Integrated Water Network Designs for Batch Processes

Kai-Fang Cheng and Chuei-Tin Chang*

Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan 70101, Republic of China

A general mixed-integer nonlinear programming (MINLP) model is developed in this study to synthesize water networks in batch processes. The proposed model formulation is believed to be superior to the available ones. In the past, the tasks of optimizing batch schedules, water-reuse subsystems, and wastewater treatment subsystems were performed individually. In this study, all three optimization problems are incorporated in the same mathematical programming model. By properly addressing the issue of interaction between subsystems, better overall designs can be generated. The resulting design specifications include the following: the production schedule, the number and sizes of buffer tanks, the physical configuration of the pipeline network, and the operating policies of water flows. The network structure can also be strategically manipulated by imposing suitable logic constraints. A series of illustrative examples are presented to demonstrate the effectiveness of the proposed approach.

1. Introduction

In the literature, studies on the designs of water-reuse and wastewater-treatment networks in chemical plants were mainly concerned with the continuous processes, while very little attention has been directed toward the development of water conservation strategies for batch operations. Takama et al.[1] first defined the design problem of optimizing the continuous water network in a refinery. They devised a superstructure in which all possible network connections can be included. In order to avoid analyzing the interactions between water-reuse and wastewater-treatment subsystems in continuous processes, various different approaches were then proposed to optimize these two components *individually*.[2−13] On the other hand, Huang et al.[14] and Tsai and Chang[15] developed a comprehensive mathematical programming model and its solution procedures to generate an integrated network design comprising the aforementioned two subsystems. Later, Gunaratnam et al.[16] also performed a similar study with the same approach.

It has been well-recognized that batch processes are suitable for producing multiple products in small quantities. When compared with its continuous counterpart, a batch production scheme is clearly more flexible. Specifically, the process configuration of a batch plant can be easily adjusted to meet the market demand.[17] However, since waters are consumed and/or generated intermittently, the water-network designs for batch processes are obviously more complicated than the continuous ones. Almato et al.[18,19] and Puigjaner et al.[20] used Gantt charts to specify the time periods in which waters are charged to or discharged from water-using operations. They adopted the method of simulated annealing to obtain the optimal solution of the corresponding mathematical model. Wang and Smith[21] developed a modified version of the pinch method to minimize the amount of wastewater discharged from a batch process. In a later study, Kim and Smith[22] proposed a mixed-integer nonlinear programming (MINLP) formulation to automate the design procedure of such discontinuous water-reuse systems. Majozi[23,24] combined the design models for batch scheduling and water-reuse subsystem design to minimize the total volume of consumed freshwater. He assumed that the mass load or outlet pollutant concentration of every water user is constant and the number and volumes of buffer tanks is fixed. It can be observed that the charging and discharging time periods of each water user were identical in these works. In addition, the capacity and concentration constraints were not imposed on the sinks and thus the treatment capacities of the wastewaters were essentially assumed to be unlimited in the aforementioned studies. On the other hand, McLaughlin et al.[25] indicated that a wastewater-treatment unit should be designed to handle the peak processing rate. Thus, the flow rate and also pollutant concentrations of every wastewater stream should be equalized (or controlled) within certain desirable ranges before entering the treatment unit. Chang and Li[26,27] developed mathematical models to design the stand-alone water equalization systems for batch processes and also to synthesize water-reuse networks equipped with buffer tanks for equalization purposes.

Notice that the available design methods can only be used for synthesizing the subsystems of a batch water network, i.e., the batch schedule, the water-reuse network, and the wastewater-treatment network. In the present study, the three optimization problems are incorporated in a single mixed-integer nonlinear programming (MINLP) model for generating the integrated water networks in batch processes. To illustrate the proposed approach, the interactions between subsystems are first described in section 2. The mathematical programming models used for batch scheduling and water-reuse network design are presented in sections 3 and 4, respectively. Three examples are then provided in section 5 to show the potential benefits that can be achieved by integrating the scheduling model and the design model of a water-reuse network. The design model of a wastewater-treatment network is given in section 6. Two additional examples are presented in section 7 to demonstrate the advantages of simultaneously optimizing water-reuse and wastewater-treatment networks. The design method of a fully integrated water network is explained with a final example in section 8.

2. Subsystems of Batch Water Networks

As mentioned previously, a comprehensive design of the water network in a batch process consists of three components, i.e., the batch schedule, water-reuse network design, and wastewater-treatment network design. Naturally, the correspond-

* To whom correspondence should be addressed. Tel.: 886-6-2757575 ext 62663. Fax: 886-6-2344496. E-mail: ctchang@mail.ncku.edu.tw.

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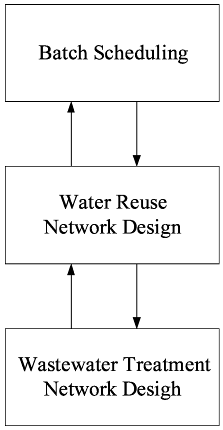

Figure 1. Components in an integrated batch water-network design.

ing design procedures are interrelated, and their general relations are depicted in Figure 1. Notice that every subsystem can be independently synthesized by ignoring the variations in the inputs from its neighbor(s). In fact, these components have already been individually discussed in various studies. To facilitate explanation of the integrated design strategy, the mathematical programming models used for the subsystem designs are first reviewed in the following. By combining these models so as to optimize more than one subsystem simultaneously, the benefits of the proposed approach can then be clearly demonstrated.

3. Batch Scheduling

The main challenge of production scheduling is to specify the appropriate time interval and allocate the suitable unit(s) to perform every task of the batch process in order to maximize profit. The conventional state-task network (STN)[28] is adopted in this study to represent the batch production process. A mathematical programming model can be formulated accordingly to identify the optimal schedule.

3.1. Time Models and Set Definitions. It has been well-established that the complexity of a scheduling model is linked directly to the embedded time model. There are two common alternatives, i.e., the discrete-time model and the continuous-time model. In the former case, the entire time horizon is divided into a finite number of time intervals with constant duration. On the other hand, the concept of event point is adopted in the latter approach to represent the precedence order of various events.[29,30] Although it has been suggested that the event-point-based model is simpler, the discrete-time model is still adopted in the present study. This is due to the need to integrate the scheduling model with the other two components in overall water network design. Let us assume that the entire time horizon can be divided into N_I equal intervals. In particular, the number of time intervals is computed in this study according to the following equation:

$$N_\mathrm{I} = \frac{H}{\mathrm{DT}} \tag{1}$$

where H is a fixed horizon time, and DT is the length of the time interval. These time intervals are collected in a set, i.e., $\mathbf{T} = \{1, 2, 3, \cdots, N_\mathrm{I} - 1, N_\mathrm{I}\}$, and their boundary points are collected in another $\mathbf{N} = \{0, 1,2, 3, \cdots, N_\mathrm{I} - 1, N_\mathrm{I}\}$.

To be able to present the mathematical model succinctly, it is necessary to first provide the definitions of a number of sets to classify the tasks, units, and states in the batch schedules, i.e.

$$\mathbf{I} = \{i \mid i \text{ is the label of a task}\}$$

$$\mathbf{I}_j = \{i \mid i \text{ is the label of a task for which unit } j \text{ can be used}\}$$

$$\mathbf{I}_s^{\mathrm{in}} = \{i \mid i \text{ is the label of a task whose input is state } s\}$$

$$\mathbf{I}_s^{\mathrm{out}} = \{i \mid i \text{ is the label of a task whose output is state } s\}$$

$$\mathbf{J} = \{j \mid j \text{ is the label of a unit}\}$$

$$\mathbf{J}_i = \{j \mid j \text{ is the label of a unit to which task } i \text{ can be assigned}\}$$

$$\mathbf{S} = \{s \mid s \text{ is the label of a state}\}$$

$$\mathbf{S}_p = \{s \mid s \text{ is the label of a state corresponding to product } p\}$$

$$\mathbf{S}_r = \{s \mid s \text{ is the label of a state corresponding to raw material } r\}$$

3.2. Model Formulation. The constraints and objective function of the conventional scheduling model[31] are summarized as follows:

- Material balances

$$S_{\mathrm{s,n}} = S_{\mathrm{s,n}-1} - \sum_{i \in \mathbf{I}_s^{\mathrm{in}}} \sum_{j \in \mathbf{J}_i} \rho_{s,i}^{c} \mathrm{BS}_{i,j,n} + \sum_{i \in \mathbf{I}_s^{\mathrm{out}}} \sum_{j \in \mathbf{J}_i} \rho_{s,i}^{p} \mathrm{BE}_{i,j,n} - D_{\mathrm{s,n}} + R_{\mathrm{s,n}} \quad \forall\, s \in \mathbf{S}, \quad \forall\, n \in \mathbf{N}\ (n \geq 1) \tag{2}$$

where $S_{s,n}$ represents the amount of material stored in state s at time point n; $D_{s,n}$ is the amount of material sold in state s at time point n; $R_{s,n}$ is the amount of material purchased in state s at time point n; $\mathrm{BS}_{i,j,n}$ is the amount of material that starts task i in unit j at time point n; $\mathrm{BE}_{i,j,n}$ is the amount of material that ends task i in unit j at time point n; $\rho_{s,i}^{c}$ denotes the proportion of input to task i from state s; ρ_{si}^{p} denotes the proportion of output from task i to state s. Notice that only$\rho_{s,i}^{c}$ and ρ_{si}^{p} are design parameters, while the rest of the aforementioned quantities are all variables.

- Allocation constraints

$$\sum_{i \in \mathbf{I}_j} (\mathrm{WS}_{i,j,n} + \mathrm{WP}_{i,j,n}) \leq 1, \quad \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N} \tag{3}$$

$$\sum_{i \in \mathbf{I}_j} (\mathrm{WP}_{i,j,n} + \mathrm{WE}_{i,j,n}) \leq 1, \quad \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N} \tag{4}$$

$$\mathrm{WS}_{i,j,n-1} + \mathrm{WP}_{i,j,n-1} = \mathrm{WP}_{i,j,n} + \mathrm{WE}_{i,j,n}, \quad \forall\, i \in \mathbf{I}_j, \quad \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N}\ (n \geq 1) \tag{5}$$

where $\mathrm{WS}_{i,j,n}$, $\mathrm{WP}_{i,j,n}$, and $\mathrm{WE}_{i,j,n}$ are binary variables. $\mathrm{WS}_{i,j,n}$ equals 1 if unit j starts tasks i at time point n; $\mathrm{WP}_{i,j,n}$ assumes the value 1 if unit j is processing tasks i at time point n; $\mathrm{WE}_{i,j,n}$ assumes the value 1 if unit j ends tasks i at time point n.

