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Optimization of Water Consumption in Industrial Systems Using Linear and Nonlinear Programming

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Abstract: The awareness of the danger to the environment resulting from the over extraction and stricter discharge regulations, has caused the price of freshwater and waste treatment facilities to rise. Therefore, there is a growing interest in the process industries to reduce both freshwater consumption and wastewater production. Water minimization techniques can effectively reduce overall fresh water demand and the overall effluent generated as well as lower costs of fresh water and effluent treatment costs. In the context of the paper two different situations are considered, re-use and regeneration re-use. The optimization model is formulated for single and multiple contaminant(s) system in the class of Linear Programming (LP) and Nonlinear Programming (NLP), respectively. For this a superstructure that entails all possible recycle and reuse possibilities is used as the basis for the formulation. After that GUI was created for input data and showing results of optimization. With this results water network can be designed among water using operations. The proposed method was compared with several literature examples for validity. Results showed that this program can find the same or better results in some test problems.

Key words: Wastewater minimization, reuse regeneration, recycle, network design

INTRODUCTION

Process plants such as petrochemical, petroleum refining, pulp and paper, etc. consume water in large amounts. After utilizing the water, the processes generate wastewater which may contain several contaminants. Many industrial users of fresh water are under increasing pressure to reuse water within their facilities. Their goal is to minimize the amount of water that is discharged, either to a receiving stream or a publicly owned treatment works. There are a variety of reasons for this pressure such as: the cost of fresh water; the cost of additional treatment to reach discharge limits; water availability and environmental awareness and community relations. Before treating the wastewater, it is better to minimize the quantity of wastewater that appears during the process. If the quantity of wastewater was minimized, the freshwater consumption would be reduced and at the same time, capacity of the wastewater treatment system would be increased. The optimum water usage network leads to a minimum freshwater consumption and wastewater treatment. As presented by Wang and Smith (1994, 1995) the wastewater quantity can be reduced by the followings:

Reuse: Wastewater can be re-used directly in other operations. This might require wastewater being blended with wastewater from other operations and/or freshwater.

Regeneration reuse: When the wastewater is refined and reused in another operation or process. It will also be frequently mixed with wastewater from other operations or freshwater.

Regeneration-recycling: In this case water can re-enter processes in which it has previously been used.

Process changes: Process changes reduce the inherent demand for water, for example, using air coolers instead of cooling towers.

Several studies have been reported showing the application of these approaches. Wang and Smith have developed a new approach for wastewater minimization using water pinch technology (Wang and Smith, 1994, 1995). Water pinch analysis embedded in wastewater minimization techniques offers simple methods and beneficial results when applied to water using industries. This approach is based on the use of a limiting water

profile that identifies the maximum inlet and outlet concentrations of pollutants in water being used in the process. These inlet and outlet concentrations limits, account for corrosion, fouling, maximum solubility, etc. Note that this method is based upon a plot of contaminant concentration vs. mass load. Although this approach has been a major step in understanding water system design, it has several limitations. Especially for multiple contaminants, the graphical approach is difficult to extend and has several drawbacks. Methods provided later for wastewater minimization were basically integration techniques. These techniques can include graphical approaches (Crittenden, 2001; Mann and Liu, 1999; Wang and Smith 1995; Tainsh and Rudman, 1999; El-Halwagi, 1997; Hallale and Frase, 2000) and mathematical programming (Bagajewicz, 2000; Bagajewicz *et al.*, 2000; Prakotpol and Srinophakun, 2004; Doyle and Smith, 1997; Rossiter and Nath, 1995; Savelski and Bagajewicz, 2003; El-Halwagi and Spriggs, 1995). Each method varies significantly in scope and approach. Mathematical optimization is the most suitable approach for wastewater minimization, for both new and retrofit applications. Bagajewicz (2000) presented a review of the mathematical programming procedures for designing and retrofitting water networks, with an emphasis on refinery processes. They concluded that mathematical programming can efficiently produce globally optimal and sub-optimal solutions if conceptual insights are made to properly build the models.

