A Mathematical Programming Model for Wastewater Equalization in Batch Processes*

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Abstract

The demands for fresh process waters and heating/cooling utilities arise intermittently in batch plants. Due to equipment constraints, the quality and flow rate of each resulting wastewater stream are required to be controlled within specified ranges before treatment/regeneration. In this paper, a general mathematic model is developed to design the optimal buffer system for equalizing the flow rates and contaminant concentrations of its outputs. Three examples are provided to illustrated the effectiveness of proposed model.

1 Introduction

Sufficient water supply is a prerequisite for running any chemical process. This is because water may be used in almost every aspect of plant operation. In the process system, it may be considered not only as a reactant in reactors but also as a mass-separating agent (MSA) in various separation processes such as absorption, extraction, leaching and stripping. In the utility system, water is constantly consumed in boilers and cooling towers to generate steam and cooling water. Furthermore, it can be utilized for equipment cleaning, fire fighting and various other miscellaneous operations. After these usages, wastewaters are inevitably created. They should be treated/regenerated and then either reused/recycled within the plant boundary or discharged to the environment.

Although water is one of many abundant natural resources on earth, its demand has been increased dramatically in modern age due to rapid economic expansion in many regions worldwide. Consequently, there are real incentives to develop proper water management methodologies with special emphasis on industrial water conservation. In the literature, the related publications in this area are almost all concerned with the *continuous processes*. Takama *et al.* [1] first studied the optimal water allocation problem in a refinery. A superstructure including all possible reuse options and network connections was built and an iterative decomposition procedure was used to solve the model. In later studies, the water networks in continuous processes were classified into two subsystems, that is, the water-using and wastewater-treatment systems. Most researchers focused on the design issues concerning either one of these two subsystems in order to avoid analyzing the complex interactions between them, e.g., see [2] – [12]. An integrated approach for the overall system design remained a challenge until a general nonlinear programming (NLP) model was developed by Huang *et al.* [13]. In a subsequent work, Tsai and Chang [14] adopted Genetic Algorithm to identify the optimum solution of the same problem.

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* **Keywords:** Batch Process, Water Equalization, Mathematical Programming Model

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It should be noted that, in practice, batch processing has received increasing attention in recent years. It is the predominant means of manufacturing low-volume high-value commercial products, e.g., specialty chemicals, biochemicals and pharmaceuticals, polymers, electronic materials, ceramics and coatings, etc. It has been well recognized that the batch production schemes are especially suitable for accommodating frequent changes in market demands owing to their inherent operation flexibilities [15]. When compared with the continuous counterparts, the benefits of reduced inventories and/or shortened response time can often be achieved with batch processes. However, very few published studies addressed the important issues of water management in batch plants. In fact only the wastewater-reuse problem has been discussed in depth. For example, Wang and Smith [16] proposed a modified version of the Pinch Method to minimize the total amount of discharged wastewater. Almato *et al.* [17, 18] and Puigjaner *et al.* [19] developed a NLP model to optimize water reuse in batch processes. Recently, Kim and Smith [20] contructed a MINLP model to automate the design procedure for discontinuous water systems.

An additional point should be brought up here that, in the water-reuse strategy mentioned above, the practical constraints of the wastewater treatment units are not considered in sufficient detail. For example, since the demands for heating/cooling utilities in a batch plant arise intermittently and their quantities vary drastically with time, the generation rates of the resulting spent waters must also be time dependent [21]. A buffer tank can thus be used at the entrance of each utility system to maintain a steady throughput, see Figure 1. On the other hand, McLaughlin *et al.* [22] indicated that the capital cost of a wastewater treatment operation is usually proportional to its capacity. Thus, for economic reasons, flow equalization is needed to reduce the maximum flow rate of wastewater entering the treatment system. In addition, since the biological-treatment unit is included in most cases, the “shock loads” (mainly in concentration) must be avoided at all times so that the embedded bacteria can always be kept in an active state [23]. In this situation, a buffer system may also be installed to equalize the wastewater flow rates and pollutant concentrations simultaneously. Thus, the water equalization systems in batch processes can be described with the general representation given in Figure 1. The inputs in this representation can be the spent utility waters or wastewaters generated from various batch operations, and the outputs can be considered to be the feeds to different utility-producing equipments, wastewater-treatment units and/or discharge points.

