

# A DIVIDING APPROACH FOR THE SYNTHESIS OF WATER NETWORKS INVOLVING BATCH AND CONTINUOUS UNITS

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## Abstract

This paper presents a mathematical model for the synthesis of water networks, where both batch and continuous units are involved. For cases where the number of batch units is greater than that of continuous units, a dividing approach is proposed. By treating continuous operation as a combination of batch operations, the original design problem is simplified and the resultant problem is to synthesize a batch water network. The model can then be formulated as a mixed-integer nonlinear program based on a superstructure that includes all possible network connections. A modified literature example is solved to illustrate the proposed approach.

## Keywords

Batch and continuous units, Process integration, Water reuse/recycle, Network synthesis, Mathematical optimization.

## Introduction

Water is one of the most important natural resources being widely used in various process industries. However, rapid industrial growth has led to serious water pollution in the world. In addition, the growing concern about high consumption and waste of water for industrial applications calls for efficient and responsible use of water in industry. Other reasons tied to this need include the predicted scarcity of industrial water, increasingly stringent environmental regulations for wastewater disposal, and the rising costs of fresh water and effluent treatment.

To make efficient use of water, water recovery via *water network synthesis* has been commonly accepted as an effective means, with *reuse*, *recycle*, and *regeneration* as options for reducing industrial water withdrawals and discharges. Over the past decades, various *process integration* techniques for water network synthesis have been developed for continuous and batch processes (Bagajewicz, 2000; Foo, 2009; Jeżowski, 2010; Gouws et al., 2010)

based on *pinch analysis* and *mathematical optimization* approaches. The latter is preferred when a systematic strategy that leads to an optimal solution is required.

While previous works on water network synthesis are restricted to addressing systems with all continuous or batch units, there are cases where both types of units exist. In this paper, a mathematical model is developed for the synthesis of water networks involving batch and continuous units, focusing on the special case where batch units are in the majority. Application of the model is demonstrated through an illustrative example.

## Problem Statement

The problem addressed in this paper can be formally stated as follows. Given is a set of water-using units  $i \in \mathcal{I}$ . A few of them are continuous units ( $i \in \mathcal{I}^c \subset \mathcal{I}$ ), but

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most are batch ones ( $i \in \mathcal{I}^b \subset \mathcal{I}$ ). Water is required for these units to remove a set of contaminants  $c \in \mathcal{C}$  with fixed mass loads. Available for service are a set of fresh water sources  $w \in \mathcal{W}$  that supply water of different qualities. Before using fresh water, it is first considered to reuse/recycle the effluent from the units. To facilitate the allocation of reusable water, a set of storage tanks  $s \in \mathcal{S}$  for intermediate water storage may be used. The objective is to synthesize an optimum water network that achieves the minimum fresh water consumption, while satisfying all process constraints.

### Solution Approach

Since the problem involves batch and continuous units, the main challenge is to integrate units of different operating modes. While continuous units operate nonstop for a long duration (e.g. 8000 h/y), batch units are often operated shortly (for a few hours) and cyclically. In addition, water intake and discharge of a batch unit are found at the beginning and end of the operation respectively. The inlet and outlet water of a continuous unit, by contrast, is continuously fed and discharged during the operation.

For dealing with the case where the number of batch units is greater than that of continuous units, it is proposed to take continuous operation as a combination of batch operations. This can be achieved by dividing the operating time of continuous units into a number of time intervals, according to the start and end times of the batch unit operations. In any time interval  $(t, t + 1)$ , the inlet water fed to the continuous units is treated as if it were charged at time point  $t$  through water storage, as illustrated in Figure 1. Meanwhile, the outlet water from those units is treated as if it were discharged at time point  $t + 1$ . The original problem can thus be converted into a simpler one where only batch units are involved in water network synthesis.

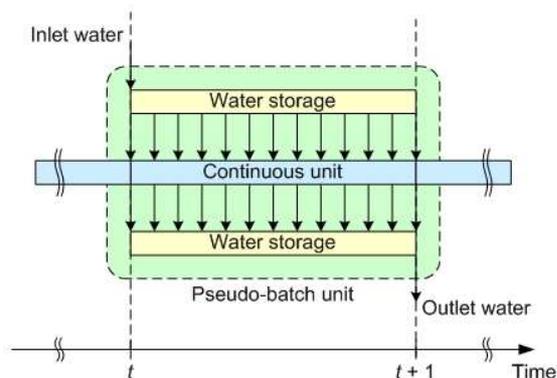


Figure 1. Illustration of a pseudo-batch unit

Note that the approach of approximating a continuous unit as a number of batch units has been applied before in

the synthesis of reactor networks (Lakshmanan and Biegler, 1996; Schweiger and Floudas, 1999).

