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Synthesis of Total Water Networks for Batch Processes Considering the Impact of Contaminants

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This article develops a systematic methodology to consider the impacts of contaminants on regeneration network when synthesizing the integrated water network for batch processes. The method is based on the improved state-space superstructure where full configurations of the network are incorporated and concentrate streams of two outflows regeneration modules can be reused and further purified. To bridge the gap to industrial applications, regeneration modules with variable removal efficiencies for different types of contaminants and the inhibitory impact of toxic substances on regeneration network are considered. On these basis, an overall mixed-integer nonlinear programming (MINLP) model is formulated. The results of the case study show that the further reuse of concentrate streams decreases the fresh water consumption and cost-optimal network can be achieved when considering the effects of contaminants. In addition, the toxic substances in wastewater for regeneration also lead to the integration of different regeneration technologies.

1. Introduction

Wastewater minimization in batch plants has gained increasing attention from both academic and industrial communities because of stringent environmental legislation and growing application of batch processes. Wang and Smith (1995) first applied water pinch method to minimize wastewater generation in batch processes. Mathematical optimization-based approaches were also developed, such as optimization models considering water indirect reuse (Almató et al., 1999) and all possible recycle and reuse opportunities (Chen et al., 2008). After water reuse/recycle was deeply investigated, regeneration was introduced by many researchers to further reduce effluent. Liu et al. (2009) introduced a single semi-continuous regenerator for the single contaminant system, and Pintarič et al. (2014) introduced a batch regenerator when investigating various economic objectives. While the integration of various regeneration processes was considered by Cheng and Chang (2007) with economic objective and Tokos et al. (2013) with economic and environmental objectives. The different regeneration modes (batch and semi-continuous) and the selection of various regeneration technologies are considered by Wang et al. (2016), and the approach is improved to consider complex regeneration network and address multi-contaminant system (Dong et al., 2016). Although two outflows regeneration technologies like ultrafiltration and reverse osmosis have been involved in the work of Dong et al. (2016), opportunities that concentrate streams can be further reused and cleaned by regeneration modules are neglected to simplify the network structure. The majority of these works investigate the single contaminant systems and less attention has been paid to the effects of contaminants on regeneration subsystem. The research of Dong et al. (2016) related to total water network synthesis assumes that removal efficiencies for different contaminants in the regenerators are identical. This simplification cannot guarantee the true efficiency of the regeneration network, and even leads to infeasible design schemes, because the purification efficiencies always vary with different contaminants. It is common that wastewater generated from industrial production (i.e. the productions of fine organic chemicals) contains toxic substances that can contaminant certain regeneration processes. For example, heavy metals can greatly inhibit anaerobic process and nitrogen removal by nitrification/denitrification. This inhibitory impact of toxic substances on regeneration network has never been taken into consideration in previous studies. This paper aims to consider the effects of contaminants on the regeneration network and further reuse of concentrate stream from two outflows regeneration modules.

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2. Problem statement

Given is a set of batch water-using processes $i \in I$ with specific mass loads of each contaminant $c \in C$ under a predefined production schedule. The water-using processes are assumed to operate in truly batch mode. During the time horizon of interest, a set of fresh water sources $f \in F$ and end-of-pipe treatments $e \in E$ are available. For further water reuse, a set of batch regeneration modules ($br \in BR$) and semi-continuous regeneration modules ($cr \in CR$) with various candidate technologies are involved to purify the wastewater. Three sets of storage tanks ($u_b \in U_b$, $v_p \in V_p$ and $v_c \in V_c$) are installed for wastewater, purified water and concentrate streams from two outflows semi-continuous regeneration modules. The objective is to consider the effects of contaminants when synthesizing the water network of batch processes.

3. Superstructure

The formulated model relies on the superstructure (Figure 1) that consists of four blocks: distribution network (DN), water-using operator (WO), storage operator (SO) and regeneration operator (RO). The superstructure is adapted from our previous work (Dong et al., 2016), and the modifications are detailed below.

(1) Original four sets of tanks designated before and after the regeneration modules are replaced by three sets of tanks for waste water, purified water and concentrate water, in order to ensure the full configurations of the network and reduce the number of sets of storage tanks.

