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Optimal design of wastewater equalization systems in batch processes

Chuei-Tin Chang^{a,*}, Bao-Hong Li^b

^a Department of Chemical Engineering, National Cheng Kung University, Tainan 70101, Taiwan, ROC
 ^b Department of Chemical Engineering, Dalian Nationalities University, Dalian 116600, China

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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 limits before treatment/regeneration. In this paper, a general mathematical programming 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 illustrate the effectiveness of proposed approach. © 2005 Elsevier Ltd. All rights reserved.

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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 massseparating 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, Kuriyama, Shiroko, and Umeda (1980) first studied the optimal water allocation problem in a refinery. A superstructure including all possible reuse options and network connections were 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 (Bagajewicz, 2000; Feng & Seider, 2001; Galan & Grossmann, 1998; Hernandez-Suarez, Castellanos-Fernandez, & Zamora, 2004; Kuo & Smith, 1997,1998; Li, Fan, & Yao, 2002a; Li, Hui, & Smith, 2002b; Wang & Smith, 1994a,b; Wang, Feng, & Zhang, 2003; Yang, Lou, & Huang, 2000) focused on the design issues concerning either one of these two subsystems in order to avoid analyzing the complex interactions between them. An integrated approach for the overall system design remained a challenge until a general non-linear programming (NLP) model was developed by Huang, Chang, Ling, and Chang (1999). In a subsequent work, Tsai and Chang (2001) adopted genetic algorithm to identify the optimum solution of the same problem.

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

^{*} Corresponding author. Tel.: +886 6 275 7575x62663; fax: +886 6 234 4496. *E-mail addresses:* ctchang@mail.ncku.edu.tw (C.-T. Chang),

libh@dlnu.edu.cn (B.-H. Li)

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Nomenclature

Indices

- *e* the label of a batch unit from which the wastewater or spent water is generated, $e = 1, 2, ..., N_E$
- *i* the label of the time interval $[\theta_{i-1}, \theta_i)$, $i = 1, \dots, N_{\text{I}}$
- k the label of a pollution index, e.g. the concentration of a contaminant, which affects water quality; $k = 1, 2, ..., N_{K}$
- *o* the label of a discharge point, a wastewatertreatment unit or an utility-producing device, $o = 1, 2, ..., N_{O}$
- t the label of a buffer tank, $t = 1, 2, ..., N_T$

Parameters

- α a cost constant
- θ_i the *i*th time instance when wastewater generation begins or ends
- $C_{o,k}^{L}$ the lower limits of the concentration of pollutant k in the wastewater stream entering sink o
- $C_{o,k}^{U}$ the upper limits of the concentration of pollutant k in the wastewater stream entering sink o
- D_i the length of subinterval in time interval *i* $F_o^{\rm L}$ the permitted minimum flowrate of wast
- $F_o^{\rm L}$ the permitted minimum flowrate of wastewater discharged to sink *o*
- $F_o^{\rm U}$ the permitted maximum flowrate of wastewater discharged to sink *o*
- $G_{e,i}$ the wastewater generation rate from source *e* in time interval *i*
- LB^V a user-specified lower bound on the total transported water volume through any single connection line in a production cycle
- $M_{\rm I}$ the chosen number of subintervals in interval *i*
- $N_{\rm E}$ the number of sources of spent waters or wastewaters entering the equalization system
- $N_{\rm I}$ the number of time intervals
- $N_{\rm K}$ the number of pollutant indices
- $N_{\rm O}$ the number of discharge points
- $N_{\rm T}$ the number of buffer tanks
- NB_e^S the maximum allowable numbers of output branches from splitters at source e
- NB_o^M the maximum allowable numbers of input branches connected to the mixers at sink o
- NB_t^M the maximum allowable numbers of input branches connected to the mixers at the entrance of buffer tank *t*
- NB_t^S the maximum allowable numbers of output branches from splitters at exit of buffer tank *t*
- UB^F the upper bound of flowrate that must not be exceeded in any pipeline at any time