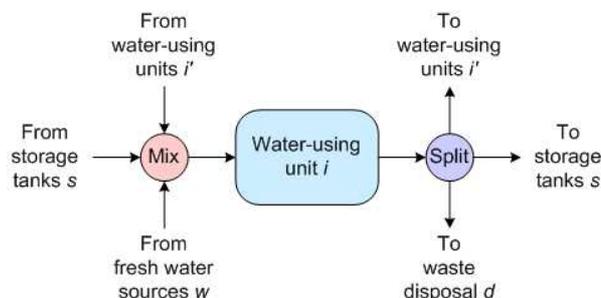


Figure 2. Water-using unit

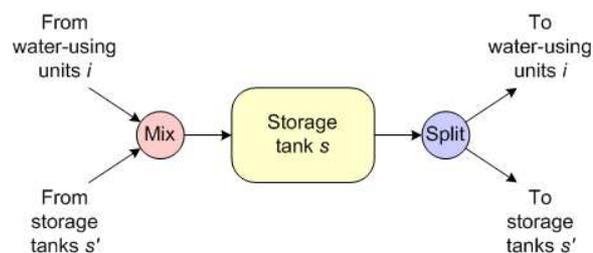


Figure 3. Storage tank

### Mathematical Model

Having treated all continuous units as pseudo-batch units, the resultant problem is almost to synthesize a batch water network. In this paper, the model of Chen et al. (2009) is adapted to perform the synthesis task. The presented model consists of mass balance equations and logical constraints, which is based on a superstructure that includes all possible network connections between water-using units and storage tanks. To address the time dimension in batch processes, a set of time points  $t \in \mathcal{T}$  are defined, and index  $t$  is used through the model to represent time dependence.

#### Mass Balance for Water-using Units

Figure 2 shows the schematic diagram of a water-using unit ( $i$ ). As shown, its inlet water may come from other water-using units  $i'$ , storage tanks  $s$ , and/or fresh water sources  $w$ . The outlet water of unit  $i$  may be sent to other water-using units  $i'$ , storage tanks  $s$ , and/or waste disposal systems  $d$ . Equations (1) and (2) describe the inlet and outlet water balances respectively for unit  $i$  at time point  $t$ . If the operation of unit  $i$  finishes and starts immediately at the same time point, the outlet flow of the unit

must occur prior to its inlet flow. Based on the assumption that no water loss or gain is found in the unit operation, Eq. (3) depicts the water balance around unit  $i$ . Note that  $\Delta_i$  is the number of time intervals between the start and end of unit  $i$  operation, which reflects the processing time needed to achieve the desired effect.

$$q_{it}^{\text{in}} = \sum_{i' \in \mathcal{I}} q_{i't} + \sum_{s \in \mathcal{S}} q_{sit} + \sum_{w \in \mathcal{W}} q_{wit} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (1)$$

$$q_{it}^{\text{out}} = \sum_{i' \in \mathcal{I}} q_{i't} + \sum_{s \in \mathcal{S}} q_{ist} + \sum_{d \in \mathcal{D}} q_{idt} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (2)$$

$$q_{it}^{\text{in}} = q_{it'}^{\text{out}} \quad \forall i \in \mathcal{I}, t, t' \in \mathcal{T}, t' = t + \Delta_i \quad (3)$$

The lower and upper bounds on the inlet and outlet water flows of a unit are set by Eqs. (4) and (5), where  $Y_{it}^{\text{in}}$  and  $Y_{it}^{\text{out}}$  are binary parameters indicating the start and end times of the water-using operations. These two equations ensure reasonable amounts of water entering and leaving a unit at the beginning and end of the operation. Additionally, no water will enter or leave the unit if it is not time for the operation to start or finish.

$$Q_i^L Y_{it}^{\text{in}} \leq q_{it}^{\text{in}} \leq Q_i^U Y_{it}^{\text{in}} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (4)$$

$$Q_i^L Y_{it}^{\text{out}} \leq q_{it}^{\text{out}} \leq Q_i^U Y_{it}^{\text{out}} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (5)$$

Apart from the water balances, contaminant balances need to be considered for the units. Equations (6) and (7) describe the contaminant balances at the inlet of unit  $i$  and around it, respectively. Note that  $M_{ict}$  is the mass load for unit  $i$  operation started at time point  $t$ . The maximum inlet and outlet concentrations for a water-using unit are specified by Eqs. (8) and (9).