(2) The concentrate streams from two outflows regeneration modules are allowed to be directly reused and regenerated for further reuse, which can decrease the fresh water consumption and effluent discharge.

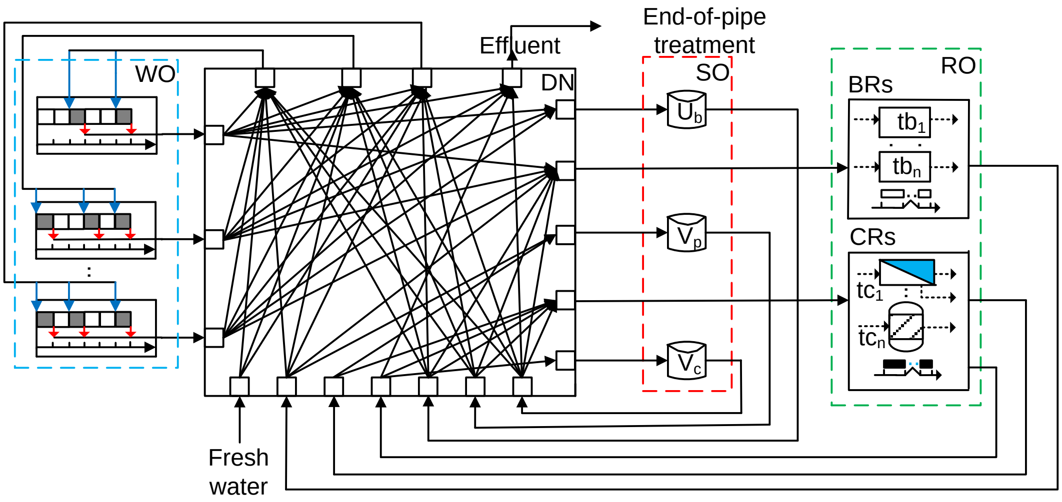

Figure1: State space superstructure for batch water network

4. Model formulation

The mathematical model is formulated on the basis of uniform discrete time representation, where constraints for WO can refer to our previous work (Dong et al., 2016).

4.1 Constraints for DN

Mass balances for the mixers attached to the upper and right sides of DN are given as Eq(1) and Eq(2), when the water is transferred in truly batch mode. If water is transferred in semi-continuous mode, flow rate balances around the mixers will be formulated. It should be pointed out that mass and flow rate balances are both presented when truly batch and semi-continuous mode are involved at the same time. For the splitters attached to the lower and left sides of DN, mass and flow rate balances are shown by Eq(3) and Eq(4).

$$m_{mx,t}^{in} = \sum_{sp \in SP_{mx}} m_{sp,mx,t} \quad mx \in MX, t \in T \tag{1}$$

$$f_{mx,t}^{in} = \sum_{sp \in SP_{mx}} f_{sp,mx,t} \quad mx \in MX, t \in T \tag{2}$$

$$m_{sp,t}^{\text{out}} = \sum_{mx \in \text{MX}_{sp}} m_{sp,mx,t} \quad sp \in \text{SP}, t \in \text{T} \tag{3}$$

$$f_{sp,t}^{\text{out}} = \sum_{mx \in \text{MX}_{sp}} f_{sp,mx,t} \quad sp \in \text{SP}, t \in \text{T} \tag{4}$$

4.2 Constraints for SO

The overall mass balance around the storage tanks is formulated as constraint (5).

$$q_{sr,t} = q_{sr,t-1} + m_{sr,t}^{\text{in}}\big|_{sr \neq v_c} - m_{sr,t}^{\text{out}} + \Delta\text{T} f_{sr,t-1}^{\text{in}}\big|_{sr \neq u_b} - \Delta\text{T} f_{sr,t-1}^{\text{out}} \quad \forall sr \in \text{SR}, t \in \text{T} \tag{5}$$

In order to ensure the feasibility of mass balance in storage tanks, constraints (6) - (8) are given.