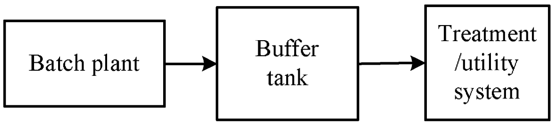

Figure 1: The use of buffer system for wastewater equalization in batch plants.

From the above discussions, it is clear that wastewater equalization is a common practice required in almost every industrial batch process. A typical example can be found in Renda *et al.* [24], in which the authors tried to equalize wastewater generated in a yeast plant by rescheduling and adding new production equipments. Despite this apparent need in practical applications, the development of systematic design strategies for wastewater equalization systems has not been attempted until recently. In a preliminary study, Li *et al.* [25] adopted both a conceptual design approach and also a mathematical programming model to eliminate the possibility of producing an unnecessarily large combined water flow at any instance by using a buffer tank and by rescheduling the batch recipe. Later, Hui *et al.* [26] used a two-tanks configuration to remove peaks in the profile of total wastewater flow rate and also in that of one pollutant concentration.

There are several obvious drawbacks in the present approach to solve the equalization problem. First of all, it may not be enough simply to eliminate the peaks in the time profiles of total flow rate and pollutant concentration. As mentioned before, it is necessary to ensure that the equalized water flows satisfy the operation constraints imposed upon the downstream facilities. In many cases, each water flow is required to be continuous and its flow rate and pollutant concentrations must be maintained within specific upper and/or lower limits. Secondly, the implied assumption of a single *combined* wastewater stream may not be appropriate for the design of optimal water treatment system. The distributed treatment strategy has long been advocated by various researchers [8]–[12] on the ground that pollutants at higher concentrations can be removed more efficiently than those at the average concentrations in most cases. Finally, the system designs obtained under the constraint of a single pollutant are clearly not useful in many industrial problems. The development of a systematic procedure is therefore needed to equalize multiple pollutant concentrations and feed rates to separate downstream units.

2 Problem Statement

To facilitate a precise description of our design problem, let us first introduce the definitions of two unit sets:
E = { e | e is the label of a batch unit from which the wastewater or spent water is generated; e = 1, 2, $\cdots$, N_E }
O = { o | o is the label of a discharge point, a wastewater-treatment unit or an utility-producing device; o = 1, 2, $\cdots$, N_O }
In this paper, the units in **E** are regarded as the *sources* of spent waters or wastewaters entering the equalization system and the elements in **O** are referred to as the *sinks* of these waters leaving the same system.

As mentioned previously, the equalization system consists of a set of interconnected buffer tanks. These tanks can be represented with another unit set defined as follows:
T = { t | t is the label of a buffer tank; i= 1, 2, $\cdots$, N_T}

On the basis of the above definitions, the design task of a water equalization system can be stated as follows: Given the N_E sources in set **E** and N_O sinks in set **O**, the goal of equalization system design is to synthesize a cost-effective network of buffer tanks and their operating policies that can properly distribute the waters generated from the sources to the sinks. For this design problem, it is assumed that the following additional parameters are available:

- the durations, flow rates and pollutant concentrations of the intermittent water flow leaving every source, and
- the upper and lower limits of the flow rate and pollutant concentrations imposed upon the continuous water stream entering each sink.

A proper design of the water equalization system includes at least the following specifications: (1) the number of buffer tanks (N_T) and their sizes, (2) the network configuration, and (3) the time profiles of the flow rate and pollutant concentrations of the water stream in every branch of the water network.

3 Superstructure

Similar to other optimization study in process synthesis, it is necessary to first build a superstructure in which all possible flow configurations can be embedded. A simple construction procedure of the superstructure is presented below:

1. Place a mixing node at the inlet of every buffer tank and every sink.
2. Place a splitting node at outlet of every source and every buffer tank.
3. Connect the split branches from each source to all mixing nodes.
4. Connect the split branches from each buffer tank to all mixing nodes *except* the one before the same tank.

This flow connection scheme is presented in Figure 2.