$$q_{it}^{\text{in}} c_{ict}^{\text{in}} = \sum_{i' \in \mathcal{I}} q_{i't} c_{i'ct}^{\text{out}} + \sum_{s \in \mathcal{S}} q_{sit} c_{sct}^{\text{out}} + \sum_{w \in \mathcal{W}} q_{wit} c_{wc} \quad \forall c \in \mathcal{C}, i \in \mathcal{I}, t \in \mathcal{T} \quad (6)$$

$$q_{it}^{\text{in}} c_{ict}^{\text{in}} + M_{ict} = q_{it'}^{\text{out}} c_{ict'}^{\text{out}} \quad \forall c \in \mathcal{C}, i \in \mathcal{I}, t, t' \in \mathcal{T}, t' = t + \Delta_i \quad (7)$$

$$c_{ict}^{\text{in}} \leq C_{ic}^{\text{in}, \text{max}} \quad \forall c \in \mathcal{C}, i \in \mathcal{I}, t \in \mathcal{T} \quad (8)$$

$$c_{ict}^{\text{out}} \leq C_{ic}^{\text{out}, \text{max}} \quad \forall c \in \mathcal{C}, i \in \mathcal{I}, t \in \mathcal{T} \quad (9)$$

### Mass Balance for Storage Tanks

Figure 3 shows the schematic diagram of a storage tank ( $s$ ). As shown, its inlet water may come from water-using units  $i$  and/or other storage tanks  $s'$ . The outlet water of tank  $s$  may be sent to water-using units  $i$  and/or other storage tanks  $s'$ . Equations (10) and (11) describe the inlet and outlet water balances respectively for tank  $s$  at time point  $t$ . If there is water entering and leaving a tank at the same time point, it is assumed that the inlet flow occurs prior to the outlet flow.

$$q_{st}^{\text{in}} = \sum_{i \in \mathcal{I}} q_{ist} + \sum_{s' \in \mathcal{S}} q_{s'st} \quad \forall s \in \mathcal{S}, t \in \mathcal{T} \quad (10)$$

$$q_{st}^{\text{out}} = \sum_{i \in \mathcal{I}} q_{sit} + \sum_{s' \in \mathcal{S}} q_{s's't} \quad \forall s \in \mathcal{S}, t \in \mathcal{T} \quad (11)$$

Equation (12) depicts the water balance around tank  $s$ , where the amount of water stored at a time point ( $t$ ) is equal to that at the previous time point ( $t - 1$ ) adjusted by the amounts of water entering and leaving at the same time point. Note that  $Z^{\text{cyc}}$  is a binary parameter indicating the mode of batch operation;  $Z^{\text{cyc}} = 0$  means single operation for which there is no initial water stock, while  $Z^{\text{cyc}} = 1$  means cyclic operation. For the latter case, the water stored at the last time point ( $T$ ) of a cycle is taken as the initial water stock for the next cycle. The upper bound on the amount of water stored in a tank and its inlet flow is set by Eqs. (13) and (14).

$$q_{st} = Z^{\text{cyc}} q_{s,T} \Big|_{t=1} + q_{s,t-1} \Big|_{t>1} + q_{st}^{\text{in}} - q_{st}^{\text{out}} \quad \forall s \in \mathcal{S}, t \in \mathcal{T} \quad (12)$$

$$q_{st}^{\text{in}} \leq Q_s^{\text{max}} \quad \forall s \in \mathcal{S}, t \in \mathcal{T} \quad (13)$$

$$q_{st} \leq Q_s^{\text{max}} \quad \forall s \in \mathcal{S}, t \in \mathcal{T} \quad (14)$$

In addition to the water balances, contaminant balances for the tanks are needed. Equations (15) and (16) describe the contaminant balances at the inlet of tank  $s$  and around it, respectively.

$$q_{st}^{\text{in}} c_{sct}^{\text{in}} = \sum_{i \in \mathcal{I}} q_{ist} c_{ict}^{\text{out}} + \sum_{s' \in \mathcal{S}} q_{s's't} c_{s'ct}^{\text{out}} \quad \forall c \in \mathcal{C}, s \in \mathcal{S}, t \in \mathcal{T} \quad (15)$$

$$q_{st} c_{sct}^{\text{out}} = Z^{\text{cyc}} q_{s,T} c_{sc,T}^{\text{out}} \Big|_{t=1} + q_{s,t-1} c_{sc,t-1}^{\text{out}} \Big|_{t>1} + q_{st}^{\text{in}} c_{sct}^{\text{in}} - q_{st}^{\text{out}} c_{sct}^{\text{out}} \quad \forall c \in \mathcal{C}, s \in \mathcal{S}, t \in \mathcal{T} \quad (16)$$