$$q_{sr,t} \le w_{sr} \text{Q}_{sr}^{\max} \quad \forall sr \in \text{SR}, t \in \text{T} \tag{6}$$

$$q_{sr,t} \ge f_{sr,t}^{\text{out}} \Delta\text{T} \quad \forall sr \in \text{SR}, t \in \text{T}, t < \text{N} \tag{7}$$

$$f_{sr,t}^{\text{in}} f_{sr,t}^{\text{out}} \le 0 \quad \forall sr \in \text{SR}, sr \neq u_b, t \in \text{T} \tag{8}$$

4.3 Constraints for RO

The concentration balances around the batch and semi-continuous regeneration modules are respectively presented by constraints Eq(9) and Eq(10), where $\text{Rc}_{tb,c}$ and $\text{Rc}_{tc,c}$ are the removal ratios for contaminants.

$$\begin{gathered} c_{br,c,t'}^{\text{out}} - \text{M}(2 - w_{br,t} - w_{br,tb}) \le c_{br,c,t}^{\text{in}}(1\text{-Rc}_{tb,c}) \le c_{br,c,t'}^{\text{out}} + \text{M}(2 - w_{br,t} - w_{br,tb}) \\ \forall br \in \text{BR}, tb \in \text{TB}, c \in \text{C}, t, t' \in \text{T}, t' = t + \Delta\text{t}_{tb} \end{gathered} \tag{9}$$

$$\begin{gathered} c_{cr,c,t}^{\text{out}} - \text{M}(2 - w_{cr,t} - w_{cr,tc}) \le c_{cr,c,t}^{\text{in}}(1\text{-Rc}_{tc,c}) \le c_{cr,c,t}^{\text{out}} + \text{M}(2 - w_{cr,t} - w_{cr,tc}) \\ \forall cr \in \text{CR}, tc \in \text{TC}, c \in \text{C}, t \in \text{T} \end{gathered} \tag{10}$$

The limitations for the inlet concentrations are imposed by additional constraints Eq(11) and Eq(12), in order to consider the inhibitory impact of toxic substances on the regeneration processes and the variation of removal efficiency with concentration of contaminants.

$$\sum_{tb \in \text{TB}} w_{br,tb} \text{C}_{tb,c}^{\text{in,min}} \le c_{br,c,t}^{\text{in}} \le \sum_{tb \in \text{TB}} w_{br,tb} \text{C}_{tb,c}^{\text{in,max}} \quad \forall br \in \text{BR}, t \in \text{T} \tag{11}$$

$$\sum_{tc \in \text{TC}} w_{cr,tc} \text{C}_{tc,c}^{\text{in,min}} \le c_{cr,c,t}^{\text{in}} \le \sum_{tc \in \text{TC}} w_{cr,tc} \text{C}_{tc,c}^{\text{in,max}} \quad \forall cr \in \text{CR}, t \in \text{T} \tag{12}$$

Other mass balance constraints for RO are similar to those in the work of Dong et al. (2016).

4.4 Objective function

The objective function for the problem is to minimize the total annual cost determined by Eq(13), which encompasses the fresh water cost, the cost of treatment, the cost of storage tanks, capital and operational cost of regeneration modules.

$$\begin{aligned} \min TAC = & \Big(\sum_{sr \in \text{SR}} \text{ICS}_{sr} w_{sr} + \sum_{br \in \text{BR}} \sum_{tb \in \text{TB}} w_{br,tb} \text{IC}_{tb} + \sum_{cr \in \text{CR}} \sum_{tc \in \text{TC}} w_{cr,tc} \text{IC}_{tc} \Big) + \text{NTC} \Big(\sum_{br \in \text{BR}} \sum_{t \in \text{T}} \sum_{tb \in \text{TB}} m_{br,tb,t}^{\text{in}} \text{OC}_{tb} \\ & + \sum_{cr \in \text{CR}} \sum_{t=1}^{\text{N}-1} \sum_{tc \in \text{TC}} f_{cr,tc,t}^{\text{in}} \Delta\text{TOC}_{tc} + \sum_{e \in \text{E}} \Big(\sum_{cr \in \text{CR}} \sum_{t=1}^{\text{N}-1} f_{cr,e,t} \Delta\text{T} + \sum_{t \in \text{T}} m_{e,t}^{\text{in}} \Big) \text{Ce}_e + \sum_{f \in \text{F}} \sum_{t \in \text{T}} m_{f,t}^{\text{out}} \text{Cf}_f \Big) \end{aligned} \tag{13}$$

5. Case study

A multi-contaminant case study is introduced to explore the impact of contaminants on the total water network for batch plants. Limiting data of water-using operations is given in Table 1, relative parameters for regeneration modules in Table 2.