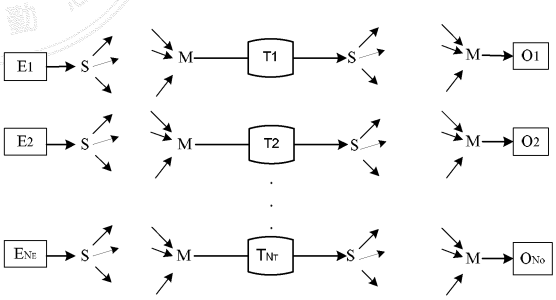

Figure 2: Superstructure of equalization system.

4 Mathematical Model

For formulation convenience, a species set is used for characterizing multiple water contaminants in the equalization system, i.e.,
K= { k | k is the label of a pollutant or an index of pollutants which affects water quality; k=1, 2, $\cdots$, N_K }

In addition, due to the intermittent nature of wastewater flow, it is also necessary to divide the entire period of production cycle into distinct time intervals. Specifically, let us label the time instances when wastewater generation begins or ends as θ_1, θ_2, $\cdots$, θ_{N_J-1}, and express the whole period of production cycle as $[\theta_0, \theta_{N_J}]$. These time instances are arranged in the following order

$$\theta_0 \leq \theta_1 < \theta_2 < \cdots < \theta_{N_J-1} \leq \theta_{N_J}$$

The maximum common divisor DT of the durations of above time intervals, i.e., $\theta_j - \theta_{j-1}$ and $j = 1, 2, \cdots, N_J$, is then selected to further divide $[\theta_0, \theta_{N_J}]$ into smaller equally-spaced unit intervals. An interval set can then be defined accordingly, i.e.,
I= { i | i is the label of the unit time interval ; i = 1, $\cdots, N_I\}$
where the total number of unit time intervals N_I can be determined according to

$$N_I = \frac{\theta_{N_J} - \theta_0}{DT} \qquad (1)$$

On the basis of the definitions of unit sets, species set and interval set, the constraints of mathematical programming model can be formulated as follows

4.1 Buffer tanks

Since the water volumes and pollutant concentrations in the buffer tanks are time-variant, it is necessary to describe their transient behaviors during each time interval defined in **I** with dynamic models. These models are usually expressed in the form of ordinary differential equations (ODEs). To simplify model formulation and to reduce the computation load of optimization, the water volumes in the buffer tanks is calculated by:

$$v_{t,i} = v_{t,i-1} + \left(f^{in}_{t,i} - f^{out}_{t,i}\right) DT \quad t \in \mathbf{T}, \quad i \in \mathbf{I} \qquad (2)$$

In the above equation, $v_{t,i}$ represents the water volume in tank t at the time interval i; $f^{in}_{t,i}$ and $f^{out}_{t,i}$ denote respectively the input and output wastewater flow rates of tank t during time interval i. DT is the duration of each time interval in set **I**.

The water volume in tank t at any instance should of course be less than the storage capacity of the buffer tank. This constraint can be written as

$$v^{max}_t \geq v_{t,i} \quad t \in \mathbf{T}, \qquad i \in \mathbf{I} \qquad (3)$$

in which v^{max}_t is the needed size of buffer tank t.

The component balance equations of each pollutant can also be formulated in a similar fashion, i.e.,

$$v_{t,i}c^{out}_{t,i,k} = v_{t,i-1}c^{out}_{t,i-1,k} + (f^{in}_{t,i}c^{in}_{t,i,k} - f^{out}_{t,i}c^{out}_{t,i,k})DT$$
$$t \in \mathbf{T}, \quad i \in \mathbf{I}, \quad k \in \mathbf{K} \qquad (4)$$

In above equation, $c^{in}_{t,i,k}$ and $c^{out}_{t,i,k}$ denote respectively the concentrations of pollutant k in the inlet and outlet streams of tank k at time interval i.