In the present study, we used a mathematical approach to minimization of water consumption. The main goal was to reduce the flow rate of technological wastewater with wastewater reuse or regeneration-reuse; the freshwater consumption would consequently be reduced.

Mass transfer operations: 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 (Savelski and Bagajewicz, 2003). We begin by defining the system as a mass transfer problem in which the contaminant is transferred from a contaminant rich process stream to a water stream. The process contains a certain amount of water to reduce fixed content of contaminant. This water is considered as a contaminant-rich stream. It transfers some contaminants to a contaminant-lean stream (water). The contaminants may correspond to the Total Suspended Solids (TSS), Total

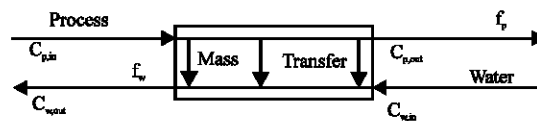


Fig. 1: Countercurrent contact between a contaminant-rich process stream and a contaminant-lean water stream (Mann and Liu, 1999)

Dissolved Solids (TDS), Total Organic Carbon (TOC) and the Biochemical Oxygen Demand (BOD) or similar quantities whose concentration levels limit the reuse of the effluent water in the other operations (Bagajewicz, 2000). The water using operation represented by the mass transfer of these two streams is shown in Fig. 1.

Each rich stream (process stream) has a mass flowrate f_p and has to be brought from a supply composition C_p^{in} to a target composition C_p^{out} . Therefore, each lean stream (water) will have a mass flowrate f_w an initial composition C_w^{in} and a final composition C_w^{out} . From Fig. 1 the mass to be transferred in this unit, Δm , can be determined by establishing a mass balance on the solute:

$$\Delta m = f_p (C_p^{in} - C_p^{out}) = f_w (C_w^{out} - C_w^{in}). \quad (1)$$

From Fig.1, the contaminant concentration of the water inlet and outlet is limited by the concentration at the outlet and inlet of the rich stream, respectively. The lean stream (water) entering any unit operation must have a lower contaminant concentration than the concentration of the rich stream outlet and the wastewater leaving must have a lower concentration than the concentration of the rich stream inlet.

Problem statement: The design of a water system involves a number of freshwater sources available to satisfy the demands of each water-using operation, both in terms of volume and concentration level of certain contaminants. A water treatment operation is available to reduce the freshwater consumption in the site and/or to achieve the environmental limits imposed on the wastewater discharge. The design task is to find the network configuration that will minimize the wastewater generation (and thus minimize demand for freshwater).

The method addressed in this study to design water system can be stated as follows. For each water using operation, given:

The contaminant mass load: The maximum inlet and outlet concentrations, determine the minimum amount of wastewater that can be achieved through the exploitation of reuse and recycle opportunities.

A set of contaminants to be analyzed which may be present in the freshwater sources and/or picked up in the water-using operations.

The operations set are then separated in two subsets: A subset of water-using operations, each one described by its limiting water profile for each contaminant in terms of its maximum inlet concentration, its maximum outlet concentration and either the mass load of contaminant to be transferred, or the limiting flow rate for the operation.

A subset of water treatment operations, its performance for the removal of contaminants specified as a removal ratio.

The following assumptions are made

- All data for the limiting water profiles is available and certain.
- The number of water using and water treatment operations is fixed.
- Mass flow rate of each stream remains essentially unchanged as it passes through the network.
- In single contaminant system the outlet concentration of any unit operation is equal to the limiting outlet concentration in order to maximize water reuse.

Modeling the wastewater network

Single contaminant-Water reuse/recycle model: The design of a water network for wastewater minimization can be described with reference to a set of water-using operations I . $I = \{i | i = 1, 2, \dots, n\}$.

n is the total number of operations in the system. Each user is assigned water demands of different quantity and quality. General schematic diagram of a water-using operation is shown in Fig. 2. This water-using operation receives freshwater in addition to recycled water streams from other units.

In this kind of problem, all of the decision variables can be divided into three groups:

- Freshwater flowrate (F_i);
- Wastewater flowrate (W_i);
- Reused water flowrate ($F_{i,j}$).

