process 3 to feed process 4, or vice versa, although possible, does not provide any savings.

5.2. Example 2

This example is taken from Olesen and Polley [8]. The system involves six processes and their corresponding data is given in Table 2. The minimum flowrate reported is 157.14 ton/h. Olesen and Polley [8] obtained a realizing network by methods of inspection. Fig. 4 shows this network. The target is met, so the solution is optimal but constitutes a degenerate alternative of the solution network depicted in Fig. 5, which is obtained using WaterSave, satisfies all necessary conditions of optimality and meets the 157.14 ton/h target.

Table 3 shows the results for the network obtained using WaterSave. All processes have reached both maximum inlet and outlet concentration through maximum reuse. All the necessary conditions of optimality are satisfied by this solution.

6. Multicomponent systems

Necessary conditions of optimality for multicomponent systems have been presented recently [19]. The necessary conditions of maximum outlet concentration hold for at least one component. The monotonicity holds only for

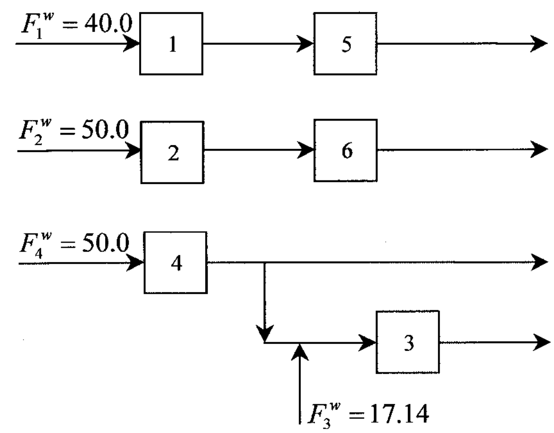

Fig. 4. Solution of Example 2 [8].

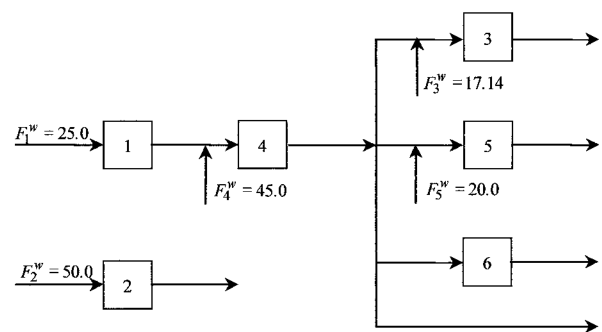

Fig. 5. Solution of Example 2 (Watersave).

Table 3
Solution of Example 2 corresponding to Fig. 5

Process number	Type of process	Fresh water intake (ton/h)	Wastewater reuse (ton/h)	C_{in} (ppm)	C_{out} (ppm)
1	H	25.0	0.0	0	80
2	H	50.0	0.0	0	100
3	T	17.14	5.714	25	200
4	I	45.0	25.0	28.57	100
5	T	20.0	20.0	50	800
6	WWU	0.0	5.714	100	800
Total flowrate (ton/h)		157.14	56.428		

special components called "key" components. A method to design multicomponent systems has also been developed [20] and capital as well as retrofit considerations are discussed in Bagajewicz et al. [21].

7. Conclusions

Necessary conditions of optimality in water allocation problems have been presented. These conditions state that optimal structures satisfy monotonicity of the outlet concentrations when one process sends its wastewater to another. In addition, conditions under which the inlet or the outlet concentrations reach their maximum have been discussed. Finally, a new design methodology has been introduced and the results of a literature example problem, solved using WaterSave, depicted. Extensions to multicomponent problems have been produced.

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