4.2 Splitting nodes

The water balance at each source can be written as:

$$G_{e,i} = \sum_{t \in \mathbf{T}} f_{e,t,i} + \sum_{o \in \mathbf{O}} f_{e,o,i} \qquad e \in \mathbf{E}, \quad i \in \mathbf{I} \qquad (5)$$

where, $G_{e,i}$ is the wastewater generation rate from source e in time interval i; $f_{e,t,i}$ represents the water flow rate from source e to buffer tank t in time interval i; $f_{e,o,i}$ is the water flow rate from source e to sink o in time interval i.

On the other hand, the water balance equation for the splitting node at the outlet of each buffer tank can be expressed as

$$f^{out}_{t,i} = \sum_{t' \in \mathbf{T}; t' \neq t} f_{t,t',i} + \sum_{o \in \mathbf{O}} f_{t,o,i} \quad t \in \mathbf{T}, \quad i \in \mathbf{I} \qquad (6)$$

where, $f_{t,t',i}$ represents the water flow rate from buffer tank t to another buffer tank t' in time interval i; $f_{t,o,i}$ is the water flow rate from tank t to sink o in time interval i.

Finally, it should be noted that the pollutant concentrations of the wastewater flow before any splitting node should be the same as those in every the split stream.

4.3 Mixing nodes

The water balance at the inlet mixing node of each buffer tank can be written as:

$$f^{in}_{t,i} = \sum_{e \in \mathbf{E}} f_{e,t,i} + \sum_{t' \in \mathbf{T}; t' \neq t} f_{t',t,i} \qquad t \in \mathbf{T}, \quad i \in \mathbf{I} \qquad (7)$$

where, $f_{t',t,i}$ represents the water flow rate from buffer tank t' to a different tank t in time interval i and the other variables in this equation has already defined previously. The material balances of water contaminants about the same mixing node can be expressed as:

$$f_{t,i}^{in} c_{t,i,k}^{in} = \sum_{e \in \mathbf{E}} f_{e,t,i} C_{e,i,k} + \sum_{t' \in \mathbf{T}; t' \neq t} f_{t',t,i} c_{t',i,k}^{out}$$

$$t \in \mathbf{T}, \quad i \in \mathbf{I}, \quad k \in \mathbf{K} \qquad (8)$$

where $C_{e,i,k}$ represents the concentration of pollutant k in the wastewater generated by source e during interval i.

Similarly, the water balance equation for the mixing node at each sink can be written as

$$f_{o,i}^{sink} = \sum_{t \in \mathbf{T}} f_{t,o,i} + \sum_{e \in \mathbf{E}} f_{e,o,i} \qquad o \in \mathbf{O}, \quad i \in \mathbf{I} \qquad (9)$$

The mass balances of the pollutants around the mixing node before every sink can be written as:

$$f_{o,i}^{sink} c_{o,i,k}^{sink} = \sum_{t \in \mathbf{T}} f_{t,o,i} c_{t,i,k}^{out} + \sum_{e \in \mathbf{E}} f_{e,o,i} C_{e,i,k}$$

$$o \in \mathbf{O}, \quad i \in \mathbf{I}, \quad k \in \mathbf{K} \qquad (10)$$

where, $f_{o,i}^{sink}$ represents the wastewater flow rate discharged to sink o during time interval i and $c_{o,i,k}^{sink}$ is the concentration of pollutant k in the wastewater discharged to sink o at time interval i.

The operation requirements of the treatment unit imposed at the entrance of each sink are assumed to be:

$$C_{o,k}^{L} \leq c_{o,i,k}^{sink} \leq C_{o,k}^{U} \qquad F_{o}^{L} \leq f_{o,i}^{sink} \leq F_{o}^{U}$$

$$o \in \mathbf{O}, \quad i \in \mathbf{I}, \quad k \in \mathbf{K} \qquad (11)$$

where, $C_{o,k}^{L}$ and $C_{o,k}^{U}$ represent respectively the lower and upper limits of the concentration of pollutant k in the wastewater stream entering sink o and, similarly, F_{o}^{L} and F_{o}^{U} are the permitted minimum and maximum flow rate of wastewater discharged to sink o.