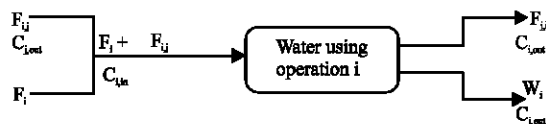


Fig. 2: Superstructure model of any operation of water reuse

The possible number of freshwater and wastewater stream is equal to the number of unit operation. So, there are $2n$ variables which represent the flowrate of these streams. They are: $F = [F_1, F_2, \dots, F_n]$ and $W = [W_1, W_2, \dots, W_n]$.

Also there are $n^2 - n$ variables that represent the flowrates of reused stream. All of the possible reused streams from any operations to the others can be represented by this matrix:

$$F = \begin{bmatrix} 0 & F_{1,2} & F_{1,3} & \dots & F_{1,n} \\ F_{2,1} & 0 & F_{2,3} & \dots & F_{2,n} \\ F_{3,1} & F_{3,2} & 0 & \dots & F_{3,n} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ F_{n,1} & F_{n,2} & F_{n,3} & \dots & 0 \end{bmatrix}$$

The objective function for the problem can be defined as below:

$$\text{Objective function} = \min \sum_i F_i \quad (2)$$

The objective function expressed by Eq. 2 is subject to the following constraints:

Inlet and outlet set of constraints: To maximize water reuse, the inlet and outlet concentrations of contaminants from a water-using unit are forced to be equal to a limiting inlet and outlet concentrations. These limiting concentrations may be specified based on a number of considerations, such as solubility limits, operating conditions, in addition to regeneration and process design limits. Hence, the maximum inlet and outlet concentration of contaminants will be forced to be equal to pre-specified limit $C_{i,in}^{\max}$ and $C_{i,out}^{\max}$, respectively ($C_{i,in} = C_{i,in}^{\max}$, $C_{i,out} = C_{i,out}^{\max}$).

$$C_{i,in} = \frac{\sum_{j \neq i} F_{i,j} C_{j,out}}{\sum_{j \neq i} F_{i,j} + F_i} \leq C_{i,in}^{\max} \Rightarrow \sum_{j \neq i} F_{i,j} C_{j,out} - (\sum_{j \neq i} F_{i,j} + F_i) C_{i,in}^{\max} \leq 0 \quad (3)$$

$$C_{i,out} = \frac{(\sum_{j \neq i} F_{i,j} + F_i) C_{i,in} + \Delta m_i}{\sum_{j \neq i} F_{j,i} + W_i} \leq C_{i,out}^{\max} \Rightarrow (\sum_{j \neq i} F_{i,j} + F_i) C_{i,in} + \Delta m_i - (\sum_{j \neq i} F_{j,i} + W_i) C_{i,out}^{\max} \leq 0 \quad (4)$$

Total mass balance: The water mass balance around each unit operation i in Fig. 2 is:

$$F_i + \sum_{j \neq i} F_{i,j} - W_i - \sum_{j \neq i} F_{j,i} = 0 \quad (5)$$

Partial mass balance, for the contaminant: The contaminant mass balance around each operation can be formulated as follows:

$$\sum C_{j,out} F_{i,j} + \Delta m_i - C_{i,out} (W_i + \sum F_{j,i}) = 0 \quad (6)$$

All concentrations and flow rates are positive:

$$F_i, F_{i,j}, F_{j,i}, W_i, C_{i,in}, C_{i,out} \geq 0 \quad \forall i, j \in n \quad (7)$$

Finally a Linear Programming (LP) based on Eq. 3-7 is formulated to minimization of wastewater generation and fresh water consumption.

Single contaminant-water regeneration/recycle model:

Water consumption can be further reduced if we allow intermediate regeneration. Many different types of process can be used to regenerate wastewater, for example gravity settling, filtration, membranes, activated carbon, biological treatment, etc. The superstructure model with the regeneration process included can be shown in Fig. 3. According to Fig. 3 $F_{r,i}$ and $F_{i,r}$ are streams to and from a regeneration process. The outlet contaminant concentration of regeneration process is C_r .