The annual investment of each storage tank is set as 1,000 \$/y, and the costs of fresh water and end-of-pipe treatment are assumed to be 1 \$/t and 5 \$/t. Total number of cycles in a year is set as 800. The problem is implemented in GAMS 23.4 by the DICOPT solver, using CPLEX as the MILP solver and MINOS as the NLP solver.

Table 1: Limiting data for water-using processes of the case

Operation	Contaminant	$[M_i^{min}, M_i^{max}]$ (t)	$C_{i,c}^{max}$ (μg c/g water) in	$C_{i,c}^{max}$ (μg c/g water) out	Start time (h)	End time (h)	$MI_{i,c}$ (kg)
P1	A/B/C	[0,200]	0/0/0	20/400/50	0	0.5	4/80/10
P2	A/B/C	[0,300]	50/200/50	100/1,000/12,000	1	2	15/240/3,585
P3	A/B/C	[0,150]	10/50/300	200/100/1,200	2	3.5	28.5/7.5/135
P4	A/B/C	[0,200]	30/100/200	75/200/1,000	1	2	9/20/160
P5	A/B/C	[0,100]	150/200/350	300/1,000/1,200	4	4.5	15/80/85
P6	A/B/C	[0,150]	0/0/50	150/300/2,500	5.5	6.5	22.5/45/367.5
P7	A/B/C	[0,50]	100/150/220	200/1,500/1,000	8	10	5/67.5/39