The objective function (obj) of our optimization problem is the sum of installed costs and treatment costs, i.e.,

$$obj = \sum_{t \in \mathbf{T}} \text{instcost}_t + \sum_{o \in \mathbf{O}} \text{treatcost}_o \qquad (12)$$

The installed cost of each buffer tank is determined according to

$$\text{instcost}_t = \alpha (v_t^{max})^{0.6} \qquad t \in \mathbf{T} \qquad (13)$$

where, α is a constant[27]. On the other hand, the treatment cost of wastewater discharged to sink o can be computed with the following formula:

$$\text{treatcost}_o = \gamma_o DT \sum_{i \in \mathbf{I}} f_{o,i}^{sink} \qquad o \in \mathbf{O} \qquad (14)$$

where γ_o is the treatment cost per unit volume of wastewater discharged to sink o.

5 Illustration Examples

To illustrate the implementation procedure of the proposed approach, a series of three examples are presented here. All problems were solved with module *conopt3* under the GAMS environment [28].

5.1 Example 1

The simple flow equalization problem for spent utility is studied in this example. It is assumed that there is only one buffer tank in this case. Because also concentration of pollutant is not involved in this example, it is unnecessary to use bypass branch for flow rate equalization. The combined flow rate of spent water generated during a production cycle is plotted in Figure 3 as a function of time. The cycle time is 20 hours and the chosen duration of each unit interval is 0.5 hour.

Let us first consider the requirement of equalizing water flow rate to its average value of 6.125 m^3/hr (see the dashed line in Figure 3). Let us further assume that the treatment cost of spent utility water is negligible and the objective function can be reduced to the total size of buffer tank. Consequently, the minimum size of buffer tank was found to be 24.5 m^3. The variation of water volume in the buffer tank is presented in Figure 4. If the requirements on the input flow to the utility system can be relaxed to within ±10% of the average value, it is possible to reduce the buffer size to 22.05 m^3. This represents a 8.2% saving. The flow rate profile of the equalized stream in this case is provided in Figure 5.

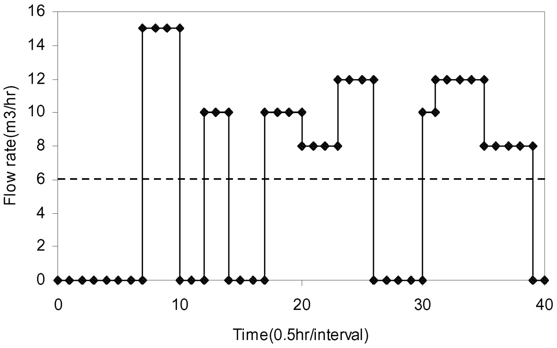

Figure 3: The flow rate profile of spent utility water in a batch process (Example 1).

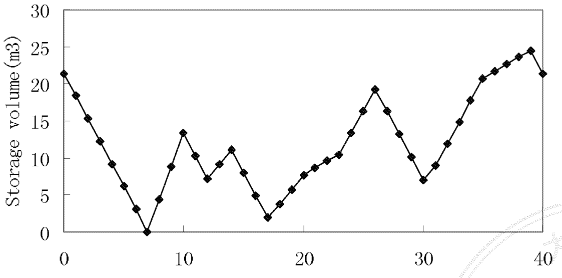

Figure 4: The volume profile of stored water in the buffer tank (Example 1).

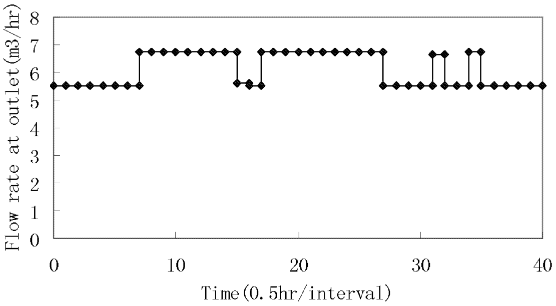

Figure 5: The flow rate profile of wastewater stream equalized to satisfy the relaxed constraints (Example 1).