When regeneration process is included, there are $2n$ variables more than water reuse without regeneration. These adding variables are the flowrate of regenerated water to each operation and wastewater from each operation to regeneration process. These decision variables can be represented by the matrix:

$$FR = \begin{bmatrix} FR_{1,r} & FR_{r,1} \\ FR_{2,r} & FR_{r,2} \\ \vdots & \vdots \\ FR_{n,r} & FR_{r,n} \end{bmatrix}$$

Although there are $2n$ variables more, there is only one constraint excesses. It is the mass balance around regeneration process:

$$\sum_i FR_{i,r} = \sum_i FR_{r,i} \quad (\text{Number of } i \text{ equal to number of unit operation}) \quad (8)$$

According to Fig. 3 Eq. 3-7 can be modified to develop constraints on the contaminant concentration at

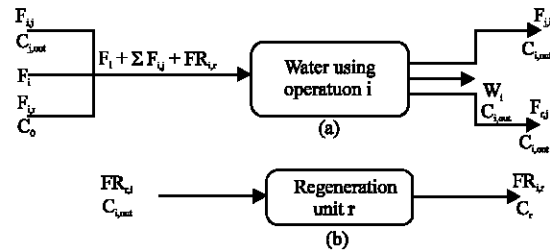


Fig. 3: Superstructure model when a regeneration process included

the inlet and outlet of each operation as well as mass balance on water across each operation:

$$\sum_{j \neq i} F_{i,j} C_{j,out} + FR_{i,r} C_r - (\sum_{j \neq i} F_{i,j} + F_i + FR_{i,r}) C_{i,in}^{max} \leq 0 \quad (9)$$

$$\begin{aligned} & (\sum_{j \neq i} F_{i,j} + F_i + FR_{i,r}) C_{i,in} + \Delta m_i - \\ & (\sum_{j \neq i} F_{j,i} + W_i + FR_{r,i}) C_{i,out}^{max} \leq 0 \end{aligned} \quad (10)$$

$$F_i + \sum_{j \neq i} F_{i,j} + FR_{i,r} - W_i - \sum_{j \neq i} F_{j,i} - FR_{r,i} = 0 \quad (11)$$

$$\begin{aligned} & \sum C_{j,out} F_{i,j} + FR_{i,r} C_r + \Delta m_i - C_{i,out} \\ & (W_i + \sum F_{j,i} + FR_{r,i}) = 0 \end{aligned} \quad (12)$$

$$\begin{aligned} & F_i, F_{i,j}, F_{j,i}, FR_{i,r}, FR_{r,i}, W_i, C_{i,in}, \\ & C_{i,out}, C_r \geq 0 \quad \forall i, j \in n \end{aligned} \quad (13)$$

The Linear Programming (LP) to optimize the water network including the regeneration process is to minimize Eq. 2 subject to Eq. 8-13.

Multi-contaminant formulation: In the multiple contaminants system, formulation of wastewater minimization is similar to single contaminant system and only contaminant balance and constraints from maximum inlet and outlet concentrations have to be modified for each type of contaminant. From water pinch analysis we know that for all water-using operations, in the optimal solution, at least one of the contaminants will reach its maximum permissible value (Doyle and Smith, 1997). With this information the contaminant k balance around operation i is:

$$\sum C_{j,k,out} F_{i,j} + \Delta m_{i,k} - C_{i,k,out} (W_i + \sum F_{j,i}) = 0 \quad (14)$$

Also, the constraints from the maximum inlet and outlet concentration of contaminant k to operation i are:

$$\sum_{j \neq i} F_{i,j} C_{j,k,out} - (\sum_{i \neq j} F_{i,j} + F_i) C_{i,k,in}^{\max} \leq 0 \quad (15)$$

$$(\sum_{j \neq i} F_{i,j} + F_i) C_{i,k,in} + \Delta m_{i,k} - (\sum_{i \neq j} F_{j,i} + W_i) C_{i,k,out}^{\max} \leq 0 \quad (16)$$

For the multiple contaminants system, the outlet concentration of each contaminant from any operations can not be fixed. Since, they are unknown. Then Eq. 14-16 form nonlinear constraints. Therefore, the nonlinear programming is used to minimize Eq. 2 subject to Eq. 14-16.