### Logical Constraints

Since treating continuous units as pseudo-batch units involves water storage to change the pattern of water intake and discharge (Figure 1), no direct water reuse/recycle is allowed for the continuous units, although fresh water and wastewater can be fed and discharged at any time without storage tanks. Equation (17) ensures that the outlet water of a continuous unit will not be directly reused by any other units, while Eq. (18) ensures that a continuous unit will not reuse water from any other units directly.

$$\sum_{i' \in \mathcal{I}} \sum_{t \in \mathcal{T}} q_{i't} = 0 \quad \forall i \in \mathcal{I}^c \quad (17)$$

$$\sum_{i' \in \mathcal{I}} \sum_{t \in \mathcal{T}} q_{i't} = 0 \quad \forall i \in \mathcal{I}^c \quad (18)$$

The inlet and outlet flows of a storage tank must be prevented from occurring in the same time interval. This is to provide sufficient time for water to be well mixed in the tank before being dispatched to units or other tanks. Therefore, a continuous unit is not allowed to send water to a tank at a time point ( $t$ ) if the unit has received water from the tank at the previous time point ( $t - 1$ ). To take this constraint into account, two binary variables  $y_{ist}$  and  $y_{sit}$  are defined to indicate if there is water sent from unit  $i$  to tank  $s$  at time point  $t$ , and if there is water sent from tank  $s$  to unit  $i$  at time point  $t$ , respectively. Equations (19) and (20) are introduced to correlate the binary variables with the corresponding water flows (continuous variables). These equations ensure a reasonable amount of water transferred between a unit and a tank if the connection exists, while if it does not exist, the water flow goes to zero. Having defined the binary variables, the constraint is then given by Eq. (21).

$$Q_{is}^L y_{ist} \leq q_{ist} \leq Q_{is}^U y_{ist} \quad \forall i \in \mathcal{I}, s \in \mathcal{S}, t \in \mathcal{T} \quad (19)$$

$$Q_{si}^L y_{sit} \leq q_{sit} \leq Q_{si}^U y_{sit} \quad \forall i \in \mathcal{I}, s \in \mathcal{S}, t \in \mathcal{T} \quad (20)$$

$$y_{si,t-1} + y_{ist} \leq 1 \quad \forall i \in \mathcal{I}^c, s \in \mathcal{S}, t \in \mathcal{T}, t > 1 \quad (21)$$

### Objective Function

For maximum water recovery, the objective is set to minimize the consumption of fresh water for water-using operations, as given in Eq. (22):

$$\min_{\mathbf{x} \in \Omega} \phi = \sum_{w \in \mathcal{W}} \sum_{i \in \mathcal{I}} \sum_{t \in \mathcal{T}} q_{wit} \quad (22)$$

$$\mathbf{x} \equiv \left\{ \begin{array}{l} c_{ict}^{\text{in}}, c_{ict}^{\text{out}}, c_{sct}^{\text{in}}, c_{sct}^{\text{out}}, q_{idt}, q_{iit}, q_{ist}, q_{it}^{\text{in}}, \\ q_{it}^{\text{out}}, q_{sit}, q_{ss't}, q_{st}, q_{st}^{\text{in}}, q_{st}^{\text{out}}, q_{wit}, y_{ist}, y_{sit} \\ \forall c \in \mathcal{C}, d \in \mathcal{D}, i, i' \in \mathcal{I}, s, s' \in \mathcal{S}, t \in \mathcal{T}, w \in \mathcal{W} \end{array} \right\} \quad (23)$$

$$\Omega = \{ \mathbf{x} \mid \text{Equations (1)-(21)} \} \quad (24)$$

where  $\mathbf{x}$  is a vector of the variables involved, while  $\Omega$  is a feasible searching space defined by the constraints. Note that the model is a mixed-integer nonlinear program (MINLP).

### Illustrative Example

An example adapted from Majozi (2005) is solved to illustrate the proposed approach. This example involves five batch units (A-E) and a continuous unit (F). Table 1 shows the operating data for the water-using units. Note that the contaminant mass load in unit F is given as the total amount over the 7.5-h cycle time. In other words, the instantaneous mass load of unit F is  $187.5/7.5 = 25$  kg/h. From the Gantt chart shown in Figure 4, it can be seen that seven time points are defined according to the start and end times of the batch operations, and the operation of unit F is divided into six batch sub-operations. A single uncontaminated fresh water source is available for use.