Table 1: Process data of wastewater in Example 2

Prod. Line	t_s	t_f (hr)	Flow rate (m^3/hr)	COD (mg/L)
1	0.5	2.5	10	900
1	5.0	7.0	5	1500
1	10.5	14.5	15	2000
2	2.5	4.5	10	3000
2	7.0	9.0	20	2500
2	11.5	13.5	15	2400
2	17.0	19.0	6	1800
3	6.0	8.0	5	4000
3	9.5	11.5	2	2000
3	17.0	19.0	4	3000

5.2 Example 2

A food company owns three production lines for (1) frozen fruits and vegetables, (2) canned and frozen fruit juices and (3) canned fruits and vegetables. Wastewaters are created when washing raw materials, cleaning tables, walls, belts, floors and so forth. All wastewaters generated within the same production line are collected to a single sewage and thus form a wastewater stream. Its flow rate varies with time and is discontinuous. *COD* (Chemical Oxygen Demand) is used to characterize the amount of pollutants in a wastewater stream. The process data of all the wastewaters in this company are given in Table 1. The production cycle is 20 hour. From Table 1, it is clear that the duration of unit interval can be set at 0.5 hr. Since these waters are too polluted to be processed by the municipal treatment facility, they must be pretreated before leaving the plant. Thus, the flow rate and *COD* of wastewater must be equalized according to the operation constraints of the pretreatment system. Specifically, the variation of equalized flow rate should be limited within the range [10.16, 11.24] m^3/hr and *COD* variation must be controlled within [2125, 2348] mg/L. We used a superstructure with two buffer tanks, three sources and one sink. Since there is only one sink, the second term in objective function (12) can be dropped.

The minimum installation cost can be obtained by solving the mathematical program, i.e., 14.85 cost unit. The volumes of buffer tanks are 47.46 and 13.26 m^3 respectively. It was found that that all branches embedded in superstructure were selected in the solution. However, the total volumes of transported wasterwaters in two of them, i.e., the branches from E_3 to T_2

and from T_2 to T_1, are very small. To simplify the network structure, these two branches were removed from superstructure and the optimization process was repeated. The resulting cost increased to 16.94 cost unit, and the corresponding buffer volumes were found to be 10.0 and 71.52 m^3 respectively. This equalization structure is shown in Figure 6. The flow rate and COD profiles at the sink are shown in Figure 7 and 8 respectively. In addition, the volume profiles of stored waters in the two buffer tanks are presented in Figure 9 and 10 respectively.

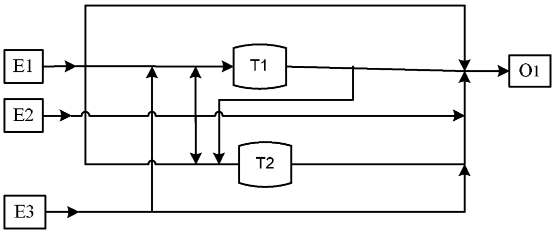

Figure 6: The equalization structure obtained in Example 2.

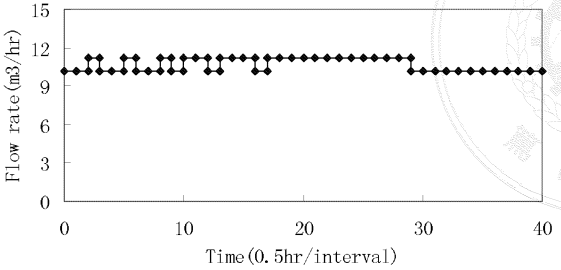

Figure 7: Flow rate of wastewater at the sink (Example 2).

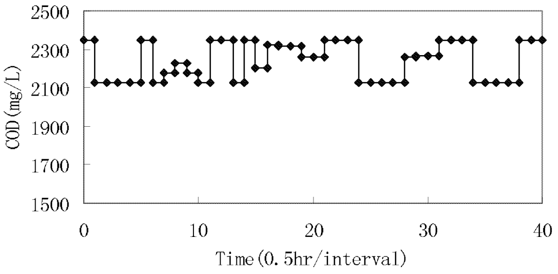

Figure 8: COD of wastewater at the sink (Example 2).

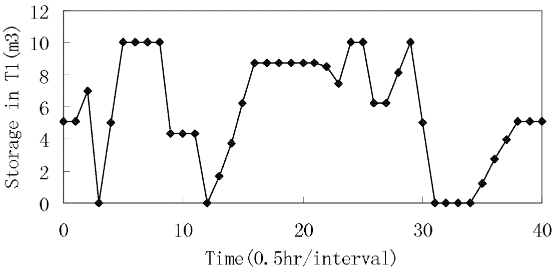

Figure 9: Volume of stored wastewater in tank 1 (Example 2).