Optimization software and Graphic User Interface (GUI): The mathematical formulation of the single contaminant and multiple contaminants systems are LP and NLP, respectively. Theses LP and NLP models are then solved

using available methods or software. In this study Lingo software was used for optimization and a graphic user interface was built in order to make the program easy and convenient. The user just inputs the limiting process data (maximum inlet and outlet concentrations and mass transfer) into the blank form of GUI and the program will formulate the optimization model and solve for the solution automatically. Then the optimum results are returned to the user for design water network. Figure 4 shows GUI for input the process data.

Literature example and computational results: Several problems are used to validate this program. The data for the literature example (Prakotpol and Srinophakun, 2004) is shown in Fig. 4 (GUI). The literature example involves

Operation	Mass transfer [kg/h]	Max.inlet.Co [ppm]	Max.outlet.Co [ppm]
1	6.25	0	250
2	15	50	300
3	7.5	150	400
4	14	300	500

Fig. 4: Graphic user interface for input data

Operation	Fresh water	Wastewater	Water Reuse		
1	25	0	X12 = 0	X13 = 0	X14 = 0
2	49.37	0	X21 = 3.75	X23 = 0	X24 = 0
3	15	19.375	X31 = 0	X32 = 15	X34 = 0
4	0	70	X41 = 21.25	X42 = 38.12	X43 = 10.63

Fig. 5: Results of single contaminant-water reuse

four water using operations for which the limiting concentrations and water quantities are specified. For this example the model was solved within 2 CPU seconds in a 1.82-GHz, Pentium processor. The results from Lingo software based LP is shown in Fig. 5. These results are used to construct the optimum water-using network and compared to the results from (Castro *et al.*, 1999), as shown in Fig. 6.

Limiting process data of another example problem are shown in GUI in Fig. 7. Here we assume a regeneration unit that enable to reduce contaminant concentration to 25 ppm. The optimum water using networks that are

constructed from the results of LP solution and Pinch technology (Mann and Liu, 1999) are shown in Fig. 8.

As shown as in Fig.6 and Fig.8 the minimum fresh water consumption and minimum wastewater generated are the same at 89.375 and 30 ton hr⁻¹, respectively. However, there are some differences in parts of streams and configurations. The designer should decide which configuration is better based on capital cost investment such as piping and operating cost. This program was tested on other literature examples for multiple contaminants system. Results were similar but as same as single contaminant problems sometimes configurations of networks were different.

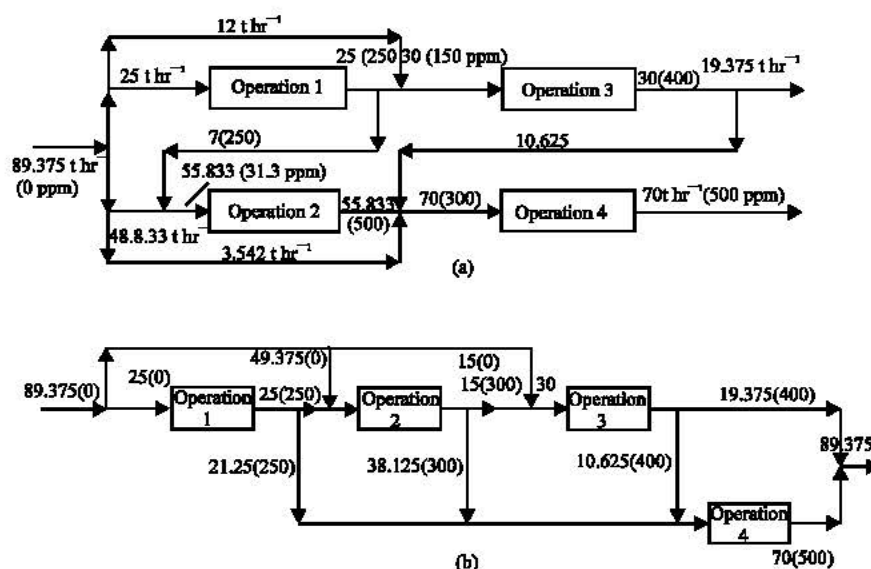


Fig. 6: Design network based (a) literature (Castro *et al.*, 1999) and (b) results from LP