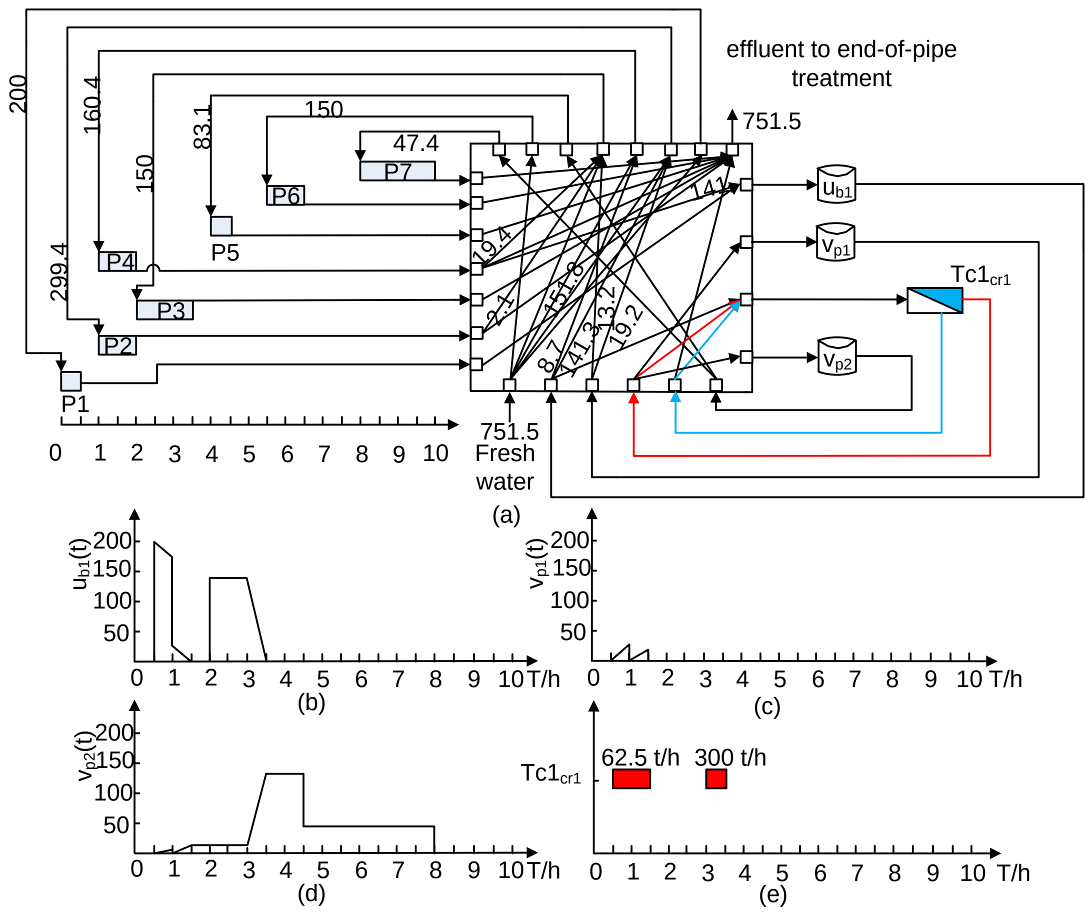

Figure 2: (a) Resultant network configuration for Scenario B; (b) - (d) Variations of residue water in storage tanks; (e) The schedule of the regeneration module

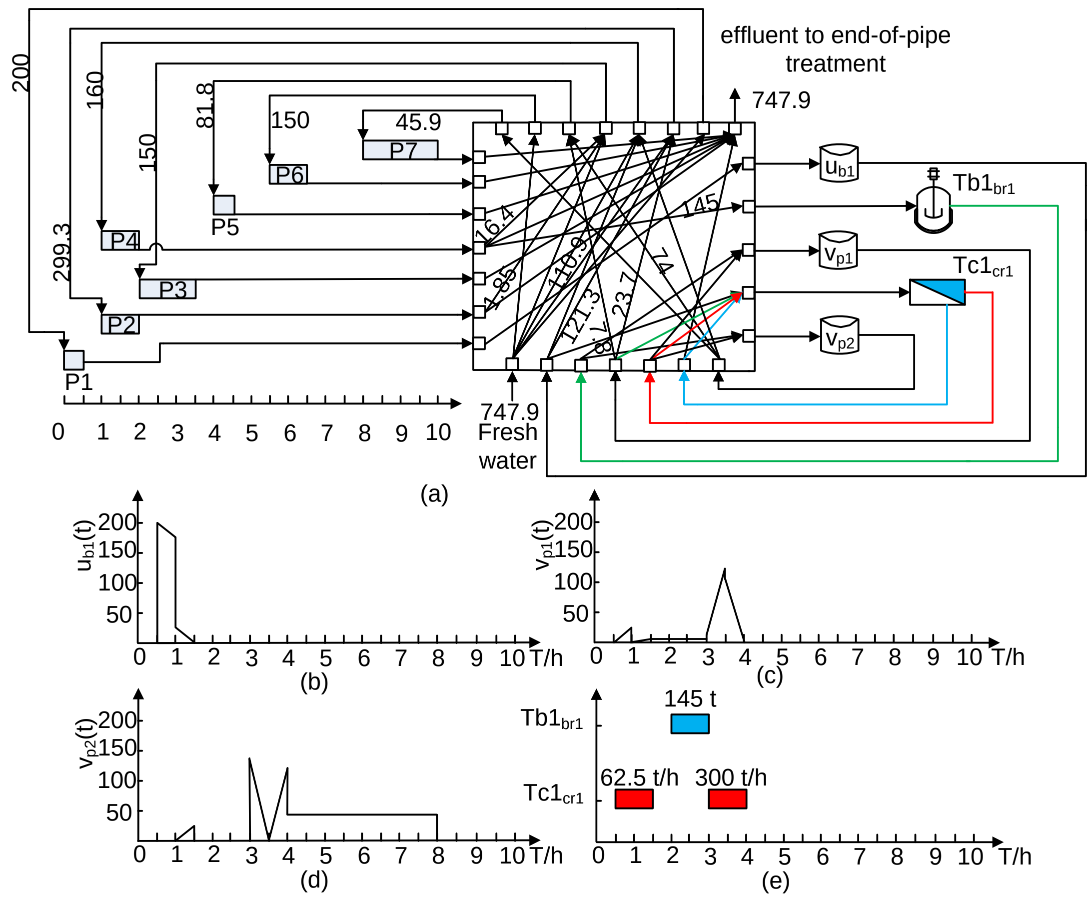

Figure 3: (a) Resultant network configuration for Scenario C; (b) - (d) Variations of residue water in storage tanks; (e) Schedules of regeneration modules