- Capacity constraints

$$B_{i,j}^{\min} \mathrm{WS}_{i,j,n} \leq \mathrm{BS}_{i,j,n} \leq B_{i,j}^{\max} \mathrm{WS}_{i,j,n}, \quad \forall\, i \in \mathbf{I}_j, \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N} \tag{6}$$

$$B_{i,j}^{\min} \mathrm{WP}_{i,j,n} \leq \mathrm{BP}_{i,j,n} \leq B_{i,j}^{\max} \mathrm{WP}_{i,j,n}, \quad \forall\, i \in \mathbf{I}_j, \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N} \tag{7}$$

$$B_{i,j}^{\min}\mathrm{WE}_{i,j,n} \le \mathrm{BE}_{i,j,n} \le B_{i,j}^{\max}\mathrm{WE}_{i,j,n}, \quad \forall\, i \in \mathbf{I}_j, \forall\, j \in \mathbf{J}, \forall\, n \in \mathbf{N} \quad (8)$$

where $\mathrm{BP}_{i,j,n}$ is the amount of material being processed by task i in unit j at time point n; $B_{i,j}^{\min}$ and $B_{i,j}^{\max}$ are design parameters denoting, respectively, the minimum and maximum capacities of task i in unit j.

- Storage constraints

$$S_{s,n} \le M_s, \quad \forall\, s \in \mathbf{S}, \forall\, n \in \mathbf{N} \quad (9)$$

where M_s denotes the maximum storage capacity of state s, which is a design parameter.

- Purchase and demand constraints

$$D_{s,n} \ge d_s, \quad \forall\, s \in \mathbf{S}_p, \forall\, n \in \mathbf{N} \quad (10)$$

$$D_{s,n} = 0, \quad \forall\, s \notin \mathbf{S}_p, \forall\, n \in \mathbf{N} \quad (11)$$

$$R_{s,n} \le r_s, \quad \forall\, s \in \mathbf{S}_c, \forall\, n \in \mathbf{N} \quad (12)$$

$$R_{s,n} = 0, \quad \forall\, s \notin \mathbf{S}_c, \forall\, n \in \mathbf{N} \quad (13)$$

where d_s and r_s are two parameters representing the minimum demand for product s and the maximum supply of raw material s, respectively.

- Other constraints

$$\mathrm{TE}_{i,j} = \mathrm{TS}_{i,j} + \tau_i, \quad \forall\, j \in \mathbf{J}, \forall\, i \in \mathbf{I}_j \quad (14)$$

$$\mathrm{WP}_{i,j,0} = 0, \quad \forall\, j \in \mathbf{J}, \forall\, i \in \mathbf{I}_j \quad (15)$$

$$\mathrm{WE}_{i,j,0} = 0, \quad \forall\, j \in \mathbf{J}, \forall\, i \in \mathbf{I}_j \quad (16)$$

$$\mathrm{WS}_{i,j,N_\mathrm{I}} = 0, \quad \forall\, j \in \mathbf{J}, \forall\, i \in \mathbf{I}_j \quad (17)$$

$$\mathrm{WP}_{i,j,N_\mathrm{I}} = 0, \quad \forall\, j \in \mathbf{J}, \forall\, i \in \mathbf{I}_j \quad (18)$$

where $\mathrm{TS}_{i,j}$ and $\mathrm{TE}_{i,j}$ represent, respectively, the start and end times of task i assigned to unit j; τ_i is the parameter denoting the processing time of task i.

- Objective function

$$\mathrm{obj}_{\mathrm{schedule}} = \sum_{n\in\mathbf{N}} \sum_{s\in\mathbf{S}_p} C_s^P D_{s,n} - \sum_{n\in\mathbf{N}} \sum_{s\in\mathbf{S}_r} C_s^R R_{s,n} \quad (19)$$

where C_s^R and C_s^P are the cost coefficients of raw material and product, respectively.

Constraint 2 is the material balance of state s between time point n and $n - 1$. Constraint 3 enforces the limitation that only one task can be started or processed in the same unit at the same time point. In the same way, constraint 4 ensures that only one task can be processed or ended in the same unit at the same time point. Constraint 5 shows that if task i is started or processed in unit j at time point $n - 1$, it must be processed or ended at time point n. In order to limit the range of task i assigned to unit j, it is necessary to impose constraints 6−8. The upper bound of the storage capacity of state s at time point n is provided in constraint 9. Constraints 10−13 show the upper and lower bounds of the amounts of purchased raw material $R_{s,n}$ and sold product $D_{s,n}$, respectively. Constraint 14 shows that the end time of task i assigned to unit j must equal the sum of its start time and processing time. Constraints 15 and 16 show that tasks can only be started at the first time point. Constraints 17 and 18 show that tasks can only be ended at the final time point. Finally, the objective function is presented in eq 19.

4. Water-Reuse Network Design

Having determined the production schedule and the water generation and/or consumption rates of every task in the schedule, one can then design the water-reuse network accordingly. The following mathematical programming model can be adopted for this purpose.

4.1. Sets. In order to describe the proposed mathematical programming model clearly, let us first introduce the following set definitions:

$$\mathbf{SA} = \{sa \mid sa \text{ is the label of an external water source}\}$$

$$\mathbf{SB} = \{sb \mid sb \text{ is the label of a water-generating operation without consuming any usable water}\}$$

$$\mathbf{S} = \mathbf{SA} \cup \mathbf{SB} = \{s \mid s \text{ is the label of a water source of the water-reuse network}\}$$

$$\mathbf{OA} = \{oa \mid oa \text{ is the label of a water sink in the environment}\}$$

$$\mathbf{OB} = \{ob \mid ob \text{ is the label of a wastewater-treatment unit}\}$$

$$\mathbf{OC} = \{oc \mid oc \text{ is the label of a water-consuming operation without generating any wastewater}\}$$

$$\mathbf{O} = \mathbf{OA} \cup \mathbf{OB} \cup \mathbf{OC} = \{o \mid o \text{ is the label of a sink of the water-reuse network}\}$$

$$\mathbf{UA} = \{ua \mid ua \text{ is the label of a water user with non-identical charging and discharging time intervals}\}$$

$$\mathbf{UB} = \{ub \mid ub \text{ is the label of a water user with identical charging and discharging time intervals}\}$$

$$\mathbf{U} = \mathbf{UA} \cup \mathbf{UB} = \{u \mid u \text{ is the label of a water user}\}$$

$$\mathbf{B} = \{b \mid b \text{ is the label of a buffer tank in the water-reuse network}\}$$

$$\mathbf{E} = \{e \mid e \text{ is the label of an equipment which facilitates at least one operation defined in } \mathbf{U}, \mathbf{SB}, \text{ or } \mathbf{OC}\}$$

$$\mathbf{P}_e = \{p \mid p \text{ is the label of an operation carried out in equipment } e \in \mathbf{E}\}$$

$$\mathbf{K} = \{k \mid k \text{ is the label of a pollutant index}\}$$

Finally, it should be noted that

$$\bigcup_{e\in\mathbf{E}} \mathbf{P}_e = \mathbf{U} \cup \mathbf{SB} \cup \mathbf{OC}$$

4.2. Superstructure. Similar to other mathematical programming approach to process synthesis, a superstructure (Figure 2) must be constructed to incorporate all possible flow configurations. This structure can be built by implementing the following steps:

(1) Place a mixing node M at the inlet of each water user, buffer tank, and sink;

(2) Place a splitting node S at outlet of each source, water user, and buffer tank;

(3) Connect the split branches from the splitting node after each source in **SA** to all mixing nodes;

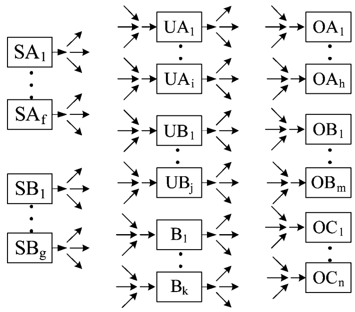

Figure 2. Superstructure of water-reuse subsystem.

(4) Connect the split branches from the splitting node after every source in **SB** and also at every water user in **U** to the mixing nodes before the buffer tanks in **B** and sinks in **OA** and **OB** but not to those before the water users in **U** and the sinks in **OC**;

(5) Connect the split branches from the splitting node after each buffer tank in **B** to all mixing nodes except the one before itself.

The labels of splitting and mixing nodes are also collected in two additional sets to facilitate a concise model formulation, i.e.

$$\mathbf{MX} = \{mx \mid mx \text{ is the label of a mixing node in the water-reuse network}\} = \mathbf{U} \cup \mathbf{B} \cup \mathbf{O}$$

$$\mathbf{SP} = \{sp \mid sp \text{ is the label of a splitting node in the water-reuse network}\} = \mathbf{S} \cup \mathbf{U} \cup \mathbf{B}$$

Let us express the sets of starting and ending nodes of the branches produced in steps 3, 4, and 5 as $\mathbf{SP}_i$ and $\mathbf{MX}_i$ ($i = 1, 2, 3$), respectively. They can be obtained according to the following conventions:

- In step 3, $\mathbf{SP}_1 = \mathbf{SA}$ and $\mathbf{MX}_1 = \mathbf{MX}$;
- In step 4, $\mathbf{SP}_2 = \mathbf{SB} \cup \mathbf{U}$ and $\mathbf{MX}_2 = \mathbf{B} \cup \mathbf{OA} \cup \mathbf{OB}$;
- In step 5, $\mathbf{SP}_3 = \mathbf{B}$ and $\mathbf{MX}_3 = \mathbf{MX}$.

Also

$$\cup_{i=1}^{3} \mathbf{SP}_i = \mathbf{SP}$$

Notice that the splitting nodes in $\mathbf{SP}_2$ are not connected to every mixing node. Upon the basis of the belief that the upstream disturbances in wastewater streams can always be smoothed with buffer tanks, this design practice is adopted mainly to facilitate better operability.