Table 1. Operating data for water-using units

Unit	$Q_i^L / Q_i^U$ (ton)	$C_{ic}^{\text{in,max}}$ (kg salt/ton water)	$C_{ic}^{\text{out,max}}$	Duration (h)	$\bar{M}_{ic}$ (kg)
A	0/1000	0	0.1	0-3	100
B	0/280	0.25	0.51	0-4	72.8
C	300/400	0.1	0.1	4-5.5	0
D	0/280	0.25	0.51	2-6	72.8
E	300/400	0.1	0.1	6-7.5	0
F	0/333.3	0.1	0.25	0-7.5	187.5

Cycle time = 7.5 h.

The optimization is carried out in the General Algebraic Modeling System (GAMS; Rosenthal, 2008) on a Core 2, 2.00 GHz processor, with BARON as the solver for MINLP.

A single storage tank with a maximum capacity of 1500 ton is considered for water reuse/recycle. The corresponding MINLP formulation involves 688 constraints, 624 continuous variables, and 84 binary variables, which is solved in 277.6 CPU s. The minimum fresh water consumption is determined as 1321.5 ton/cycle. This corresponds to an almost 50% reduction compared with the base case (2635.5 ton/cycle) where no water is recovered. Figure 5 shows the optimal network configuration. Note that all water reuse/recycle is carried out via water storage. The

level and concentration of water stored in the tank are shown in Figure 6. As shown, the actual capacity of storage required is 1015.8 ton, while the concentration varies between 0.1 and 0.2 kg salt/ton water.

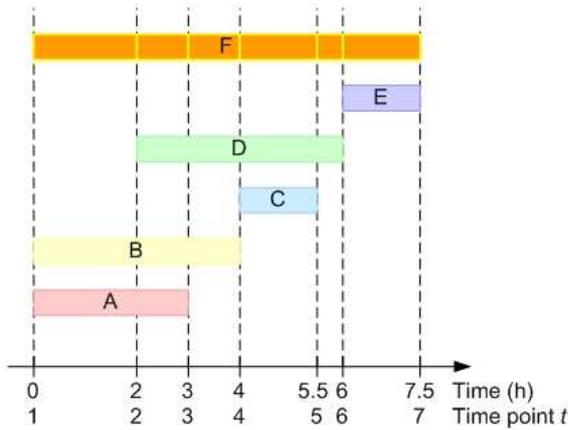


Figure 4. Gantt chart

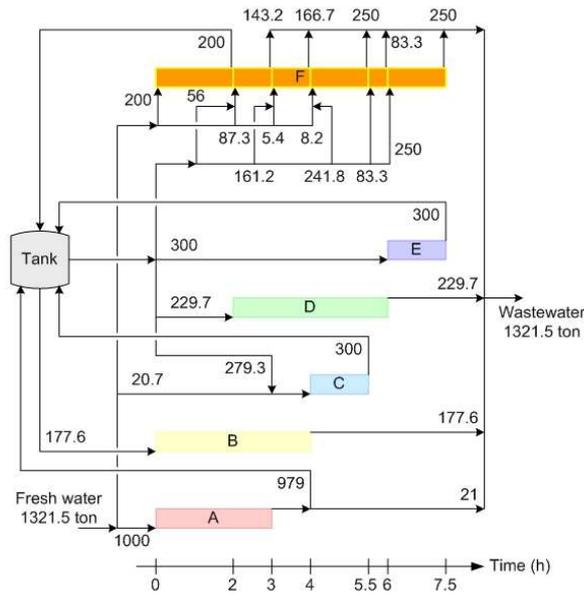


Figure 5. Optimal network configuration

### Concluding Remarks

A mathematical model for the synthesis of water networks involving batch and continuous units has been presented in this paper. For the case where batch units are in the majority, a dividing approach is proposed to convert the original problem into a simpler one that is to synthesize a batch water network. An example was solved to illustrate

the proposed approach. Other cases where the number of continuous units is large compared to that of batch units remain as the subject of future work.