Table 2: Process parameters for regeneration modules in the RO of the case

Technology	BRs			CRs		
	Tb1	Tb2	Tb3	Tc1	Tc2	Tc3
Rr	1	1	1	0.8	0.6	1
Rc (c1, c2, c3)	0.8/0.5/0	0/0.8/0.4	0/0.8/0.5	0/0.9/0.85	0.8/0.4/0.9	0.8/0.4/0.9
IC ($/y)	60,000	50,000	50,000	60,000	110,000	120,000
OC ($/t)	0.01	0.02	0.02	0.04	0.02	0.02
Capacity (t & t/h)	[50 200]	[50 300]	[50 200]	[50 300]	[50 300]	[50 200]
Duration (h)	1	1.5	1	-	-	-
$C^{in,min}$ (ppm)	15/100/0	10/100/100	10/100/100	10/100/50	0/100/50	0/100/50
$C^{in,max}$ (ppm)	300/1,200/ 1,500	50/1,200/ 1,500	50/1,200/ 1,500	20/1,200/ 1,500	300/1,200/ 1,500	300/1,200/ 1,500

Table 3: Comparison results for the case study

Scenarios	Fresh water consumption (t/y)	Total annual cost ($/y)
Scenario A (central storage tank only)	671,400	4,037,547
Scenario B (regeneration)	601,162	3,676,775
Scenario C (regeneration with maximum inlet concentration)	598,330	3,725,766

Three scenarios are analysed in this case study. Scenario A is the base scenario where only water reuse and recycle with storage tanks are involved, then the regeneration subsystem with variable removal ratios for different types of contaminants is both incorporated in Scenario B and C. In Scenario B, there are no

limitations for maximum inlet concentrations of regeneration technologies, while Scenario C considers the limitations. Before directly solving the problem, technologies Tb2 and Tc2 are firstly removed from the synthesis framework according to the pre-processing rules proposed in the paper of Dong et al. (2016).
Comparison results for these scenarios are shown in Table 3. Compared to Scenario A, the consumption of fresh water in Scenario B is reduced from 671,400 t/y to 601,162 t/y with a 10.47 % decrease, and the corresponding annual cost is reduced from 4,037,547 $/y to 3,676,775 $/y with an 8.94 % decrease. The fresh water consumption of 598,330 t/y and the annual cost of 3,725,766 $/y in Scenario C are obtained, corresponding to a 10.88 % reduction in fresh water consumption and a 7.72 % in annul investment as compared to Scenario A. The annual cost of the water network in Scenario C (3,725,766 $/y) is higher than that in Scenario B (3,676,775 $/y), while it yields a 0.47 % reduction (from 601,162 t/y to 598,330 t/y) in fresh water consumption. This is because the limitation for maximum inlet concentration of regeneration facilities calls for the integration of different technologies, resulting in higher investment for regeneration and less fresh water consumption. The corresponding design schemes for Scenario B and C are presented in Figure 2(a) and 3(a). Note that there exist direct recycle streams from both permeate and concentrate sides to the inlet of two outflows semi-continuous regeneration modules. This can further reduce the fresh water consumption and effluent, though it causes the network configuration more complex. For Scenario B and C, storage profiles of wastewater in tanks and schedules of active regeneration modules are also shown in Figure 2 and 3.

6. Conclusions

In this article, an adapted superstructure is proposed to ensure the full configurations of the network and allow concentrate streams to be reused and further purified. The regeneration processes with variable purification efficiencies for different types of contaminants and the inhibitory impact of toxic substances on regeneration network have been considered. According to these, a MINLP model is then formulated. The effectiveness of proposed methodology is demonstrated by the case study. The results show that cost-optimal network configuration can be achieved when considering the effects of contaminants. Future work should investigate the effect of contaminants on the end-of-pipe treatment and uncertainties in regeneration efficiency.

Acknowledgments

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