Operation	Mass transfer [kg/h]	Max. inlet Cc [ppm]	Max. outlet C [ppm]
1	3	0	100
2	1.75	75	100
3	3	50	150

Fig. 7: Limiting process data for a single contaminant-regeneration recycle example

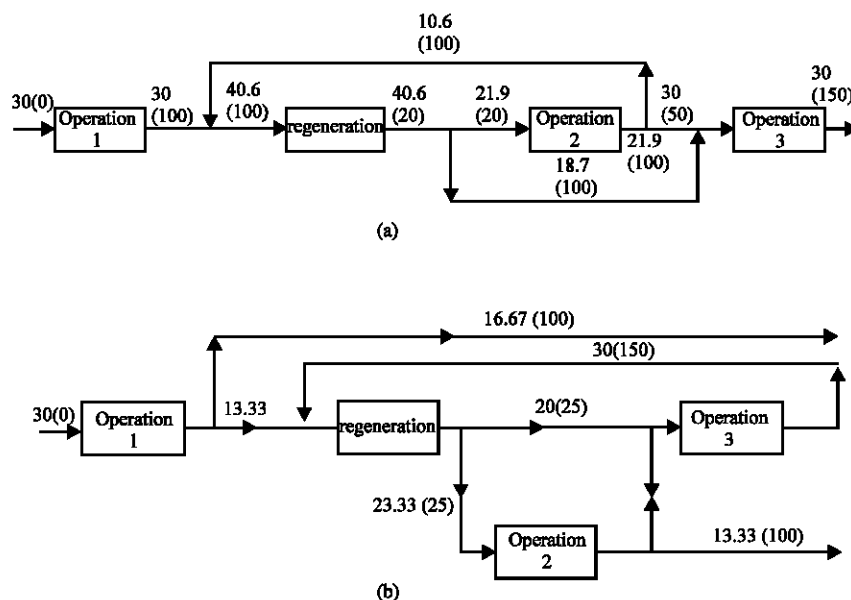


Fig 8: Design network based (a) literature (Mann and Liu, 1999) and (b) results from LP

CONCLUSIONS

In the near future, the price of fresh water and restrictions on the expansion of water usage will play an important role in water reuse projects. One way in which water usage and wastewater generation can be minimized is by reuse and regeneration reuse.

In our research, we used a mathematical approach to minimization of water consumption. Our main goal was to reduce the flow rate of technological wastewater with wastewater reuse or regeneration reuse; the freshwater consumption would consequently be reduced.

The optimization models are LP and NLP type for single and multiple contaminant(s) which are effectively solved using Lingo optimization software. These models target the minimum total fresh water subject to water and contaminant balance and maximum allowable concentration at inlet and outlet of each unit operation. After that, GUI was created in order to make this program to be used easily. Program has been tested with literature examples and the results were compared to the ones given by literatures. In single contaminant problems the program leads to obtain global optimum value. For both single and multiple contaminant(s), the results from program and literature examples reach the same value of minimum freshwater consumption but sometimes they present different configurations. These alternative configurations give the wide-vision on the analysis of the system. To decide which one is better, all the capital and operating costs must be included in the optimization. The results of the deterministic indicate that model has the same

advantages over the mass transfer-based approach of pinch technology presented by Wang and Smith. In the pinch technology the problem is difficult when there are too many contaminants but this method enables to solve problems with many operations and contaminants easily. The other main advantages of the formulation are its ability to capture the essence of time with relative exactness and its structure that renders it solvable within a reasonable CPU time.

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