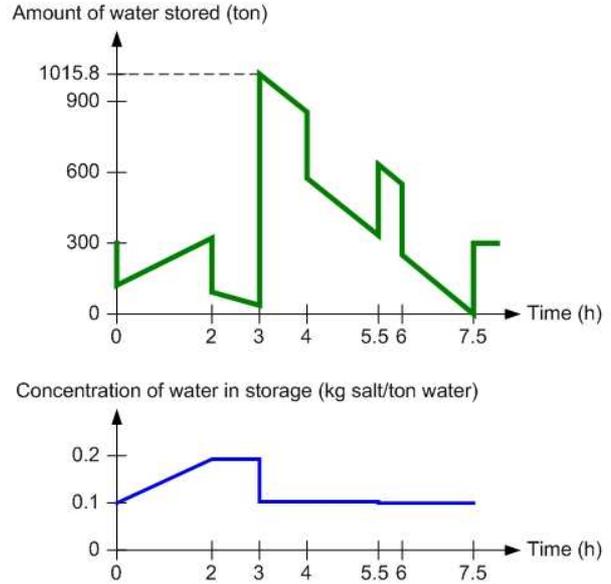


Figure 6. Storage profiles

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### Nomenclature

#### Indices and Sets

- $c \in \mathcal{C}$  contaminants
- $d \in \mathcal{D}$  waste disposal systems
- $i \in \mathcal{I}$  water-using units
- $i \in \mathcal{I}^b \subset \mathcal{I}$  batch water-using units
- $i \in \mathcal{I}^c \subset \mathcal{I}$  continuous water-using units
- $s \in \mathcal{S}$  storage tanks
- $t \in \mathcal{T}$  time points
- $w \in \mathcal{W}$  fresh water sources

#### Parameters

- $C_{ic}^{\text{in,max}}$  maximum inlet concentration of contaminant  $c$  for unit  $i$
- $C_{ic}^{\text{out,max}}$  maximum outlet concentration of contaminant  $c$  for unit  $i$
- $C_{wc}$  concentration of contaminant  $c$  in fresh water source  $w$
- $\Delta_i$  number of time intervals between the start and end of unit  $i$  operation

$M_{ict}$	mass load of contaminant $c$ for unit $i$ operation started at time point $t$
$Q_i^L$	lower bound on water flow through unit $i$
$Q_i^U$	upper bound on water flow through unit $i$
$Q_{is}^L$	lower bound on water flow from unit $i$ to tank $s$
$Q_{is}^U$	upper bound on water flow from unit $i$ to tank $s$
$Q_s^U$	maximum storage capacity of tank $s$
$Q_{si}^L$	lower bound on water flow from tank $s$ to unit $i$
$Q_{si}^U$	upper bound on water flow from tank $s$ to unit $i$
$Y_{it}^{\text{in}}$	= 0/1; indicating if unit $i$ operation starts at time point $t$
$Y_{it}^{\text{out}}$	= 0/1; indicating if unit $i$ operation finishes at time point $t$
$Z^{\text{cyc}}$	= 0/1; indicating the mode of batch operation, 0 for single operation and 1 for cyclic operation

### Variables

$c_{ict}^{\text{in}}$	inlet concentration of contaminant $c$ to unit $i$ at time point $t$
$c_{ict}^{\text{out}}$	outlet concentration of contaminant $c$ from unit $i$ at time point $t$
$c_{sct}^{\text{in}}$	inlet concentration of contaminant $c$ to tank $s$ at time point $t$
$c_{sct}^{\text{out}}$	outlet concentration of contaminant $c$ from tank $s$ at time point $t$
$q_{idt}$	water flow from unit $i$ to waste disposal system $d$ at time point $t$
$q_{ii't}$	water flow from unit $i$ to unit $i'$ at time point $t$
$q_{ist}$	water flow from unit $i$ to tank $s$ at time point $t$
$q_{it}^{\text{in}}$	inlet water flow to unit $i$ at time point $t$
$q_{it}^{\text{out}}$	outlet water flow from unit $i$ at time point $t$
$q_{sit}$	water flow from tank $s$ to unit $i$ at time point $t$
$q_{ss't}$	water flow from tank $s$ to tank $s'$ at time point $t$
$q_{st}$	amount of water stored in tank $s$ at time point $t$
$q_{st}^{\text{in}}$	inlet water flow to tank $s$ at time point $t$
$q_{st}^{\text{out}}$	outlet water flow from tank $s$ at time point $t$
$q_{wit}$	water flow from fresh water source $w$ to unit $i$ at time point $t$
$y_{ist}$	= 0/1; indicating if water is sent from unit $i$ to tank $s$ at time point $t$
$y_{sit}$	= 0/1; indicating if water is sent from tank $s$ to unit $i$ at time point $t$

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