4.3. Model Formulation. Sources. The water sources can be classified into two types, i.e., freshwater (**SA)** and secondary water (**SB)**. The flow constraints of waters from the sources in **SA** and **SB** can be expressed as

$$f_{sa,t}^{\text{source}} \leq F_{sa} \quad sa \in \mathbf{SA},\, t \in \mathbf{T} \tag{20}$$

$$f_{sb,t}^{\text{source}} = F_{sb,t} \quad sb \in \mathbf{SB},\, t \in \mathbf{T} \tag{21}$$

where, $f_{sa,t}^{\text{source}}$ and $f_{sb,t}^{\text{source}}$ represent, respectively, the flow rates of fresh water sa and secondary water sb in time interval t; F_{sa} is the maximum allowable supply rate of freshwater from source sa; $F_{sb,t}$ is the nominal supply rate of secondary water from source sb during time interval t. On the other hand, the water qualities of the freshwaters and secondary waters should be considered as known data, i.e.,

$$c_{s,k,t}^{\text{source}} = C_{s,k,t} \quad s \in \mathbf{S},\, k \in \mathbf{K},\, t \in \mathbf{T} \tag{22}$$

where $c_{s,k,t}^{\text{source}}$ denotes the pollution index k in the water stream from source s during time interval t; $C_{s,k,t}$ is a given parameter.

The material balance around the splitting node after each water source in set **SA** and **SB** can be written as

$$f_{sa,t}^{\text{source}} = \sum_{mx \in \mathbf{MX}} \text{fs}_{sa,mx,t} \quad sa \in \mathbf{SA},\, t \in \mathbf{T} \tag{23}$$

$$f_{sb,t}^{\text{source}} = \sum_{b \in \mathbf{B}} \text{fs}_{sb,b,t} + \sum_{oa \in \text{OA}} \text{fs}_{sb,oa,t} + \sum_{ob \in \mathbf{B}} \text{fs}_{sb,ob,t} \quad sb \in \mathbf{SB},\, t \in \mathbf{T} \tag{24}$$

In the above equations, fs is a variable used to denote the flow rate of each branch and its subscript denotes the flow direction. For example, $\text{fs}_{sa,mx,t}$ represents the flow rate of a stream from source sa to mixing node mx during time interval t. In the same way, $\text{cs}_{s,k,t}$ is a variable denoting the value of the kth pollution index in the split branches from splitting node s.

Finally, notice that the pollution indices in the water streams before and after a splitting node should be identical, i.e.,

$$c_{s,k,t}^{\text{source}} = \text{cs}_{s,k,t} \quad s \in \mathbf{S},\, k \in \mathbf{K},\, t \in \mathbf{T} \tag{25}$$

Water Users. The overall mass balances can be written as

$$\text{DT} \sum_{t \in \mathbf{TC}_u} f_{u,t}^{\text{in}} = \text{DT} \sum_{t' \in \mathbf{TD}_u} f_{u,t'}^{\text{out}} + \text{DV}_u \quad u \in \mathbf{U} \tag{26}$$

Here, DV_u represents the total water loss in water user u; $f_{u,t}^{\text{in}}$ and $f_{u,t'}^{\text{out}}$ denote, respectively, the input and output flow rates of water user u during interval t; $\mathbf{TC}_u$ and $\mathbf{TD}_u$ denote, respectively, the set of time intervals in which the charging and discharging operation of water user u take place.

The water users can be divided into two classes, **UA** and **UB**. Their component balances can be expressed, respectively, as

$$\text{DT} \sum_{t \in \mathbf{TC}_u} f_{ua,t}^{\text{in}} c_{ua,,k,t}^{\text{in}} + M_{ua,k} = \text{DT} \sum_{t' \in \mathbf{TD}_u} f_{ua,t'}^{\text{out}} c_{ua,k,t'}^{\text{out}} \quad ua \in \mathbf{UA},\, k \in \mathbf{K} \tag{27}$$

$$f_{ub,t}^{\text{out}} c_{ub,k,t}^{\text{out}} = f_{ub,t}^{\text{in}} c_{ub,k,t}^{\text{in}} + \mu_{ub,k} \quad ub \in \mathbf{UB},\, k \in \mathbf{K},\, t \in \mathbf{T}_{ub} \tag{28}$$

where, $c_{ua,k,t}^{\text{in}}$ and $c_{ub,k,t}^{\text{in}}$ represent the kth pollutant index in the feed stream of water user ua an ub during time interval t; $c_{ua,k,t}^{\text{out}}$ and $c_{ub,k,t}^{\text{out}}$ denote, respectively, the kth pollutant index in the output stream of water user ua and ub during time interval t; $M_{ua,k}$ is a given parameter which represents the accumulated mass load of pollutant index k in operation ua; $\mu_{ub,k}$ is the instantaneous mass load of pollutant k in water user ub; $\mathbf{T}_{ub}$ is the set of time intervals for operating water user ub. Notice that, $\mathbf{TC}_u \neq \mathbf{TD}_u$ when $u \in \mathbf{UA}$; $\mathbf{T}_u = \mathbf{TD}_u = \mathbf{TC}_u$ if $u \in \mathbf{UB}$. The mass balances around the mixing node before each water user and the splitting node after each water user can be written as

$$f_{u,t}^{\text{in}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{s,u,t} + \sum_{b \in \mathbf{B}} \text{fs}_{b,u,t} \quad u \in \mathbf{U},\, k \in \mathbf{K},\, t \in \mathbf{TC}_u \tag{29}$$

$$f_{u,t}^{\text{in}} c_{u,k,t}^{\text{in}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{sa,u,t} \text{cs}_{s,k,t} + \sum_{b \in \mathbf{B}} \text{fs}_{b,u,t} \text{cs}_{b,k,t} \quad u \in \mathbf{U},\, k \in \mathbf{K},\, t \in \mathbf{TC}_u \tag{30}$$

$$f_{u,t}^{\text{out}} = \sum_{b \in \mathbf{B}} \text{fs}_{u,b,t} + \sum_{oa \in \mathbf{OA}} \text{fs}_{u,oa,t} + \sum_{ob \in \mathbf{OB}} \text{fs}_{u,ob,t} \quad u \in \mathbf{U}, k \in \mathbf{K}, t \in \mathbf{TD}_u \tag{31}$$

$$C_{u,k,t}^{\text{out}} = \text{cs}_{u,k,t} \quad u \in \mathbf{U}, k \in \mathbf{K}, t \in \mathbf{TD}_u \tag{32}$$

The constraints of input flow rate can be written as

$$f_u^{\min} \le f_{u,t}^{\text{in}} \le f_u^{\max} \quad u \in \mathbf{U}, t \in \mathbf{TC}_u \tag{33}$$

Also, pollutant indices at the inlets and outlets of the water user may subject to additional inequality constraints in order to maintain operation efficiency, i.e.

$$c_{u,k,t}^{\text{in}} \le \eta_{u,k}^{\text{in}}, \; c_{u,k,t}^{\text{out}} \le \eta_{u,k}^{\text{out}} \quad u \in \mathbf{U}, k \in \mathbf{K}, t \in \mathbf{T} \tag{34}$$

where, $f_u^{\max}$ and $f_u^{\min}$ are the upper and lower bounds of throughput; $\eta_{u,k}^{\text{in}}$ and $\eta_{u,k}^{\text{out}}$ are given parameters.

Buffer Tanks. The buffer tanks are used in the water network to improve the chance of water reuse. The mass-balance relations around each tank can be written as

$$v_{b,t} = v_{b,t-1} + (f_{b,t}^{\text{in}} - f_{b,t}^{\text{out}})\text{DT} \tag{35}$$

$$v_{b,t} c_{b,k,t}^{\text{out}} \cong v_{b,t-1} c_{b,k,t-1}^{\text{out}} + (f_{b,t}^{\text{in}} c_{b,k,t}^{\text{in}} - f_{b,t}^{\text{out}} c_{b,k,t}^{\text{out}})\text{DT} \tag{36}$$

$$b \in \mathbf{B}, k \in \mathbf{K}, t \in \mathbf{T}$$

where $v_{b,t}$ denotes the water volume in tank b at the end of time interval t; $c_{b,k,t}^{\text{in}}$ and $c_{b,k,t}^{\text{out}}$ represent, respectively, the values of pollutant index k in the inlet and outlet streams of tank b at the end of interval t;$f_{b,t}^{\text{in}}$ and $f_{b,t}^{\text{out}}$ represent, respectively, the flow rates of input and output streams of tank b during time interval t. In addition, since the batch operations are often periodic, the process conditions of every buffer tank at the starting and ending times of any operation cycle should be kept identical, i.e.

$$v_{b,0} = v_{b,N_{\text{I}}} \tag{37}$$

$$c_{b,k,0}^{\text{out}} = c_{b,k,N_{\text{I}}}^{\text{out}} \tag{38}$$

$$b \in \mathbf{B}, k \in \mathbf{K}$$

The material balances around the mixing nodes and splitting nodes are the following:

$$f_{b,t}^{\text{in}} = \sum_{\substack{sp \in \mathbf{SP} \\ sp \ne b}} \text{fs}_{sp,b,t} \tag{39}$$

$$f_{b,t}^{\text{in}} c_{b,k,t}^{\text{in}} = \sum_{\substack{sp \in \mathbf{SP} \\ sp \ne b}} \text{fs}_{sp,b,t} \text{cs}_{sp,k,t} \tag{40}$$

$$f_{b,t}^{\text{out}} = \sum_{\substack{mx \in \text{MX} \\ mx \ne b}} \text{fs}_{b,mx,t} \tag{41}$$

$$c_{b,k,t}^{\text{out}} = \text{cs}_{b,k,t} \tag{42}$$

$$b \in \mathbf{B}, k \in \mathbf{K}, t \in \mathbf{T}$$

The total volume of water in a buffer tank at any instance should be larger than zero and less than the storage capacity. The corresponding constraints can be written as

$$v_b^{\max} \ge v_{b,t} \ge 0 \quad b \in \mathbf{B}, t \in \mathbf{T} \tag{43}$$