Binary variables

 $n_{e,o}$ a binary variable to signify whether or not the branch from source *e* to sink *o* is selected

- $n_{e,t}$ a binary variable to signify whether or not the branch from source *e* to tank *t* is selected
- $n_{t,o}$ a binary variable to signify whether or not the branch from tank *t* to sink *o* is selected
- $n_{t,t'}$ a binary variable to signify whether or not the branch from tank *t* to tank *t'* is selected

Variables

- $c_{o,i,j,k}^{\text{sink}}$ the concentration of pollutant k in the wastewater discharged to sink o at time $\theta_{i-1} + jD_i$
- $c_{t,i,j,k}^{\text{in}}$ the concentration of pollutant k in the inlet streams of tank t at time instance $\theta_{i-1} + jD_i$
- $c_{t,i,j,k}^{\text{out}}$ the concentration of pollutant k in the outlet streams of tank t at time instance $\theta_{i-1} + jD_i$
- $f_{e,o,i}$ the water flow-rate from source *e* to sink *o* in time interval *i*
- $f_{e,t,i}$ the water flow-rate from source *e* to buffer tank *t* in time interval *i*
- $f_{t,o,i}$ the water flow-rate from buffer tank *t* to sink *o* in time interval *i*
- $f_{t,t',i}$ the water flow-rate from buffer tank *t* to buffer tank *t'* in time interval *i*
- $f_{o,i}^{\text{sink}}$ the wastewater flow-rate discharged to sink *o* during time interval *i*
- $f_{t,i}^{\text{in}}$ the input wastewater flow-rate of tank *k* during time interval *i*
- $f_{t,i}^{\text{out}}$ the output wastewater flow-rate of tank *k* during time interval *i*
- $v_{t,i,j}$ the water volume in tank *t* at the time instance $\theta_{i-1} + jD_i$
- v_t^{max} the needed size of buffer tank t

operation flexibilities (Rippin, 1991). 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 (1995) proposed a modified version of the Pinch method to minimize the total amount of discharged wastewater. Almato, Sanmarti, Espuna, and Puigjaner (1997), Almato, Espuna, and Puigjaner (1999) and Puigjaner, Espuna, and Almato (2000) developed a NLP model to optimize water reuse in batch processes. Recently, Kim and Smith (2004) constructed 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 (Winkel, Zullo, Verheijen, & Pantelides, 1995). A buffer tank can thus be used at the en-

trance of each utility system to maintain a steady throughput. On the other hand, McLaughlin, McLaugh, and Groff (1992)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 (Nemerow, 1971). In this situation, a buffer system may also be installed to equalize the wastewater flow-rates and pollutant concentrations simultaneously. The inputs of this equalization system 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.

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 Tumsen, Velioglu, and Hortacsu (1996), 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. (2002a,b) 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, Li, and Smith (2003) 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 (Galan & Grossmann, 1998; Hernandez-Suarez et al., 2004; Kuo & Smith, 1997; Li et al., 2002a,b; Wang & Smith, 1994b) 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.

The rest of this paper is organized as follows. A formal definition of the equalization system design problem is first presented in the next section. To facilitate the formulation of the mathematical programming model, a superstructure of the buffer network is then given in Section 3. The mixed-integer non-linear program is outlined accordingly in the following section. With this model, a minimum-cost design can be obtained under the constraints imposed upon the network structure, and also upon the flow-rates and concentrations at the inlet(s) and outlet(s) of every buffer tank, mixing node and splitting node in the equalization system. Finally, three illustration examples are provided at the end of this paper to demonstrate the effectiveness of the proposed approach.

2. Problem statement

To facilitate a precise description of our design problem, let us first introduce the definitions of two unit sets:

 $E = \{e | e \text{ is the label of a batch unit from which the wastewater}$ or spent water is generated; $e = 1, 2, ..., N_E\}$ (1)

 $O = \{o | o \text{ is the label of a discharge point,} \}$

a wastewater-treatment unit or an utility-producing

device;
$$o = 1, 2, ..., N_0$$
 (2)

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:

$$\mathbf{T} = \{t | t \text{ is the label of a buffer tank; } i = 1, 2, \dots, N_{\mathrm{T}}\}$$
(3)

On the basis of the above definitions, the design task of a water equalization system can be stated as follows: Given the $N_{\rm E}$ sources in set E and $N_{\rm O}$ 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 number of buffer tanks to be used,
- 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.

