# A RAPID DESIGN METHOD FOR WATER-USING SYSTEM WITH MULTIPLE CONTAMINANTS

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## Abstract

In this paper, a rapid design method for water-using system with multiple contaminants is developed. It uses a combination of linear programming and necessary conditions of optimality to generate the optimal or sub-optimal solution. The new method consists of five steps and the main steps are that water-using processes are arranged according to their maximum outlet concentration and a list is formed; for each process on the list, linear programming model is used to determine its freshwater consumption and wastewater usage from its precursors, and then it is deleted from the list and the remaining problem is updated; repeat previous step until there is no process on the list. The new method has been illustrated by two cases; the obtained solutions are optimal or near optimal.

# Keywords

Water-using system, Design, Multiple contaminants, Linear programming.

# Introduction

Water has been used in abundant quantities by chemical, petrochemical, petroleum refining and other processes. In recent years, fresh water scarcity and stricter environmental regulation on industrial effluents force people to find ways for freshwater minimization, which corresponds to wastewater minimization. Wastewater reuse is an effective way for freshwater minimization when we exclude the possibility of making fundamental changes to processes to reduce their inherent demand for water, for example, air cooler substitutes for water cooler.

In 1980, Takama et al (1980) addressed an approach for optimal water allocation in petroleum refinery based on superstructure. Wang and Smith (1994) proposed the concept of "water pinch", which originated from mass integration (El-Halwagi and Manousiouthakis, 1989). "Water Pinch" is very helpful to understand characters of water-using network. At present, the necessary condition of optimality proposed by Bagajewicz and Savelski (2000,2004) is another important tool to understand and design water-using network. Up to now, water-using network with single contaminant can be optimized routinely and there are several methods available to be chosen; as far as water-using network with multiple contaminants is concerned, available design methods have some defects due to its intrinsic complexity. For example, superstructure model needs too much computing time to find a feasible solution and initial values of variables are difficult to be found; concentration shifts (Wang and Smith, 1994) are required when pinch method is adopted, which are tedious for multiple contaminants; tree search has been proposed to find the global optimal solution, which is in fact an effective enumeration method.

In this paper, linear programming step by step borrowed from Hu et al (2002) and the arranging process for water-using processes with multiple contaminants learned from Wang et al (2003) are combined together to form a rapid design method used for water-using system with multiple contaminants. In general, the global optimality is not guaranteed by the new method, but it is simple and practical.

## **Definitions and Necessary Conditions of Optimality**

*Partial Wastewater Provider (PWP):* this is a process whose wastewater is partially reused by other process, that means, a portion of its wastewater is sent directly to treatment;

Set of Precursors of process j: this is the set of all processes that send wastewater to process j;

#### Necessary conditions of Optimality:

If a solution to water-using network is optimal, then at every partial wastewater provider (PWP), the outlet concentration of a key component is not lower than the concentration of the same key component in the combined wastewater stream coming from all the precursors.

The key component is defined as:

$$\mathbf{G}_{j,s}^{W} = \mathbf{L}_{j,s} / \mathbf{C}_{\text{out},j,s}^{\text{max}} \tag{1}$$

In which  $G_{j,s}^{w}$  is the minimum freshwater consumption for process j based on Contaminant s;  $C_{out,j,s}^{max}$  is the maximum outlet concentration of process j for contaminant s;  $L_{j,s}$  is the contaminant mass to be removed.

The maximum  $G_{j,s}^{w}$  of process j is the basic freshwater consumption and the corresponding component is key component. The aim of wastewater reuse is to reduce freshwater consumption below to its basic freshwater consumption

It should be pointed out that the key contaminant (constrains the freshwater consumption) of each process is different and related to the water source to the process and sometimes there is more than one key component. In our design procedure, the wastewater stream in which all contaminant concentrations are not satisfied with increasing monotonicity is excluded from the precursor set of process j.

### **Design procedures**

A design method composed of five steps is addressed below:

Step 1: Calculate the basic freshwater consumption required by each process.

Step 2: Arrange water-using processes according to their maximum outlet concentration.