Water Sinks. All wastewaters which cannot be reused should be discharged into the water sinks. As mentioned before, they can be divided into three groups. The mass balance around the mixing nodes before the sinks in sets **OA** and **OB** can be written as

$$f_{o,t}^{\text{sink}} = \sum_{sp \in \mathbf{SP}} \text{fs}_{sp,o,t} \tag{44}$$

$$f_{o,t}^{\text{sink}} c_{o,k,t}^{\text{sink}} = \sum_{sp \in \mathbf{SP}} \text{fs}_{sp,o,t} c_{sp,k,t} \tag{45}$$

$$o \in \mathbf{OA} \cup \mathbf{B}, k \in \mathbf{K}, t \in \mathbf{T}$$

Also, the corresponding constraints for the sinks in **OC** should be

$$f_{oc,t}^{\text{sink}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{sa,oc,t} + \sum_{b \in \mathbf{B}} \text{fs}_{b,oc,t} \tag{46}$$

$$f_{oc,t}^{\text{sink}} c_{oc,k,t}^{\text{sink}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{sa,oc,t} \text{cs}_{sa,k,t} + \sum_{b \in \mathbf{B}} \text{fs}_{b,oc,t} \text{cs}_{b,k,t} \tag{47}$$

$$oc \in \mathbf{OC}, k \in \mathbf{K}, t \in \mathbf{T}$$

The upper and lower bounds of flow rates and pollutant indices in the wastewaters discharged to the sinks in **OA** and **OB** can be written as

$$\lambda_o^{\min} \le f_{o,t}^{\text{sink}} \le \lambda_o^{\max}, \quad \theta_{o,k}^{\min} \le c_{o,k,t}^{\text{sink}} \le \theta_{o,k}^{\max}, \quad o \in \mathbf{OA} \cup \mathbf{OB}, k \in \mathbf{K}, t \in \mathbf{T} \tag{48}$$

where $\lambda_o^{\max}$ and $\lambda_o^{\min}$ represent, respectively, the minimum and maximum flow rates allowed by sink o;$\theta_{o,k}^{\max}$ and $\theta_{o,k}^{\min}$ denote the corresponding minimum and maximum values of pollutant index k. For the sinks in **OA**, $\lambda_o^{\min} = 0$ and $\theta_{o,k}^{\min} = 0$. On the other hand, the flow rates of wastewater streams delivered to the sinks in **OC** are required to be maintained at time-variant nominal levels; the equality constraint is shown below

$$f_{oc,t}^{\text{sink}} = \lambda_{oc,t} \quad oc \in \mathbf{OC}, t \in \mathbf{T} \tag{49}$$

where $\lambda_{oc,t}$ is the nominal flow rate required by sink oc in interval t. Finally, the constraints imposed upon the pollution indices in the above wastewater streams should be the same as those adopted for the sinks in **OA**.

Structural Constraints. From a practical standpoint, there is an obvious need to eliminate any branch that is used to transfer only a negligible amount of water during the entire production cycle. To prevent generating such branches in solving the proposed model, it is necessary to add the following constraints:

$$\sum_{t \in \mathbf{T}} \text{fs}_{sp,mx,t} \ge y_{sp,mx} \text{LB}^{\text{v}} \tag{50}$$

$$\text{fs}_{sp,mx,t} \le y_{sp,mx} \text{UB}^{\text{F}} \tag{51}$$

$$sp \in \mathbf{SP}_{\text{i}}, mx \in \mathbf{MX}_i, sp \ne mx, t \in \mathbf{T}$$

where $i = 1, 2, 3$; LB^{V} denotes a user-specified lower bound of the total transported water volume through any branch during a production cycle; UB^{F} is the upper bound of flow rate that must not be exceeded in any branch; $y_{sp,mx} \in \{0,1\}$ signifies whether or not the corresponding branch is selected in the optimal network configuration. If $y_{sp,mx} = 0$, $\text{fs}_{sp,mx,t}$ will be forced to zero according to eqs 50 and 51.

The number of buffer tanks embedded in the superstructure is usually larger than what is actually needed in the optimal solution. To remove the unreasonably small tanks in the system design, it is often necessary to impose a lower bound on the tank size. If buffer tank b does not exist, i.e., $x_b = 0$, the connecting branches in the superstructure should also be eliminated all together. These constraints are shown below:

$$x_b V^L \le \upsilon_b^{\max} \quad b \in \mathbf{B} \tag{52}$$

$$x_b \ge y_{b,mx} \quad mx \in \mathbf{MX}, b \ne mx \tag{53}$$

$$x_b \ge y_{sp,b} \quad sp \in \mathbf{SP}, b \ne sp \tag{54}$$

where $x_b \in \{0,1\}$ is used to reflect whether or not tank b exists; V^L is the lower limit of the tank volume.

As mentioned previously, more than one water-using operation may be carried out with the same equipment. In other words, the superstructure used in this study is only a fictitious process configuration. Additional structural constraints must therefore be incorporated in the mathematical programming model to automatically translate the optimal solution into the actual pipeline network of the resulting system design. Notice first that, if a branch in the superstructure is not used to facilitate the operation of a water user, it can be regarded as a physical pipeline. This feature can be characterized as follows:

$$z_{i,j} = y_{i,j} \quad i \in \mathbf{SA} \cup \mathbf{B}, j \in \mathbf{B} \cup \mathbf{OA} \cup \mathbf{OB} \tag{55}$$

where $z_{i,j} \in \{0,1\}$ $(i \ne j)$ is used to signify the existence of a pipeline from i to j. The binary values associated with the rest of the connection branches can be interpreted according to the logic operators suggested by Raman and Grossmann,[32] i.e.

$$z_{e',e} \le \sum_{p \in \mathbf{P}_e} y_{e',p} \quad e' \in \mathbf{SA} \cup \mathbf{B}, e \in \mathbf{B} \tag{56}$$

$$z_{e',e} \ge y_{e',p} \quad e' \in \mathbf{SA} \cup \mathbf{B}, e \in \mathbf{E}, p \in \mathbf{P}_e \tag{57}$$

$$z_{e,e'} \le \sum_{p \in P_{e'}} y_{p,e'} \quad e \in \mathbf{E}, e' \in \mathbf{B} \cup \mathbf{OA} \cup \mathbf{OB} \tag{58}$$

$$z_{e,e'} \ge y_{p,e'} \quad e \in \mathbf{E}, e' \in \mathbf{B} \cup \mathbf{OA} \cup \mathbf{OB}, p \in \mathbf{P}_e \tag{59}$$

To simplify the network structure, it is also desirable to limit the numbers of pipelines attached to the mixing and splitting nodes in the actual pipeline network. These inequality constraints can be written in the following forms:

$$\sum_{sa \in \mathbf{SA}} z_{sa,e} + \sum_{b \in \mathbf{B}} z_{b,e} \le \mathrm{NM}_e \quad e \in \mathbf{E} \tag{60}$$

$$\sum_{b \in \mathbf{B}} z_{e,b} + \sum_{oa \in \mathbf{OA}} z_{e,oa} + \sum_{ob \in \mathbf{OB}} z_{e,ob} \le \mathrm{NS}_e \quad e \in \mathbf{E} \tag{61}$$

$$\sum_{sa \in \mathbf{SA}} z_{sa,b} + \sum_{\substack{b' \in \mathbf{B} \\ b' \ne b}} z_{b',b} + \sum_{e \in \mathbf{E}} z_{e,b} \le \mathrm{NM}_b \quad b \in \mathbf{B} \tag{62}$$

$$\sum_{e \in \mathbf{E}} z_{b,e} + \sum_{\substack{b' \in \mathrm{B} \\ b' \ne b}} z_{b,b'} + \sum_{oa \in \mathbf{OA}} z_{b,oa} + \sum_{ob \in \mathrm{OB}} z_{b,ob} \le \mathrm{NS}_b \quad b \in \mathbf{B} \tag{63}$$

$$\sum_{e \in \mathbf{E}} z_{sa,e} + \sum_{b \in \mathbf{B}} z_{sa,b} + \sum_{oa \in \mathbf{OA}} z_{sa,oa} + \sum_{ob \in \mathbf{OB}} z_{sa,ob} \le \mathrm{NS}_{sa} \quad sa \in \mathbf{SA} \tag{64}$$

$$\sum_{sa \in \mathbf{SA}} z_{sa,o} + \sum_{b \in \mathbf{B}} z_{b,o} + \sum_{e \in \mathbf{E}} z_{e,o} \le \mathrm{NM}_o \quad o \in \mathbf{OA} \cup \mathbf{OB} \tag{65}$$

where NM_e and NS_e denote the upper bounds of the pipeline numbers connected to mixing node and splitting node of equipment e respectively; NM_b and NS_b denote the upper bounds of the pipeline numbers connected to mixing node and splitting node of buffer tank b respectively; NS_{sa} denotes the upper bound of the pipeline number connected to the splitting node of source sa; NM_o denote the upper bound of the pipeline number connected to mixing node of sink o.

Objective Function. The objective function of our optimization problem is the sum of the annual water cost, annualized installation cost, and annual treatment cost, i.e.,

$$\mathrm{obj}_{\mathrm{reuse}} = \Gamma_{\mathrm{SA}}\Phi_{\mathrm{SA}} + \Gamma_{\mathrm{B}}\Phi_{\mathrm{B}} + \Gamma_{\mathrm{OB}}\Phi_{\mathrm{OB}} \tag{66}$$

where Γ_{SA}, Γ_{B}, and Γ_{OB} assume only binary values. They are used in this formulation to account for various different combinations of objective functions used in practical applications. The function Φ_{SA} represents the annual cost of consumed freshwater from **SA**; Φ_{B} and Φ_{OB} denote the annualized installation cost and annual treatment cost, respectively. The annual water and treatment costs are calculated with the following formulas:

$$\Phi_{\mathrm{SA}} = N_{\mathrm{cycle}}\mathrm{DT} \sum_{sa \in \mathbf{SA}} \varphi_{sa}\Big(\sum_{t \in \mathbf{T}} f_{sa,t}^{\mathrm{source}}\Big) \tag{67}$$

$$\Phi_{\mathrm{OB}} = N_{\mathrm{cycle}}\mathrm{DT} \sum_{ob \in \mathbf{OB}} \varphi_{ob}\Big(\sum_{t \in \mathbf{T}} f_{ob,t}^{\mathrm{sink}}\Big) \tag{68}$$

where N_{cycle} is the number of production cycles carried out per year; φ_{sa} is the raw-material cost per unit volume of consumed freshwater from source sa; φ_{ob} is the treatment cost per unit volume of wastewater discharged to sink ob. The annualized installation cost of buffer tanks is determined according to

$$\Phi_{\mathrm{B}} = \sum_{b \in \mathbf{B}} [x_b \alpha_b + \beta_b (\upsilon_b^{\max})^{0.6}] \tag{69}$$

where α_b is the fixed charge and β_b is the cost coefficient of tank b.