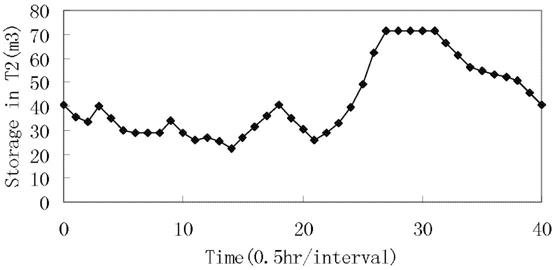

Figure 10: Volume of stored wastwater in tank 2 (Example 2).

5.3 Example 3

Let us assume that there is another facility located in the vicinity of the company described in Example 2. This plant has two production lines and its wastewaters can be characterized not only by *COD* but also by *SS* (Suspend Solids). The corresponding process data are given in Table 2. Notice that the wastewaters generated in the first plant are rich in organic compounds, while those generated in the second are dominated by *Suspend Solids.* Consequently, two types of wastewater sinks are considered in this example. One is used for the reduction of organic chemicals and the other for the treatment of suspended solids. The operational limits imposed upon the inputs to these two kinds of treatment systems are listed in Table 3. Again we assumed that their unit treatment costs are the same and thus the second term in equation (12) can be neglected. The number of buffer tanks used in the superstructure is still chosen to be 2. Our design objective is to obtain an minimum-cost wastewater equalization system that satisfies the requirements of treatment systems at the sinks.

Table 2: Process data of wastewater in Example 3

Prod. Line	t_s	t_f	Flow rate	COD	SS
	(hr)		(m^3/hr)	(mg/L)	
1	0.5	2.5	10	900	20
1	5.0	7.0	5	1500	30
1	10.5	14.5	15	2000	40
2	2.5	4.5	10	3000	50
2	7.0	9.0	20	2500	50
2	11.5	13.5	15	2400	30
2	17.0	19.0	6	1800	20
3	6.0	8.0	5	4000	80
3	9.5	11.5	2	2000	30
3	17.0	19.0	4	3000	40
4	2.0	3.5	10	120	600
4	5.0	7.5	15	200	100
4	10.0	15.0	12	80	300
5	3.0	6.0	12	130	100
5	7.5	10.0	15	150	800
5	12.0	15.0	14	130	500
5	18.0	20.0	16	80	300

Table 3: Limitations imposed by wastewater treatment systems (Example 3).

Sink	Flow(m^3/hr)		COD(mg/L)		SS(mg/L)	
	min	max	min	max	min	max
1	8	12	2000	2500	0	50
2	10	14	0	150	300	500

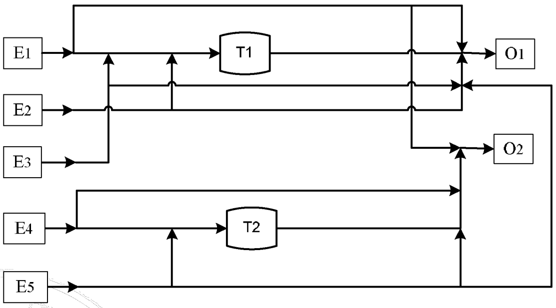

Figure 11: Optimal equalization structure in Example 3

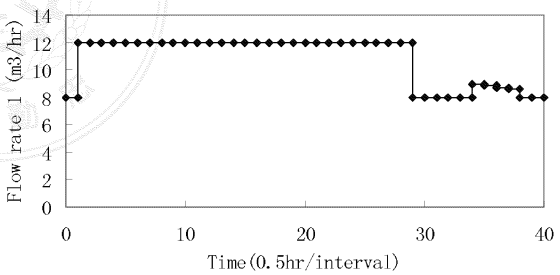

Figure 12: Flow rate profile at sink 1 (Example 3)

The proposed mathematical programming model was solved to obtain the optimal design the equalization system. The minimum cost was determined to be 30.35 cost unit. The corresponding sizes of the two buffer tanks are 78.48 and 108.47 m^3 respectively. Again, by removing the seldom-used branches from the superstructure, the optimization was solved a second time. The resulting cost is 31.23 cost unit, and the corresponding sizes of two buffer tanks are 75.25 and 122.05 m^3 respectively. The simplified network structure is shown in Figure 11. The profiles of equalized flow rate and pollutant indices are provided in Figure 12 to 17.