To simplify model formulation, these parameters are considered to be constant in the search process. The uncertainty issues are not addressed in the present study.

Thus, a proper design of the water equalization system includes at least the following specifications: (1) the needed size of each buffer tank, (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 equalization network.



Fig. 1. Superstructure of equalization system.

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 Fig. 1.

4. Mathematical programming model

For formulation convenience, a species set is used for characterizing multiple water contaminants in the equalization system, i.e.:

 $K = \{k | k \text{ is the label of a pollution index}, \}$

e.g. the concentration of a contaminant,

which affects water quality;
$$k = 1, 2, ..., N_{\rm K}$$
 (4)

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 $\theta_1, \theta_2, \ldots, \theta_{N_I-1}$, and express the whole period of production cycle as $[\theta_0, \theta_{N_I}]$. These time instances are arranged in the following order:

$$\theta_0 \le \theta_1 < \theta_2 < \dots < \theta_{N_{\rm I}-1} \le \theta_{N_{\rm I}} \tag{5}$$

In this paper, an interval set is defined accordingly for the identification of the time intervals in $[\theta_0, \theta_{N_I}]$, i.e.:

I = {*i*|*i* is the label of the time interval [
$$\theta_{i-1}, \theta_i$$
);

$$i = 1, \dots, N_{\mathrm{I}} \} \tag{6}$$

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

• 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 computation load, every time intervals is further divided into several equallyspaced subintervals and the corresponding ODEs are discreteized accordingly to a set of algebraic equations. The length of a subinterval in time interval $i \in I$ is determined with the following equation:

$$D_i = \frac{\theta_i - \theta_{i-1}}{M_i}, \quad i \in \mathbf{I}$$
(7)

where, M_i is the chosen number of subintervals in interval *i*. The durations of these subintervals D_i s are regarded as known parameters in the proposed model.

The water volumes in the buffer tanks can thus be written as:

$$v_{t,i,j} = v_{t,i,0} + (f_{t,i}^{\text{in}} - f_{t,i}^{\text{out}})jD_i, \quad t \in \mathbf{T}, \quad i \in \mathbf{I}$$
 (8)

where, $j = 0, 1, 2, ..., M_i$ and

$$v_{t,i,0} = v_{t,i-1,M_{i-1}} \tag{9}$$

In the above two equations, $v_{t,i,j}$ represents the water volume in tank t at the time instance $\theta_{i-1} + jD_i$; $f_{t,i}^{\text{in}}$ and $f_{t,i}^{\text{out}}$ denote respectively the input and output wastewater flow-rates of tank t during time interval i.

The water volume in tank *t* at any instance should of course be larger than zero and less than the storage capacity of the buffer tank. These constraints can be written as:

$$v_t^{\max} \ge v_{t,i,j} \ge 0, \qquad t \in \mathbf{T}, \quad i \in \mathbf{I}, \quad j = 1, 2, \dots, M_i$$
(10)

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

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

$$v_{t,i,j}c_{t,i,j,k}^{\text{out}} = v_{t,i,j-1}c_{t,i,j-1,k}^{\text{out}} + (f_{t,i}^{\text{in}}c_{t,i,j-1,k}^{\text{in}} - f_{t,i}^{\text{out}}c_{t,i,j-1,k}^{\text{out}})D_i,$$

 $t \in \mathbf{T}, \quad i \in \mathbf{I}, \quad j = 1, 2, \dots, M_i, \quad k \in \mathbf{K}$ (11)

where,

$$c_{t,i,0,k}^{\text{out}} = c_{t,i-1,M_{i-1},k}^{\text{out}}$$
(12)

In these two equations, $c_{t,i,j,k}^{\text{in}}$ and $c_{t,i,j,k}^{\text{out}}$ denote respectively the concentrations of pollutant *k* in the inlet and outlet streams of tank *t* at time instance $\theta_{i-1} + jD_i$.