5. Simultaneous Optimization of the Batch Schedule and Water-Reuse Subsystem Design

If the amounts of water consumed and/or generated by a water user can be assumed to be proportional to that of the process material produced in the corresponding task, the aforementioned two mathematical models can be combined for the purpose of optimizing the batch schedule and water-reuse network design simultaneously. The objective function in this case should be the net profit, i.e.

$$\mathrm{obj}_{\mathrm{int1}} = \mathrm{obj}_{\mathrm{schedule}} - \mathrm{obj}_{\mathrm{reuse}} \tag{70}$$

5.1. Example 1. Let us consider the STN shown in Figure 3. In this process, feed A is heated to produce intermediate HotA, while 50% of feed B and 50% of feed C are mixed and then reacted to form intermediate BC. 40% of HotA and 60% of BC are then mixed and reacted to form product 1 (40%) and intermediate AB (60%). On the other hand, 20% of feed C is reacted with 80% of intermediate AB to form impure E. Finally, the impure E is sent to a distillation column to separate product 2 (90%) and intermediate AB (10%). The available units, storage capacities and processing times of this process are given in Table 1. It is also assumed that the maximum amount of every feed supply is 1000 kg. For the purpose of comparing the effects of

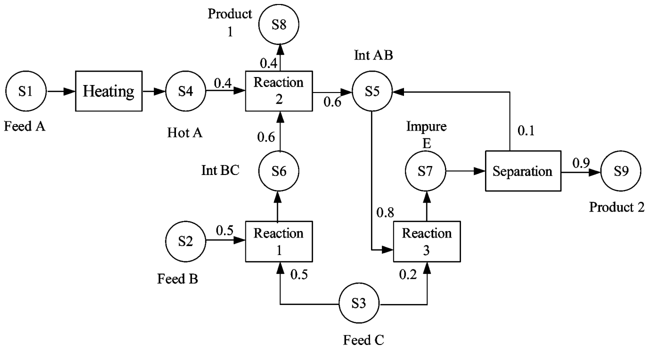

Figure 3. STN of example 1.

Table 1. Design Parameters Used in Example 1

upper limit of state	for feed (S1−S2−S3), product (S8−S9): unlimited
	for HotA (S4), ImpureE (S7): 1000 kg
	for IntAB (S5): 500 kg
	for IntBC (S6): 0 kg
equipment unit	heater: capacity 100 kg, suited for heating
	reactor1: capacity 50 kg, suited for reactions 1, 2, 3
	reactor2: capacity 80 kg, suited for reactions 1, 2, 3
	still: capacity 200 kg, suited for separation
processing of task	heating: 1 h
	reactions 1, 2: 2 h
	reaction 3: 1 h
	separation: 2 h

Table 2. Objective Values Obtained with Different Horizon Times in Example 1

time horizon (hr)	objective function (cost unit/hr)
4	341.67
5	304.58
7	301.23
8	351.43
9	338.41
10	355.33
11	344.33
12	341.67
13	360.44
14	351.43
15	351.43

varying horizon time, the objective function for this example is chosen to be

$$\Phi = \frac{\mathrm{obj}_1}{\mathrm{H}} = [\sum_{n=0}^{\mathrm{H}}(20D_{8,n} + 20D_{9,n}) - \sum_{n=0}^{\mathrm{H}}(10R_{1,n} + 10R_{2,n} + 10R_{3,n})]/\mathrm{H} \quad (71)$$

The mathematical programming model was solved with the module DICOPT within the GAMS environment. The optimal solutions corresponding to different time horizons are shown in Table 2. It can be observed that the objective function is not affected in a definite way. The Gantt chart with a time horizon of 4 h is presented in Figure 4.

5.2. Example 2. Let us next consider the batch schedule presented in Figure 4. Suppose that

• reaction 1 (RX1), separation (SEP) and heating operation (H) are water users;

• reaction 2 (RX2) is a wastewater-generating operation without consuming any usable water;

• reaction 3 (RX3) is a water-consuming operation without generating any wastewater.

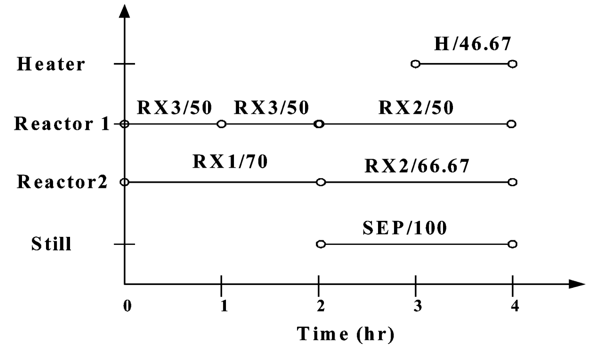

Figure 4. Gantt chart of case 1 (H = 4 hr) in example 1.

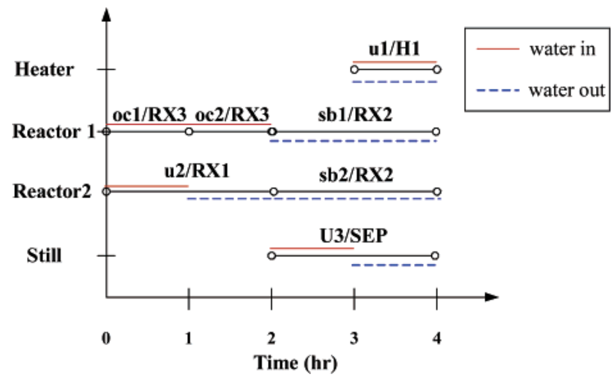

Figure 5. Gantt chart for examples 2 and 4.

Table 3. Design Parameters Used in Examples 2 and 4

operat	equip unit	nominal flow rate (m^3/hr)	start time (hr)	end time (hr)	max conc. of pollutant (ppm)
u1	e1	−46.67	3	4	0
		46.67	3	4	5
u2	e3	−35	0	1	6
		35	1	2	14
u3	e4	−50	2	3	10
		50	3	4	15
oc1	e2	−50	0	1	7
oc2	e2	−50	1	2	7
sb1	e2	25	2	4	10
sb2	e3	33.34	2	4	10

Also, it is assumed that the amounts of consumed and/or generated waters of each batch operation are directly proportional to the processing volume. The process data of all water-using operations in this system can be found in Table 3. The labels of every operation and the corresponding equipment are listed in columns 1 and 2 of this table, respectively. The nominal flow rate at its inlet and outlet are provided in column 3. A negative flow rate implies that the corresponding water stream is consumed in the operation, and a positive value represents the wastewater generation rate. The durations of the charging or discharging steps are specified in the fourth and fifth columns of Table 3. There is only one key pollutant in the water streams, and the maximum pollutant concentration in the inlet and/or outlet streams of every water-using operation are specified in column 6 of Table 3.

Only one external water source (*sa*1) is considered in this example, and its pollutant concentration is 0 ppm. The maximum water supply rate from source *sa*1 is 80 m^3/hr and, for convenience, its cost is taken to be 1 unit of value/cm^3. Also we assume that only one wastewater treatment system *ob*1 is available and the corresponding treatment cost is 3 units of value/m^3. The maximum allowable discharge rate of wastewater is 80 m^3/hr, and the pollutant concentration is required to be maintained between 5 and 10 ppm. An additional environment

Table 4. Solution Summary of Three Cases in Example 2

	scenario 1	scenario 2	scenario 3
objective value (cost unit)	620.73	110.72	79.41
freshwater cost (cost unit)	118.15	110.72	231.67
treatment cost (cost unit)	404.49	382.2	578.28
installation cost (cost unit)	98.09	1381.56	79.41
number of buffer tank	1	3	1
number of branches	12	16	14
number of pipelines	10	14	12
total amount consumed *sa*1 (m^3)	118.15	110.72	231.67
volume of buffer tank *b*1 (m^3)	98.86	30.16	52.79
volume of buffer tank *b*2 (m^3)	0	97.7	0
volume of buffer tank *b*3 (m^3)	0	100	0
total discharging vol of *ob*1(m^3)	134.83	127.4	192.76

Table 5. Design Specifications of the Water-Using Operations in Case 1 of Example 2

operation ID	flow rate (m^3/hr)	conc. (mg/L)	from/to
*u*1(*e*1)	−46.67	0	*sa*1
	46.67	5	*b*1
*u*2(*e*3)	−35	0	*sa*1
	35	8	*ob*1
*u*3(*e*4)	−50	3.12−8.31	*b*1
	50	11.13	*b*1
*oc*1(*e*2)	50	7	*b*1
*oc*2(*e*2)	50	7	*b*1
*sb*1(*e*2)	25	10	*b*1
*sb*2(*e*3)	33.34	10	*ob*1

sink *oa*1 $\in$**OA** is also assumed to be available in this example. The upper bound of its inlet pollutant concentration is set to be 2 mg/L. The number of buffer tanks embedded in the superstructure was three, and the lower bound of tank volume is 1 m^3. On the other hand, the lower bound of the total transported water volume in a split branch is set to be 1 m^3 and the upper bound of the instantaneous flow rate is 80 m^3/hr. The number of pipelines connected to the mixing or splitting points attached to every piece of equipment in the water-reuse system is chosen to be 1, while the corresponding constraints on the sources and sinks are *not* imposed. The duration of time interval is 0.5 h. Three different objective functions are adopted in this example, i.e., the total cost (case 1), the total freshwater cost (case 2), and the total installation cost of buffer tanks (case 3). Specifically, these functions can be written, respectively, as

$$\mathrm{obj}_{2,1} = \{(\sum_{t\in\mathbf{T}}\sum_{sa\in\mathbf{SA}} f^{\mathrm{source}}_{sa,t}) + 3(\sum_{t\in\mathbf{T}}\sum_{ob\in\mathbf{OB}} f^{\mathrm{sink}}_{ob1,t})\} + \sum_{b\in\mathbf{B}}[4.8x_b + 6(v_b^{\max})^{0.6}] \quad (72)$$

$$\mathrm{obj}_{2,2} = (\sum_{t\in\mathbf{T}}\sum_{sa\in\mathbf{SA}} f^{\mathrm{source}}_{sa,t}) \quad (73)$$

$$\mathrm{obj}_{2,3} = \sum_{b\in\mathbf{B}}[4.8x_b + 6(v_b^{\max})^{0.6}] \quad (74)$$

The corresponding mathematical programming models were solved with the module DICOPT within the GAMS environment. The basic features of the network designs obtained in these three cases are presented in Table 4. The more detailed information about the input and/or output streams of each water-using operation in case 1 can be found in Table 5. Also the network configurations of water-reuse systems in these cases are presented in Figures 6, 7, and 8, respectively.