List the maximum outlet concentration of each concentration for each process, and mark their serial number by  $n_{j,s}$  (j represents the water-using process, and s the contaminant). Calculate the product of serial number of every contaminant in each process by Eq. (2) and list those processes by ascending product.

$$R_{j} = \prod_{s} n_{j,s} \quad j = 1, ..., M; s = 1, ..., S$$
(2)

Step 3: Provide the first process on the list and those processes which maximum inlet concentration is 0 at least for one contaminant with their basic freshwater consumption. Delete those processes whose requirements have been satisfied from the list and add their wastewater data to the available wastewater set.

Step 4: Maximize wastewater reuse to the first process on the list. There are three cases to be considered:

Case A: if the process is a freshwater user (judged by the contaminant concentration of available wastewater and the maximum inlet concentration of the process), determine the precursor set by necessary conditions of optimality and set up a linear programming model by GAMS language to minimize freshwater consumption of the process;

Case B: if the process is a full wastewater user (no freshwater is needed), use as much wastewater of concentration close to the maximum inlet concentration as possible.

Case C: if it is hard to judge whether the process is a full wastewater user, prepare the data for the precursor set and adopt the model developed for Case A to determine the reuse usage from its precursor and the requirement of freshwater.

Delete the process from the list after its requirement is satisfied and add its wastewater data to the available wastewater set.

Step 5: Update the remaining problem and repeat Step 4 until no process is on the remaining list.

#### Linear programming model

For each FWU, a linear programming model is built to minimize its freshwater consumption and determine reuse usage from its precursor set, the model can be defined below.

Min 
$$F_i^w$$

Subject to: (i) maximum inlet concentration:

$$\sum_{i \in P_j} F_{i,j} C_{out,i,s} \leq (F_j^w + \sum_{i \in P_j} F_{i,j}) C_{in,j,s}^{\max}$$

$$j=1,...M; s=1, ..., S$$
 (3)  
(ii) maximum outlet concentration:

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$$\sum_{i \in P_j} F_{i,j} C_{out,i,s} + L_{j,s} \le (F_j^w + \sum_{i \in P_j} F_{i,j}) C_{out,j,s}^{\max}$$

$$j=1,...M; s=1,..., S$$
 (4)

(iii) maximum flowrate of precursor set of process j:

$$0 \le F_{i,j} \le F_i \quad i \in P_j \tag{5}$$

(iv) freshwater consumption constraint

$$F_j^w \ge 0 \tag{6}$$

# Illustration

## Case 1

Wang and Smith (1994) first addressed Case 1, and Savelski et al (1999) and Wang et al (2003) redesigned it. The reported global optimal solution found by tree search method is 105.60t/hr of freshwater consumption. Given data is provided in Table 1, it includes three contaminants and three water-using processes. The network connection characterized by minimum freshwater consumption is required to design.

 $C_{in}^{\max}$  $C_{out}^{\max}$ F<sup>lim</sup> (t/hr) Contaminant Process 0 15 45 1 1 2 0 400 3 0 35 2 1 20 120 34

300

45

120

20

200

12500

56

180

220

45

9500

Table 1 Specification for Case 1

Now, we design Case 1 according to the proposed steps.

Step 1: use following equation to calculate basic freshwater consumption.

$$F_j^B = \max G_{j,s}^w = \max \frac{L_{j,s}}{C_{out,j,s}^{\max}}$$
$$= \max \frac{F_j^{\lim}(C_{out,j,s}^{\max} - C_{in,j,s}^{\max})}{C_{out,j,s}^{\max}}$$

2

3

1

2

3

3

The values for these processes are 45, 33.18 and 54.82t/hr separately;

Step 2: For contaminant 1, the outlet concentration of Process 1, 2 and 3 are 15, 120 and 220ppm, and the serial number is 1, 2 and 3. The serial number for contaminant 2 and 3 are listed in Table 2. Calculate the product of serial

number of every contaminant in each process by Eq. 2 and list these processes according to its  $R_j$ . The list result is also shown in Table 2.

Table 2 Data for ordering processes of Case 1

| Process                   |   | ] | 1 |   | 2  | 2 |   |   | 3 |
|---------------------------|---|---|---|---|----|---|---|---|---|
| Contaminant               | 1 | 2 | 3 | 1 | 2  | 3 | 1 | 2 | 3 |
| $n_{j,s}$                 | 1 | 2 | 1 | 2 | 3  | 2 | 3 | 1 | 3 |
| $\mathbf{R}_{\mathbf{j}}$ |   | 2 |   |   | 12 |   |   | 9 |   |
| Order <sub>j</sub>        |   | 1 |   |   | 3  |   |   | 2 |   |

Step 3: because the maximum inlet concentration of Process 1 is zero for all contaminants, freshwater is supplied by basic freshwater consumption of 45t/hr. The concentration of produced wastewater is [15, 400, 35] ppm. Delete Process 1 from the list and add the wastewater stream to available wastewater set.