Finally, due to the cyclic nature of batch production activities, it is assumed in this study that the operating conditions at the end of each cycle are the same as the initial conditions of the next cycle. In other words, the following constraints must also be imposed:

$$v_{t,1,0} = v_{t,N_{\rm I},M_{N_{\rm I}}}, \quad t \in {\rm T}$$
 (13)

$$c_{t,1,0,k}^{\text{out}} = c_{t,N_{\text{I}},M_{N_{\text{I}}},k}^{\text{out}}, \qquad t \in \text{T}, \quad k \in \text{K}$$
(14)

• Splitting nodes

The water balance at each source can be written as:

$$G_{e,i} = \sum_{t \in \mathcal{T}} f_{e,t,i} + \sum_{o \in \mathcal{O}} f_{e,o,i}, \qquad e \in \mathcal{E}, \quad i \in \mathcal{I}$$
(15)

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. Notice that the wastewater generation rates $G_{e,i}$ s are considered to be known parameters in this model.

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

$$f_{t,i}^{\text{out}} = \sum_{t' \in \mathbf{T}; t' \neq t} f_{t,t',i} + \sum_{o \in \mathbf{O}} f_{t,o,i}, \qquad t \in \mathbf{T}, \quad i \in \mathbf{I}$$
(16)

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.

Mixing nodes

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

$$f_{t,i}^{\text{in}} = \sum_{e \in \mathcal{E}} f_{e,t,i} + \sum_{t' \in \mathcal{T}; t' \neq t} f_{t',t,i}, \quad t \in \mathcal{T}, \quad i \in \mathcal{I}$$
 (17)

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:

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

$$t \in \mathcal{T}, \quad i \in \mathcal{I}, \quad j = 0, 1, 2, \dots, M_i, \quad k \in \mathcal{K}$$
(18)

where $C_{e,i,k}$ represents the known 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:

$$f_{o,i}^{\text{sink}} = \sum_{t \in \mathcal{T}} f_{t,o,i} + \sum_{e \in \mathcal{E}} f_{e,o,i}, \qquad o \in \mathcal{O}, \quad i \in \mathcal{I}$$
(19)

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

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

 $o \in \mathcal{O}, \quad i \in \mathcal{I}, \quad j = 0, 1, 2, \dots, M_i, \quad k \in \mathcal{K}$ (20)

where, $f_{o,i}^{\text{sink}}$ represents the wastewater flow-rate discharged to sink *o* during time interval *i* and $c_{o,i,j,k}^{\text{sink}}$ is the concentration of pollutant *k* in the wastewater discharged to sink *o* at time $\theta_{i-1} + jD_i$.

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

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

$$o \in \mathrm{O}, \quad i \in \mathrm{I}, \quad j = 0, 1, 2, \dots, M_{i}, \quad k \in \mathrm{K}$$
(21)

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-rates of wastewater discharged to sink *o*. The values of these upper and lower limits are assumed to be available in advance.

• Network structure

From a practical standpoint, there is an obvious need to eliminate any pipeline that is used for transferring only a negligible amount of wastewater during the entire production cycle. To prevent generating such branches in solving the proposed model, a lower bound is imposed upon the total water volume transported through every connection line in the equalization network, i.e.:

$$\sum_{i \in \mathbf{I}} f_{e,t,i}(\theta_i - \theta_{i-1}) \ge n_{e,t} \mathbf{LB}^{\mathbf{V}}, \qquad e \in \mathbf{E}, \quad t \in \mathbf{T}$$
(22)

$$\sum_{i \in \mathbf{I}} f_{e,o,i}(\theta_i - \theta_{i-1}) \ge n_{e,o} \mathbf{LB}^{\mathbf{V}}, \qquad e \in \mathbf{E}, \quad o \in \mathbf{O} \quad (23)$$