From these results, it can be observed that only one buffer tank is selected in case 1 and its volume is 98.86 m^3. The total amount of consumed fresh water is 118.15 m^3, while that of secondary water generated from *sb*1 is 116.68 m^3. The total volume of wastewater discharged to sink *ob*1 is 134.83 m^3, while

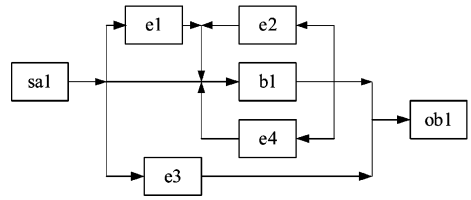

Figure 6. Network configuration of water-reuse subsystem in case 1 of example 2.

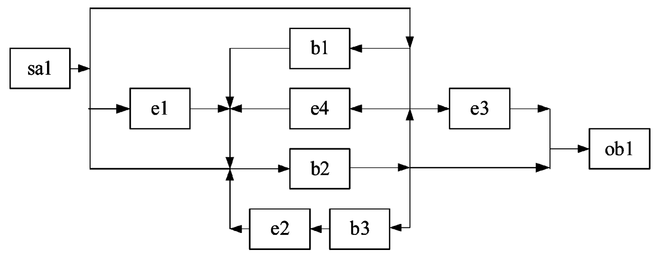

Figure 7. Network configuration of water-reuse subsystem in case 2 of example 2.

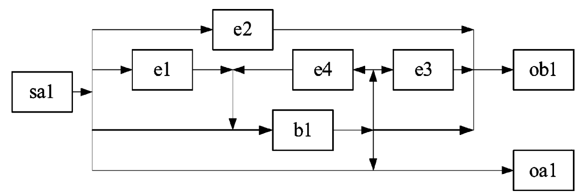

Figure 8. Network configuration of water-reuse subsystem in case 3 of example 2.

that sent to sinks *oc*1 and *oc*2 is 100 m^3. Since the freshwater cost is minimized in case 2, three buffer tanks are adopted in the optimal design and the total volume of these tanks is substantially larger than that in case 1. In addition, the network configuration becomes more complex due to the need to provide a better opportunity for water reuse. On the other hand, if the total installation cost of buffer tanks is used as the objective function, it can be found that the total amounts of consumed freshwaters and discharged wastewaters in the resulting design are significantly higher than those in case 1. This is due to the fact that the chance for reuse is reduced by cutting down the buffer volume. Notice also that sink *oa*1 is included in this network. This arrangement is introduced to satisfy the flow and/or concentration constraints of *ob*1.

5.3. Example 3. In this example, the mathematical models used for batch scheduling and water-reuse network design in the previous two examples are combined. The objective function is

$$\mathrm{obj}_3 = \mathrm{obj}_1 - \mathrm{obj}_{2,1} \quad (75)$$

The optimal design specifications in the present case are summarized in Table 6 and Figures 9 and 10. If the tasks of batch scheduling (example 1) and water-reuse network design (example 2) are performed individually, the maximum objective value obtained in the former case is 1366.68 units and the minimum of the latter is 620.72 units. Consequently, a maximum net profit of 745.95 units can be realized with the designs obtained in the previous two examples. The maximum net profit is 769.99 units in the present case, which represents an improvement of 3.2%. From Figures 5 and 9, it can be observed that the reactions are carried out in different time periods. By comparing Tables 4 (case 1) and 6, one can see that the number of buffer tanks is increased from one to two and the number of

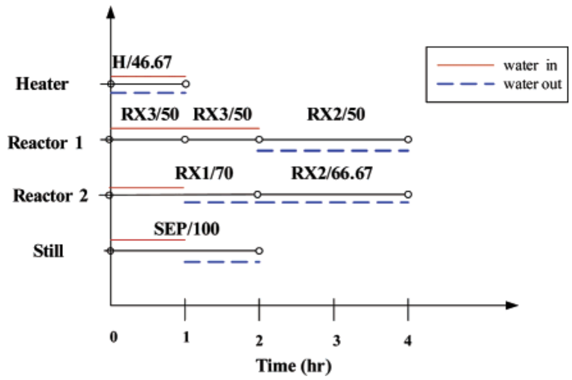

Figure 9. Gantt chart obtained in example 3.

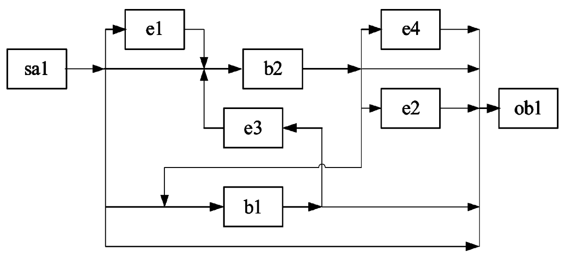

Figure 10. Network configuration of water-reuse subsystem in example 3.

Table 6. Solution Summary of Example 3

objective value (cost unit)	769.99
total income (cost unit)	2733.4
purchasing cost (cost unit)	1366.7
freshwater cost (cost unit)	1116.35
treatment cost (cost unit)	339.06
installation cost (cost unit)	81.30
number of buffer tanks	2
number of pipelines	14
yield of product 8 (kg)	46.67
yield of product 9(kg)	90
purchasing amount of feed 1 (kg)	46.67
purchasing amount of feed 2 (kg)	35
purchasing amount of feed 3(kg)	55
total amount of consumed *sa*1 (m^3)	116.35
volume of buffer tank *b*1 (m^3)	1
volume of buffer tank *b*2 (m^3)	54
volume of buffer tank *b*3 (m^3)	0
total treating volume of *ob*1 (m^3)	133.02

pipelines also becomes larger. Figures 6 and 10 also show that the network configuration of the integrated design is more complex.

6. Wastewater-Treatment Network Design

If treating effluents outside the plant boundary is not cost-effective, it may be necessary to install in-house facilities dedicated to this purpose. A mathematical programming model has been developed in this study for wastewater-treatment network design. A brief outline is given below.

6.1. Sets. The units in a wastewater-treatment network are very similar to those in a water-reuse network. Thus, the following sets are defined on the basis of those given in subsection 3.1:

$$\mathbf{SB}' = \mathbf{SB} \cup \mathbf{U} = \{sb' \mid sb' \text{ is the label of a wastewater-generating operation}\}$$

$$\mathbf{S}' = \mathbf{SA} \cup \mathbf{SB} \cup \mathbf{U} = \{s' \mid s' \text{ is the label of a source for the wastewater-treatment network}\}$$

$$\mathbf{OC}' = \mathbf{OC} \cup \mathbf{U} = \{oc' \mid oc' \text{ is the label of a wastewater-consuming operation}\}$$

$$\mathbf{O}' = \mathbf{OA} \cup \mathbf{OC} \cup \mathbf{U} = \{o' \mid o' \text{ is the label of a sink for the wastewater-treatment network}\}$$

$$\mathbf{TrA} = \{tra \mid tra \text{ is the label of a wastewater-treatment unit with nonidentical charging and discharging time intervals}\}$$

$$\mathbf{TrB} = \{trb \mid trb \text{ is the label of a wastewater-treatment unit with identical charging and discharging time intervals}\}$$

$$\mathbf{Tr} = \mathbf{TrA} \cup \mathbf{TrB} = \{tr \mid tr \text{ is the label of a wastewater-treatment unit}\}$$

$$\mathbf{B}' = \{b' \mid b' \text{ is the label of a buffer tank in the wastewater-treatment network}\}$$

As mentioned previously, every operation in set **U** in the water-reuse network needs to consume and also discharge water. Therefore, each of them can be regarded both as a source and also as a sink in a wastewater-treatment network. Notice that the wastewater-treatment units are classified as the sinks in set **OB** for water-reuse subsystem design. In the present case, **Tr** = **OB** and a different set of labels is used for identifying these units.

6.2. Superstructure. Similar to the design procedure of a water-reuse subsystem, it is necessary to build a superstructure (Figure 11) and the construction steps are given below:

(1) Place a mixing node *M* at the inlet of each wastewater-treatment unit, buffer tank, and sink;

(2) Place a splitting node *S* at the outlet of each source, wastewater-treatment unit, and buffer tank;

(3) Connect the split branches from the splitting node after each source in **SA** to all mixing nodes;

(4) Connect the split branches from the splitting node after every source in **SB′** to the mixing nodes before the buffer tanks in **B′** and sinks in **OA**;

(5) Connect the split branches from the splitting node after each buffer tank in **Tr** to all mixing nodes except the one before itself.

(6) Connect the split branches from the splitting node after each buffer tank in **B′** to all mixing nodes except the one before itself.

The labels of the splitting and mixing nodes in the wastewater-treatment network are again grouped into two additional node sets, i.e.

$$\mathbf{MX}' = \{mx' \mid mx' \text{ is the label of a mixing node in the wastewater-treatment network}\} = \mathbf{Tr} \cup \mathbf{B}' \cup \mathbf{O}'$$

$$\mathbf{SP}' = \{sp' \mid sp' \text{ is the label of a splitting node in the wastewater-treatment network}\} = \mathbf{S}' \cup \mathbf{Tr} \cup \mathbf{B}'$$

6.3. Model Formulation. First of all, it should be noted that eqs 23−25 can be used to characterize the sources of the wastewater-treatment network, i.e.

$$f^{\text{source}}_{sa,t} = \sum_{mx' \in \mathbf{MX}'} \text{fs}_{sa,mx',t} \quad sa \in \mathbf{SA},\ t \in \mathbf{T} \tag{76}$$

$$f^{\text{source}}_{sb',t} = \sum_{b' \in \mathbf{B}'} \text{fs}_{sb',b',t} + \sum_{o' \in \mathbf{OA}} \text{fs}_{sb',o',t} \quad sb' \in \mathbf{SB}',\ t \in \mathbf{T} \tag{77}$$

$$c^{\text{source}}_{s',k,t} = \text{cs}_{s',k,t} \quad s' \in \mathbf{S}',\ k \in \mathbf{K},\ t \in \mathbf{T} \tag{78}$$