6 Conclusion

A general nonlinear programming (NLP) model is developed in this work for optimal wastewater equalization in batch plants. The inherent fluctuations in the flow rates and multi-pollutant concentrations of the wastewater streams can be moderated with a network of buffer tanks in the resulting design. The proposed model is simple but practical. To avoid using ordinary differential equations to describe the time-variant water volumes and pollutant concentrations in the buffer tanks, the corresponding dynamic representations are discretized according to equally-spaced time intervals. Structure improvement is achieved with a two-step optimization strategy in this study. The complete superstructure is first used to create an initial system design. By

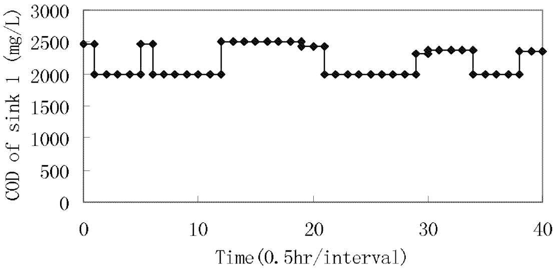

Figure 13: COD profile of COD at sink 1 (Example 3).

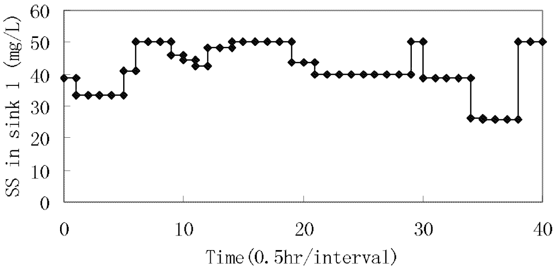

Figure 14: SS profile of SS at sink 1 (Example 3).

forbidding the branches with negligible flows in this design, the proposed model is then solved a second time to create the final network. This practice is believed to be more practical than handling the binary variables in a mixed-integer nonlinear program (MINLP). Three examples are presented in this paper to demonstrate the effectiveness of the proposed approach.

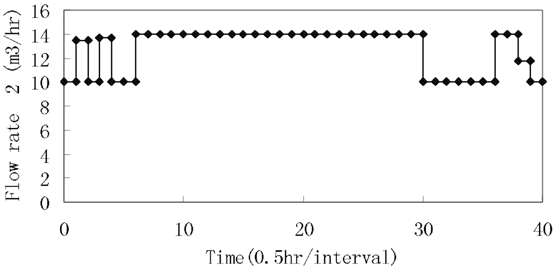

Figure 15: Flow rate profile at sink 2 (Example 3).

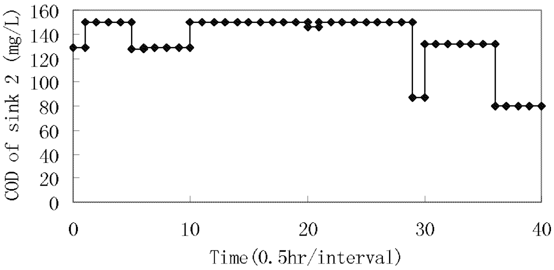

Figure 16: COD profile at sink (Example 3).

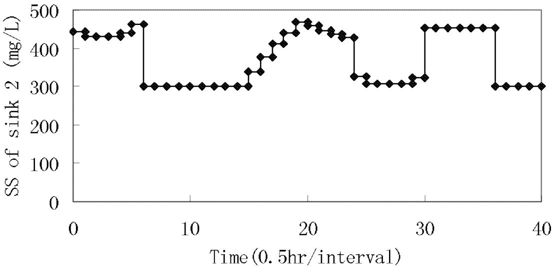

Figure 17: SS profile at sink 2 (Example 3).

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