$$\sum_{i \in \mathbf{I}} f_{t,t',i}(\theta_i - \theta_{i-1}) \ge n_{t,t'} \mathbf{LB}^{\mathbf{V}}, \qquad t, t' \in \mathbf{T}, \quad t \neq t'$$
(24)

$$\sum_{i \in \mathbf{I}} f_{t,o,i}(\theta_i - \theta_{i-1}) \ge n_{t,o} \mathbf{LB}^{\mathbf{V}}, \qquad t \in \mathbf{T}, \quad o \in \mathbf{O}$$
(25)

where, LB^{V} denotes a user-specified lower bound on the total transported water volume through any single connection line in a production cycle; $n_{e,t}$, $n_{e,o}$, $n_{t,t'}$ and $n_{t,o}$ are binary variables used to signify whether or not the corresponding line is selected in the optimal network configuration.

On the other hand, the maximum water flow-rate in each pipeline must also be limited to a level that is achievable with commercially available equipments. The corresponding inequality constraints can be written as:

$$f_{e,t,i} \le n_{e,t} \mathrm{UB}^{\mathrm{F}}, \qquad e \in \mathrm{E}, \quad t \in \mathrm{T}, \quad i \in \mathrm{I}$$
 (26)

$$f_{e,o,i} \le n_{e,o} \mathrm{UB}^{\mathrm{F}}, \qquad e \in \mathrm{E}, \quad o \in \mathrm{O}, \quad i \in \mathrm{I}$$
 (27)

$$f_{t,t',i} \le n_{t,t'} \mathrm{UB}^{\mathrm{F}}, \qquad t, t' \in \mathrm{T}, \quad t \neq t', \quad i \in \mathrm{I}$$
(28)

$$f_{t,o,i} \le n_{t,o} \mathrm{UB}^{\mathrm{F}}, \qquad t \in \mathrm{T}, \quad o \in \mathrm{O}, \quad i \in \mathrm{I}$$
 (29)

Here, UB^F is the upper bound of flow-rate that must not be exceeded in any pipeline at any time. It can be clearly observed from Eqs. (22)-(29) that, if a particular connection line is excluded from the equalization network, i.e. the corresponding

binary variable is set to be 0, then its flow-rate must also be maintained at zero throughout the whole production cycle.

Finally, in order to further simply the network structure, the following constraints are also introduced:

$$\sum_{o \in \mathcal{O}} n_{e,o} + \sum_{t \in \mathcal{T}} n_{e,t} \le \mathrm{NB}_e^{\mathrm{S}}, \quad e \in \mathrm{E}$$
(30)

$$\sum_{t'\in\mathcal{T}, t\neq t'} n_{t,t'} + \sum_{o\in\mathcal{O}} n_{t,o} \le \mathrm{NB}_t^{\mathrm{S}}, \quad t\in\mathcal{T}$$
(31)

$$\sum_{e \in \mathcal{E}} n_{e,t} + \sum_{t' \in \mathcal{T}, t' \neq t} n_{t',t} \le \mathrm{NB}_t^{\mathrm{M}}, \quad t \in \mathcal{T}$$
(32)

$$\sum_{e \in \mathbf{E}} n_{e,o} + \sum_{t \in \mathbf{T}} n_{t,o} \le \mathbf{NB}_o^{\mathbf{M}}, \quad o \in \mathbf{O}$$
(33)

where, NB_e^S and NB_t^S denote respectively the maximum allowable numbers of output branches from the splitters at source *e* and at the exit of buffer tank *t*; NB_t^M and NB_o^M represent, respectively the maximum allowable numbers of input branches connected to the mixers at the entrance of buffer tank *t* and at sink *o*.

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

$$obj = \sum_{t \in \mathcal{T}} instcost_t$$
 (34)

The installed cost of each buffer tank is determined according to:

$$\operatorname{instcost}_{t} = \alpha (v_t^{\max})^{0.6}, \quad t \in \mathbf{T}$$
 (35)

where, α is a constant (Happel & Jordan, 1975).