The wastewater-treatment units can be divided into two types. Their mass and component balances can be written as follows:

$$f_{tr,t}^{\text{in}} = f_{tr,t}^{\text{out}} + l_{tr,t} \quad tr \in \mathbf{TrB},\ t \in \mathbf{T} \tag{79}$$

$$r_{tr,k} = \frac{f_{tr,t}^{\text{in}} c_{tr,k,t}^{\text{in}} - f_{tr,t}^{\text{out}} c_{tr,k,t}^{\text{out}}}{f_{tr,t}^{\text{in}} c_{tr,k,t}^{\text{in}}} \quad tr \in \mathbf{TrB},\ k \in \mathbf{K},\ t \in \mathbf{T} \tag{80}$$

$$\text{DT} \sum_{t \in \mathbf{TC}_{tr}} f_{tr,t}^{\text{in}} = \text{DT} \sum_{t \in \mathbf{TD}_{tr}} f_{tr,t}^{\text{out}} + L_{tr} \quad tr \in \mathbf{TrA},\ t \in \mathbf{T} \tag{81}$$

$$r_{tr,k} = \frac{\sum_{t \in \mathbf{TC}_{tr}} f_{tr,t}^{\text{in}} c_{tr,k,t}^{\text{in}} - \sum_{t \in \mathbf{TD}_{tr}} f_{tr,t}^{\text{out}} c_{tr,k,t}^{\text{out}}}{\sum_{t \in \mathbf{TC}_{tr}} f_{tr,t}^{\text{in}} c_{tr,k,t}^{\text{in}}} \quad tr \in \mathbf{TrA},\ k \in \mathbf{K},\ t \in \mathbf{T} \tag{82}$$

where $r_{tr,k}$ is the removal ratio of pollutant k in treatment unit tr; $\mathbf{TC}_{tr}$ and $\mathbf{TD}_{tr}$ denote, respectively, the sets of time intervals in which the charging and discharging operation take place. Also, $l_{tr,t}$ and L_{tr} denote, respectively, the water loss rate in time interval t and the total amount of water loss in a production cycle. If the loss quantity is proportional to the inlet (or outlet) flow rate, the following constraints can be imposed:

$$l_{tr,t} = \theta_{tr} f_{tr,t}^{\text{in}} \quad tr \in \mathbf{TrB},\ t \in \mathbf{T} \tag{83}$$

$$L_{tr} = \phi_{tr} \sum_{t \in \mathbf{TC}_{tr}} f_{tr,t}^{\text{in}} \quad tr \in \mathbf{TrA},\ t \in \mathbf{T} \tag{84}$$

where θ_{tr} and ϕ_{tr} are two constants whose values are between 0 and 1.

The mass balances around the mixing node before and the splitting node after each wastewater-treatment unit can be written as

$$f_{tr,t}^{\text{in}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{sa,tr,t} + \sum_{b' \in \mathbf{B}'} \text{fs}_{b',tr,t} \quad tr \in \mathbf{Tr},\ t \in \mathbf{TC}_{tr} \tag{85}$$

$$f_{tr,t}^{\text{in}} c_{tr,k,t}^{\text{in}} = \sum_{sa \in \mathbf{SA}} \text{fs}_{sa,tr,t} \text{cs}_{s,k,t} + \sum_{b' \in \mathbf{B}'} \text{fs}_{b',tr,t} \text{cs}_{b',k,t} \quad tr \in \mathbf{Tr},\ k \in \mathbf{K},\ t \in \mathbf{TC}_{tr} \tag{86}$$

$$f_{tr,t}^{\text{out}} = \sum_{b' \in \mathbf{B}'} \text{fs}_{tr,b',t} + \sum_{o' \in \mathbf{O}'} \text{fs}_{tr,o',t} \quad tr \in \mathbf{Tr},\ t \in \mathbf{TD}_{tr} \tag{87}$$

$$C_{tr,k,t}^{\text{out}} = \text{cs}_{tr,k,t} \quad tr \in \mathbf{Tr},\ k \in \mathbf{K},\ t \in \mathbf{TD}_{tr} \tag{88}$$

Similar to the water-reuse subsystem design, the objective function in the present case can be written as follows:

$$\text{obj}_{\text{treatment}} = \Gamma_{\text{SA}} \Phi_{\text{SA}} + \Gamma_{\text{B}} \Phi_{\text{B}} + \Gamma_{\text{Tr}} \Phi_{\text{Tr}} \tag{89}$$

where the definitions of freshwater cost (Φ_{SA}) and installation cost of buffer tanks (Φ_{B}) have already been given in eqs 67 and 69. The treatment costs (Φ_{Tr}) can be calculated with the following formula:

$$\Phi_{\text{Tr}} = N_{\text{cycle}} \text{DT} \sum_{tr \in \mathbf{Tr}} \varphi_{tr} \left(\sum_{t \in \mathbf{T}} f_{tr,t}^{\text{in}} \right) \tag{90}$$

where φ_{tr} is the unit cost for wastewater treatment. Finally, the constraints of buffer tanks and water sinks can be found in eqs 35−49.

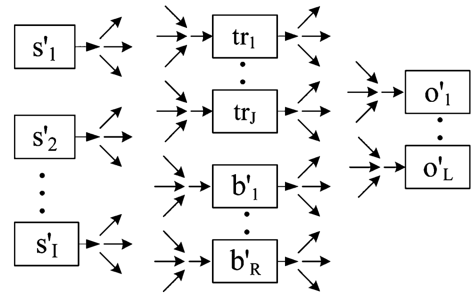

Figure 11. Superstructure of wastewater-treatment network.

7. Simultaneous Optimization of the Water-Reuse and Wastewater-Treatment Network Designs

To integrate the aforementioned models to simultaneously optimize the water-reuse and wastewater-treatment network designs, let us begin by slightly revising their set definitions. In this integrated model, the definitions of source sets (i.e., **SA**, **SB** and **S**) and the set of water users (**U**) are the same as those used in the model for water-reuse network design. The sink set **OB** must now be replaced by **Tr**, which is the set of all treatment units. Thus, the sink set for the integrated network should be

$$\mathbf{O}'' = \mathbf{OA} \cup \mathbf{OC} = \{o'' \mid o'' \text{ is the label of all sinks for the integrated network}\}$$

The construction steps of the modified superstructure are show below:

(1) Place a mixing node M at the inlet of each water user, wastewater-treatment unit, buffer tank, and sink;

(2) Place a splitting node S at the outlet of each source, water user, wastewater-treatment unit, and buffer tank;

(3) Connect the split branches from the splitting node after each source in **SA** to all mixing nodes;

(4) Connect the split branches from the splitting node after every source in **SB**, every water user in **U**, and every wastewater-treatment unit in **Tr** to the mixing nodes before the buffer tanks in **B** and sinks in **OA**, but not to those before the water users in **U** and the sinks in **OC**;

(5) Connect the split branches from the splitting node after each buffer tank in **B** to all mixing nodes except the one before itself.

Also the sets of all splitting nodes and mixing nodes are

$$\mathbf{MX}'' = \{mx'' \mid mx'' \text{ is the label of a mixing node in the integrated network}\} = \mathbf{U} \cup \mathbf{Tr} \cup \mathbf{B} \cup \mathbf{O}$$

$$\mathbf{SP}'' = \{sp'' \mid sp'' \text{ is the label of a splitting node in the integrated network}\} = \mathbf{S} \cup \mathbf{U} \cup \mathbf{Tr} \cup \mathbf{B}$$

Notice that the constraints of the integrated model have all been outlined previously in the individual models for water-reuse and wastewater-treatment network designs. Specifically,

- the mass balances at the sources should be the same as eqs 20−25;
- the model for water user can be expressed with eqs 26−34;
- the model of the wastewater-treatment unit is described in eqs 76−88;
- the tank model is given in eqs 35−43;
- the mass balances at the sinks can be written as eqs 44−49;

Table 7. Solution Summary of Example 4

objective value (cost unit)	425.785
freshwater cost (cost unit)	147.68
treatment cost (cost unit)	193.185
installation cost (cost unit)	84.92
number of buffer tanks	2
number of branches	18
number of pipelines	16
total amount of consumed *sa*1 (m^3)	147.68
volume of buffer tank *b*1 (m^3)	1
volume of buffer tank *b*2 (m^3)	59.05
volume of buffer tank *b*3 (m^3)	0
total treating volume of *trb*1 (m^3)	128.79
total discharging volume of *oa*1 (m^3)	164.35

• the structural constraints can be imposed according to eqs 50−65.

The objective function in this case can be formulated in the same form as that used in the stand-alone design of a wastewater-treatment network, i.e.

$$\mathrm{obj}_{\mathrm{int2}} == \Gamma_{\mathrm{SA}}\Phi_{\mathrm{SA}} + \Gamma_{\mathrm{B}}\Phi_{\mathrm{B}} + \Gamma_{\mathrm{Tr}}\Phi_{\mathrm{Tr}} \tag{91}$$

Two examples are presented in the following to demonstrate the benefits of integrated approach.

7.1. Example 4. Let us consider case 1 in example 2. The process data of all water-using operations in this batch plant can be found in Table 3, and the corresponding Gantt chart is presented in Figure 5. Only one external water source (*sa*1) is considered here, and its pollutant concentration is 0 ppm. The maximum water supply rate from source *sa*1 is 100 m^3/hr and its cost is 1 unit of value/m^3. We further assume that only one wastewater-treatment system *trb*1 is available. The maximum flow rate of the wastewater stream sent to this treatment unit is 100 m^3/hr, and its pollutant concentration is required to be maintained between 7 and 15 ppm. In addition, the removal ratio of *trb*1 is 0.7 and the corresponding treatment cost is 1.5 unit/m^3. An addition environment sink $oa1 \in \mathbf{OA}$ is also assumed to be present in this example. The upper bound of its inlet pollutant concentration is set to be 2.5 mg/L. The number of buffer tanks embedded in the superstructure was three and the lower bound of the tank volume was set to be 1 m^3. The lower bound of total transported water volume in each pipeline was also chosen to be 1 m^3, while the upper bound of every instantaneous flow rate was 100 m^3/hr. The maximum number of pipelines connected to a mixing or splitting point attached to every piece of water-using equipment and wastewater-treatment unit was also set to be 1. The other number constraints are again not included in the mathematical model. Finally, the objective function is

$$\mathrm{obj}_4 = \sum_{t\in\mathbf{T}}\sum_{sa\in\mathbf{SA}} f_{sa,t} + 1.5\sum_{t\in\mathbf{T}}\sum_{tr\in\mathbf{Tr}} f_{tr,t} + \sum_{b\in\mathbf{B}}(4.8x_b + 6\upsilon_b^{\,0.6}) \tag{92}$$

On the basis of a time interval of 0.5 h, the results obtained by solving the integrated model are presented in Table 7. The more detailed information about input and/or output streams of each water-using operation can be found in Table 8. The optimal network configuration is presented in Figure 12.