Step 4: maximize wastewater reuse to the first process on the list. Now, Process 3 is the first process. Comparing maximum outlet concentration of process 3 with the concentration of available wastewater (vector comparison), we can not exclude available wastewater from the precursor set of Process 3; comparing the maximum inlet concentration of Process 3 with the concentration in the precursor set, we find that Process 3 is a Freshwater User. Use the linear programming model to minimize freshwater consumption of process 3, the optimal solution is 52.162t/hr and reuse usage is 2.668t/hr. The wastewater concentration produced by Process 3 is [102.862, 45, 9500] ppm. The key components are Contaminant 2 and 3. They constrain the minimum freshwater consumption simultaneously, not just Contaminant 3 which constrains the basic freshwater consumption of Process 3. Delete Process 3 from the list and update the remaining problem. The available wastewater flowrate of Process 1 becomes:



Figure 1 The Network for Case 1

42-2.668=43.332t/hr

Step 5: only Process 2 is on the list. Similar to Process 3, Process 2 is also a Freshwater User. Using the linear model to find the freshwater consumption is 8.440t/hr, the reuse usages from its precursor set (including Process 1 and 3) are 25.492 and 0.069 t/hr respectively. The key components are Contaminant 2 and 3.

The condition to end design procedure is satisfied. The obtained solution is show in Fig. 1. The solution is as good as reported one. Comparing the freshwater consumption of each process with its basic freshwater consumption in the solution, we find that the former is not higher than the later for each process, which conforms to our expectation.

# Case 2

Case 2 comes from Wang et al (2003), involves seven water-using processes, three kinds of contaminants. Given data is shown in Table 3, the global optimal solution obtained by reference 9 is 139.3 t/hr of freshwater consumption.

Following Step 1 to 5, we obtain a solution, which freshwater consumption is 140.93t/hr and is higher than the reported optimal solution only by 1.2 percent.

| Process | Contaminant | $C_{in}^{\max}$ | $C_{out}^{\max}$ | F <sup>lim</sup> (t/h) |
|---------|-------------|-----------------|------------------|------------------------|
| 1       | 1           | 0               | 50               | 25                     |
|         | 2           | 0               | 100              |                        |
|         | 3           | 0               | 50               |                        |
| 2       | 1           | 0               | 100              | 70                     |
|         | 2           | 0               | 300              |                        |
|         | 3           | 0               | 600              |                        |
| 3       | 1           | 20              | 150              | 35                     |
|         | 2           | 50              | 400              |                        |
|         | 3           | 50              | 800              |                        |
| 4       | 1           | 50              | 600              | 40                     |
|         | 2           | 110             | 450              |                        |
|         | 3           | 200             | 700              |                        |
| 5       | 1           | 20              | 500              | 8                      |
|         | 2           | 100             | 650              |                        |
|         | 3           | 200             | 400              |                        |
| 6       | 1           | 500             | 1100             | 50                     |
|         | 2           | 300             | 3500             |                        |
|         | 3           | 600             | 2500             |                        |
| 7       | 1           | 150             | 900              | 30                     |
|         | 2           | 700             | 4500             |                        |
|         | 3           | 800             | 3000             |                        |

Table 3 Specification for Case 2

## Conclusions

A method composed of five steps is proposed to rapidly design water-using system with multiple contaminants. It first arranges water-using processes based on their maximum outlet concentration, and then a linear programming model is used to determine the freshwater consumption and reuse usages for each process. The linear programming model is built by GAMS language, which has the character that a model is independent of the data it uses. Two cases are used to illustrate the new method.

## Nomenclature

## Letters

c=concentration, ppm F, G=Flowrate, t/hr L=contaminant mass, g/hr M=the total number of processes P=precursor set S=the total number of contaminants Superscript **B**=Basic max=maximum w=freshwater **Subscripts** i=Process i in precursor set in=inlet j=process j out=outlet s=the serial number of contaminant

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