5. Illustration examples

To illustrate the implementation procedure of the proposed approach, a series of three examples are presented here. All problems were run on a personal computer with Pentium(R) 4 and CPU frequency of 2.80 GHz. Solver CPLEX is selected for Example 1 and DICOPT for Examples 2 and 3 under the GAMS environment (Brooke, Kendrik, Meeraus, & Ramam, 1998).

5.1. Example 1

A simple flow equalization problem for spent utility is studied in this example. Since the equalization of pollutant concentrations is not considered in this example, it is thus unnecessary to include any bypass branch in the superstructure. The combined flow-rate of spent water generated during a production cycle is plotted in Fig. 2 as a function of time. The cycle time is 20 h and only one buffer tank is used for equalization. Let us first consider the problem of equalizing water flow-rate exactly to its average value, i.e. $6.125 \text{ m}^3/\text{h}$, which is shown with the dashed line in Fig. 2. The minimum size of buffer tank was found to be 24.5 m^3 with the proposed mathematical programming model and the total solution time was less than 0.05 s. The variation of water volume in the buffer tank is presented in Fig. 3. Notice that



Fig. 2. The flow-rate profile of spent utility in a batch process (Example 1).



Fig. 3. Volume profile of stored water in the buffer tank (Example 1).

the water volume reaches zero at 3.5 h. This is an indication of optimum solution since, if the buffer tank is not emptied at some instances, the maximum stored volume can always reduced by lowering the initial volume while maintaining the same buffer operation policy.

If the requirements on the input flow to the utility system can be relaxed to within $\pm 10\%$ of the average value, it is possible to reduce the buffer size to 22.1 m³. The flow-rate profile of the equalized stream in this case is provided in Fig. 4. Notice that the equalized flow-rate is required to take only three distinct values and it is necessary to switch from one value to another six times in a production cycle. Since the implied demand for control facilities is moderate, this equalization strategy can be regarded as practically realizable.



Fig. 4. Flow-rate profile of equalized wastewater stream to satisfy the relaxed constraints (Example 1).

 Table 1

 Process data of generated wastewaters in Example 2

Production line	$t_{\rm s}$ (h)	$t_{\rm f}$ (h)	Flow-rate (m ³ /h)	COD (mg/L)	SS (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

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. Two pollution indices, i.e. chemical oxygen demand (COD) and suspend solids (SS), can be used to characterize the above three wastewater streams. Their process data are given in Table 1. The entire period of production cycle starts at 0 h and ends at 20 h. The effects of SS are not considered in this example due to the fact that its concentration level is quite low in all the wastewater streams. On the other hand, since the COD of these waters is too high to be processed by the municipal treatment facility, they are required to be pretreated before leaving the plant. Consequently, the flow-rate and COD of wastewater must be equalized according to the operation constraints of the pretreatment system. In particular, the variation of equalized flowrate should be limited within the range [10.16,11.24] m³/h and COD variation must be controlled in [2125,2348] mg/L. The mathematical programming model was constructed according to a superstructure with two buffer tanks, three sources and one sink.

In this example, the lower bound on the total transported water volume LB^{V} was set to be 6.0 m³; the upper bound of flow-rate UB^F was assigned a value of 50 m³/h. No limits were imposed on the branch numbers connected to the mixers and splitters in this case. The minimum installation cost was determined to be 13.98 cost unit, and the solution time was 4.5 s. The required buffer volumes in this optimal equalization system were found to be 42.5 and 12.3 m³, respectively. The optimal network configuration is shown in Fig. 5. It can be observed that two branches, i.e. the ones from E_3 to T_1 and from T_1 to T_2 , are excluded in the solution. This is apparently due to the inequality constraints imposed on the total transported volumes. The flowrate and COD profiles at the sink are presented in Figs. 6 and 7, respectively. It can be observed that both the equalized flow-rate and COD vary within the upper and lower limits required by the pre-treatment system. From Fig. 6, one can also see that the needed flow-control policy in the equalization system is quite



Fig. 5. Optimal equalization structure obtained in Example 2.



Fig. 6. Flow-rate of wastewater at the sink (Example 2).