7.2. Example 5. Let us again consider case 1 in example 2. Two wastewater-treatment units are adopted in the present example: one is operated in batch mode (*tra*1) and the other is a continuous process (*trb*1). The treatment costs of *tra*1 and *trb*1 are both 1.5 unit/m^3. The design parameters of these two treatment units are summarized as follows.

• *tra*1: The pollutant concentration at the inlet is required to be maintained between 0 and 7 ppm. The charging time interval is between 2 and 3 h, and discharging time interval is between 3 and 4 h. The removal ratio is 0.7.

• *trb*1: The pollutant concentration at the inlet is required to be maintained between 7 and 15 ppm. The unit is operated continuously between 0 and 4 h. The removal ratio is 0.5.

Two different maximum throughputs are considered in this example. In the first case, the upper bounds of the feed rates of both treatment units are chosen to be 50 m^3/hr. The corresponding objective function is the total cost, i.e.,

$$\mathrm{obj}_{5,1} = \sum_{t\in\mathbf{T}}\sum_{sa\in\mathbf{SA}} f_{sa,t} + 1.5\sum_{t\in\mathbf{T}}\sum_{tr\in\mathbf{Tr}} f_{tr,t}^{in} + \sum_{b\in\mathbf{B}}(4.8x_b + 6\upsilon_b^{\,0.6}) \tag{93}$$

These upper bounds are canged to 100 m^3/hr in the second case. The corresponding objective function is the freshwater cost, i.e.,

$$\mathrm{obj}_{5,2} = \sum_{t\in\mathbf{T}}\sum_{sa\in\mathbf{SA}} f_{sa,t} \tag{94}$$

The corresponding results shown in Figures 13 and 14 and Table 9 were obtained on the basis of a time interval of 0.5 h. When compared with case 1 of example 2, the number of buffer tanks

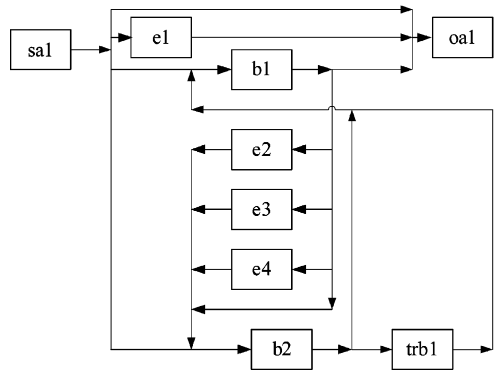

Figure 12. Network configuration of the integrated water-reuse and wastewater-treatment system in example 4.

Table 8. Design Specifications of the Water-Using Operations in Example 4

operation	flow rate (m^3/hr)	conc. (mg/L)	from/to	time period
*u*1(*e*1)	−46.67	0	*sa*1	3−4
	46.67	5	*oa*1	3−4
*u*2(*e*3)	−35	6	*b*1	0−1
	35	14	*b*2	1−2
*u*3(*e*4)	−50	3	*b*1	2−3
	50	8	*b*2	3−4
*oc*1(*e*2)	50	6	*b*1	0−1
*oc*2(*e*2)	50	7	*b*1	1−2
*sb*1(*e*2)	25	10	*b*2	2−4
*sb*2(*e*3)	33.34	10	*b*2	2−4

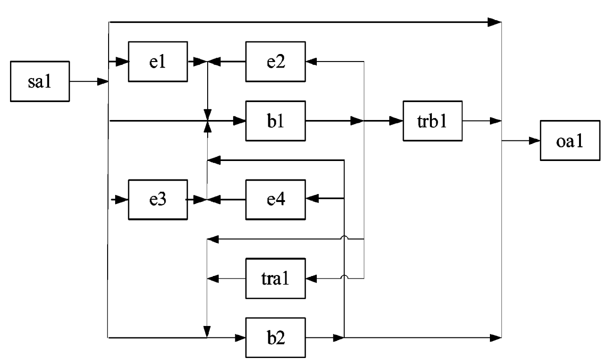

Figure 13. Network configuration of the integrated water-reuse and wastewater-treatment system in case 1 of example 5.

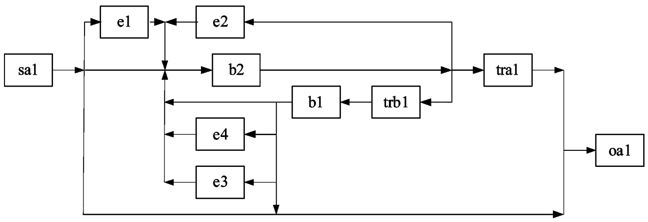

Figure 14. Network configuration of the integrated water-reuse and wastewater-treatment system in case 2 of example 5.

Table 9. Solution Summary of the Two Cases in Example 5

	scenario 1	scenario 2
objective value (cost unit)	593.63	96.46
freshwater cost (cost unit)	228.65	96.46
treatment cost (cost unit)	241.89	397.5
installation cost (cost unit)	123.09	369.92
number of buffer tanks	2	2
number of branches	20	18
number of pipelines	18	16
total amount consumed *sa*1 (m^3)	228.65	96.46
volume of buffer tank *b*1 (m^3)	123.65	62.5
volume of buffer tank *b*2 (m^3)	1	189.76
volume of buffer tank *b*3 (m^3)	0	0
total treatment volume of *tra*1 (m^3)	50	25
total treating volume of *trb*1 (m^3)	111.26	240
total discharging volume of *oa*1 (m^3)	245.35	113.135

Table 10. Solution Summary of Example 6

objective value (cost unit)	987.815
total income (cost unit)	2733.4
purchasing cost (cost unit)	1366.7
freshwater cost (cost unit)	105.1
treatment cost (cost unit)	228.705
installation cost (cost unit)	45.08
number of buffer tank	2
number of pipelines	16
yield of product 8 (kg)	46.67
yield of product 9 (kg)	90
purchasing amount of feed 1 (kg)	46.67
purchasing amount of feed 2 (kg)	35
purchasing amount of feed 3 (kg)	55
total amount of consumed *sa*1 (m^3)	105.1
volume of buffer tank *b*1 (m^3)	1
volume of buffer tank *b*2 (m^3)	14.2
volume of buffer tank *b*3 (m^3)	0
total treating volume of *ob*1 (m^3)	152.47
total discharging volume of *oa*1 (m^3)	121.77

in case 1 of the present example is increased to two. Notice from Table 9 that the volume of tank b2 is only 1 m^3. It can be deduced from Figure 13 that the main function for buffer tank *b2* is to dilute wastewater in order to satisfy the operation constraints of water user *u*3 (in *e*4), sink *oa*1, and the wastewater-treatment unit *trb*1. Also, as a result of adding a wastewater-treatment subsystem to the water-reuse network, a saving of 4.37% in cost can be achieved. However, it can also be observed that the total amount of consumed freshwater in the present case is more than that needed in case 1 of example 2. This is due to the facts that the wastewater-treatment capacities of the given treatment units are very limited and, thus, a significant amount of freshwater is used to dilute wastewater in the resulting design. Notice that, in the second case of this example, the maximum inlet flow rate of every treatment unit is increased to 100 m^3/hr. Consequently, the amount of consumed freshwater can be reduced to 87.12% of the original level.

8. Fully Integrated Water Network Design

A mathematical program can be built by combining all three components mentioned previously. The fully integrated water network design can then be obtained accordingly. The objective function to be optimized in this program is

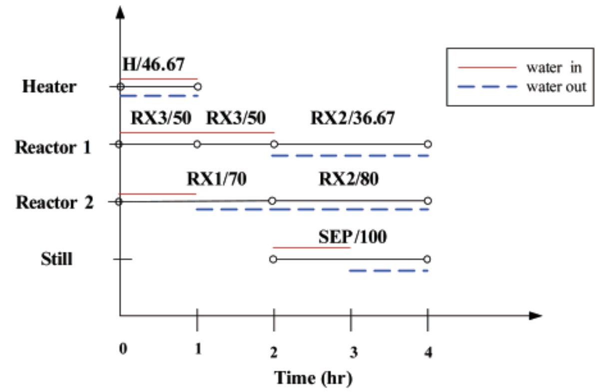

Figure 15. Optimal schedule obtained in example 6.

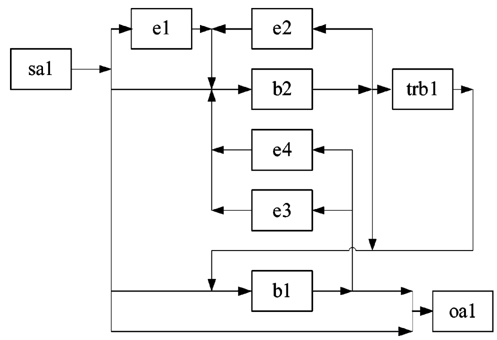

Figure 16. Network configuration of fully integrated water network in example 6.

$$\text{obj}_{\text{overall}} = \text{obj}_{\text{schedule}} - \text{obj}_{\text{int2}} \tag{95}$$

Let us use an example, which is referred to as example 6 in this paper, to demonstrate the potential impacts of the proposed practice. Specifically, let us consider the process data given in example 1 (i.e., Figure 3 and Table 1), the design parameters in example 4, and the concentration upper bounds shown in Table 3. It is also assumed in this example that the waters consumed and/or generated in each water-using operation are proportional to the process throughput. The objective function can be written as

$$\text{obj}_6 = \text{obj}_1 - \text{obj}_4 \tag{96}$$

On the basis of a time interval of 1 h, the corresponding mathematical program has been solved and the solution is summarized in Table 10. The optimal production schedule and the network configuration are presented in Figures 15 and 16, respectively. Notice that the batch schedule and water-network design are optimized separately in examples 1 and 4. Since the optimal objective values obtained in these two examples are 1366.68 and 425.785, respectively, the net profit can be computed by subtracting the latter from former, i.e., 940.895 units. In the present example, since all components are optimized simultaneously, the maximum net profit can be raised to 987.815 units, which represents a 5% improvement.

9. Conclusions

Three separate mathematical programming models are presented in this paper. They can be used individually to optimize the batch schedule, the water-reuse subsystem design, and the wastewater-treatment subsystem design. The design procedure to incorporate all three components into a single comprehensive model is also proposed for generating the optimal designs of fully integrated water networks in batch processes. The effectiveness of the integrated design approach is demonstrated with a series of case studies. It can be clearly observed that better design alternatives can always be identified with a higher degree of integration.

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