Fig. 7. COD of wastewater at the sink (Example 2).

simple and feasible. Finally, the volume profiles of stored waters in the two buffer tanks are presented in Fig. 8. Notice that again the stored volume in each tank reaches zero at more than one instance during the production cycle.



Fig. 8. Profile of storage volume in buffer tank (Example 2).

Table 2
Additional process data of generated wastewaters in Example 3

Production line	<i>t</i> _s (h)	t _f (h)	Flow-rate (m ³ /h)	COD (mg/L)	SS (mg/L)
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 the wastewater treatment systems in Example 3

Sink	Flow(m ³ /h)		COD(mg/L)		SS(mg/L)	SS(mg/L)	
	Minimum	Maximum	Minimum	Maximum	Minimum	Maximum	
1	8	12	2000	2500	0	50	
2	10	14	0	150	300	500	

5.3. Example 3

Let us expand the scope of Example 2 to include another two production lines in the company described above. The process data of these additional wastewater streams are provided in Table 2 and the duration of a cycle time is also 20 h. Notice that the wastewaters generated in the first three production lines are rich in organic compounds, while those generated in the fourth and fifth lines are dominated by suspended solids. Consequently, two types of treatment systems (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. The number of buffer tanks used in the superstructure is still chosen to be two. Our design objective here is to obtain a minimum-cost wastewater equalization system that satisfies the requirements of treatment systems at the sinks.

In this example, the lower limit on the total transported volume in a single connection line, i.e. LB^V , was chosen to be 4.0 m^3 ; the upper bound of flow-rate UB^F was set to 80 m^3 /h. In the corresponding mathematical program, the maximum num-



Fig. 9. Optimal equalization structure obtained in Example 3.



Fig. 10. Flow-rate profile at sink 1 (Example 3).

ber of output branches from each source is limited to three, and such limits on other splitters and mixers are not imposed. The proposed model was again solved to obtain the optimal design of the equalization system in this case. The total solution time is 16.1 s. The minimum cost was determined to be 32.58 cost unit. The corresponding sizes of the two buffer tanks are 93.3 and 116.6 m³, respectively. The optimal network structure is shown in Fig. 9. It can be observed that most of the organic-rich wastewaters from E_1 , E_2 and E_3 are stored in tank 1; while those generated by E_4 and E_5 (which are rich in suspended solids) are stored in tank 2. The profiles of equalized flow-rate and pollutant indices are provided in Figs. 10–15. It can be again observed that all operation requirements of the treatment units at the sinks are



Fig. 11. COD profile at sink 1 (Example 3).







Fig. 13. Flow-rate profile at sink 2 (Example 3).



Fig. 14. COD profile at sink 2 (Example 3).



Fig. 15. SS profile at sink 2 (Example 3).

satisfied and the resulting flow-control policies are simple and realizable.

6. Conclusion

A general mixed-integer non-linear programming 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 a finite number of time intervals. For practical reasons, structure simplification is achieved with inequality constraints formulated in binary variables. Three examples are presented in this paper to demonstrate the effectiveness of the proposed approach.

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References

- Almato, M., Sanmarti, E., Espuna, A., & Puigjaner, L. (1997). Rationalizing the water use in batch process industry. *Computers and Chemical Engineering*, 21, s971–s976.
- Almato, M., Espuna, A., & Puigjaner, L. (1999). Optimization of water use in batch process industries. *Computers and Chemical Engineering*, 23, 1427– 1437.
- Bagajewicz, M. (2000). A review of recent design procedures for water networks in refineries and process plants. *Computers and Chemical Engineering*, 24, 2093–2113.
- Brooke, A., Kendrik, D., Meeraus, A., & Ramam, R. (1998). GAMS: A user guide. GAMS Development Corporation.
- Feng, X. & Seider, W. D. (2001). New structure and design methodology for water networks. *Industrial & Engineering Chemistry Research*, 40, 6140– 6146.
- Galan, B. & Grossmann, I. E. (1998). Optimal design of distributed wastewater treatment networks. *Industrial & Engineering Chemistry Research*, 37, 4036–4048.
- Happel, J. & Jordan, D. G. (1975). Chemical Process Economics (2nd ed.). Marcel Dekker Inc., p. 229.
- Hernandez-Suarez, R., Castellanos-Fernandez, J., & Zamora, J. M. (2004). Superstructure decomposition and parametric optimization approach for the synthesis of distributed wastewater treatment networks. *Industrial & Engineering Chemistry Research*, 43 (9), 2175–2191.
- Huang, C. H., Chang, C. T., Ling, H. C., & Chang, C. C. (1999). A mathematical programming model for water usage and treatment network design. *Industrial & Engineering Chemistry Research*, 38, 2666–2679.
- Hui, C. W., Li, B. H., & Smith, R. (2003). Cutting the wastewater peaks for cylic batch production plants. *Engineering in Life Sciences*, 3, 77–84.
- Kim, J. K. & Smith, R. (2004). The automated design of discontinuous waster systems. Process Safety and Environmental Protection, 82 (May), 238–248.
- Kuo, W. C. J. & Smith, R. (1997). Effluent treatment system design. *Chemical Engineering Science*, 52, 4273–4290.
- Kuo, W. C. J. & Smith, R. (1998). Designing for the interactions between wateruse and effluent treatment. *Chemical Engineering Research and Design*, 76, 287–301.
- Li, B. H., Fan, X. S., & Yao, P. J. (2002a). A new method for effluent treatment system design. *Chinese Journal of Chemical Engineering*, 10 (3),273–280.
- Li, B. H., Hui, C. W., & Smith, R. (2002b). Wastewater equalization for batch production plants. *Engineering in Life Sciences*, 2, 190–194.
- McLaughlin, L. A., McLaugh, H. J., & Groff, K. A. (1992). Develop an effective wastewater treatment strategy. *Chemcal Engineering Progress*, September, 34–42.
- Nemerow, N. L. (1971). Liquid waste of industry-Theories, Practices and Treatment. Addison-Wesley Publishing Company pp. 79–82.

- Puigjaner, L., Espuna, A., & Almato, M. (2000). A software tool for helping in decision-making about water management in batch process industries. *Waste Management*, 20, 645–649.
- Tumsen, N. R., Velioglu, S. G., & Hortacsu, O. (1996). Baker's yeast plant scheduling for wastewater equalization. In G. V. Reklaitis, A. K. Sunol, D. W. T. Rippin, O. Hortacsu (Eds.), Batch Processing Systems Engineering (pp. 821-837). NATO ASI Series F, 143, Berlin: Springer Verlag.
- Rippin, D. W. T. (1991). Batch process planning. *Chemical Engineering*, May, 100–107.
- Takama, N., Kuriyama, T., Shiroko, K., & Umeda, T. (1980). Optimal water allocation in a petroleum refinery. *Computers and Chemical Engineering*, 4, 251–258.
- Tsai, M. J. & Chang, C. T. (2001). Water usage and treatment network design using genetic algorithms. *Industrial & Engineering Chemistry Research*, 40, 4874–4888.

- Wang, B., Feng, X., & Zhang, Z. (2003). A design methodology for multiplecontaminant water networks with single internal water main. *Computers and Chemical Engineering*, 27, 903–911.
- Wang, Y. P. & Smith, R. (1994a). Wastewater minimization. Chemical Engineering Science, 49, 981–1000.
- Wang, Y. P. & Smith, R. (1994b). Design of distributed effluent treatment systems. *Chemical Engineering Science*, 49 (18), 3127–3145.
- Wang, Y. P. & Smith, R. (1995). Time pinch analysis. *Chemical Engineering Research and Design*, 73, 905–914.
- Winkel, M. L., Zullo, L. C., Verheijen, P. J. T., & Pantelides, C. C. (1995). Modelling and simulation of the operation of an industrial batch plant using gPROMS. *Computers and Chemical Engineering*, 19, s571– s576.
- Yang, Y. H., Lou, H. H., & Huang, Y. L. (2000). Synthesis of an optimal wastewater reuse work. Waste Management, 20, 311–319.