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Property Integration of Water Network for Batch Processes in Multiple Production Lines

Sen Zhang, Linlin Liu*, Lei Zhang, Jian Du

Institute of Chemical Process Systems Engineering, School of Chemical Engineering, Dalian University of Technology,
Dalian, 116024, Liaoning, China
liulinlin@dlut.edu.cn

Batch operation is the main production pattern for high value-added chemicals, and the wastewater from different batch production lines features differently in properties, such as contaminant concentrations, toxicity, pH, and chemical oxygen demand. Less attention has been drawn on the batch water network design with water property considered. To address this issue, this work develops a superstructure-based optimization approach to incorporate property integration within the synthesis of batch water network. Multiple production lines are considered in the study, so in addition to the water re-using system inside each production line, the re-using across lines and the central property treatment system are included by involving intermediate storage tanks as hubs for in-line, inter-line water allocation and treatment. The property treatment system is constructed by a list of property interceptors, which operate in semi-continuous manner with optimized treating performance in different time intervals. To obtain the desired network structure, a Mixed Integer Nonlinear Programming (MINLP) model is formulated, and the operation schedule of interceptors and storage tanks are optimized as well. Finally, a multi-property case is elaborated to validate the proposed method. By considering the potential interactions among batch production lines, a 22.12 % drop in Total Annual Cost (TAC) is achieved in the case study, demonstrating the effectiveness of the method.

1. Introduction

With the increasing freshwater price and more stringent environmental regulation for the chemical process industry, effective utilization of water resource has become more crucial, and lots of works have been launched for water conservation and cost saving with Process Integration technique concerning continuous water-using processes (Khor et al., 2014). Research about batch water network synthesis also got attention due to the operating flexibility of batch production (Gouws et al., 2010). However, it should be noted that the involving of time makes the batch integration more complicated. Mathematical optimization-based approach has been adopted for relevant research, due to its capability of handling multiple water contaminants, time-related constraints and topological connection constraints, but few studies have been conducted concerning property integration together with mass integration.

Pollutant concentration is not the only constraint for water using and discharging, other properties, such as pH, toxicity and COD, are also important indexes and are often the priority with environmental limitations. It is important to integrate the water network considering properties. El-Halwagi et al. (2004) proposed the concept of property integration for Water Allocation Network (WAN), where a new concept of the cluster was introduced to track functionality and properties of the complex mixtures, which further evolved into Property Operator to indicate the mixing rules (linear or nonlinear to different properties). Ng et al. (2008) established a source-tank-interception-tank-sink representation where interceptors were used to modify the properties of streams and tanks were involved to enable mixing, storage, and dispatch of the reused/recycled water streams. Ponce-Ortega et al. (2010) summarized the property operators raised in El-Halwagi et al. (2004). They presented the rules of calculating the property operators. The nonlinearities of the system were eliminated in the proposed mass and property-based model, and the bilinear terms were handled with a relaxation approach. Vázquez-Castillo et al. (2013) presented a multi-objective optimization approach considering the water characteristics and the property-based constraints for sinks. Therein, since adjusting properties may require hazardous

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chemicals, issues to minimize the total volume of stored materials were considered along with the economic objective. Besides, Zhang et al. (2019) proposed a new method with the operator potential concept combining a Linear Programming (LP) approach to determine the allocation.

It is found from the literature review that the property integration mainly focused on batch processes in one production line. Efforts have been rarely paid to address the problem involving multiple production lines. The synchronous operation of multiple production lines is very common in fine chemical and pharmaceutical industries, and the resultant integration problem is more difficult than that of a continuous process. In this study, a superstructure-based optimization approach for the simultaneous integration of mass and properties for batch water network is presented, where the water reuse inside and across the production lines, and a semi-continuous property treatment system are involved.

2. Problem Statement

The problem addressed in this article can be stated as follows: there is a network with water sources and sinks in several batch production lines with predefined operating schedule. Each sink requires a known mass flow rate with specific properties constraints for composition, pH, toxicity, etc. A set of water sources with fixed flow rates and properties are also known. Each source can be recycled/reused through storage tanks, or treated by semi-continuous interceptors with unchanged treatment rate at each time interval and known conversion factor for each corresponding property (relevant to the treatment cost and interceptor investment). The rate can vary at different time intervals. Besides, fresh source with known property value is available to feed any sink, for which the flow rate and feeding time are to be optimized. In this study, the water reusing across production lines is allowed and a central property treatment system containing interceptors is performed to implement the in-line and inter-line water reuse, for which, storage units will be needed to overcome the time limits. In summary, the problem to be solved is to determine a cost-effective water network structure considering interactions between multiple batch production lines, where the in-line water allocation, inter-line water allocation and centralized water treatment should be well scheduled simultaneously.

3. Optimization model for batch water integration containing intermediate tanks between multiple production lines

3.1 Superstructure of water network

The time is described in Figure 1. Cycle N is divided into time points and time intervals according to the operating time of units. A set t = {1,2, …, T} is used to express time points and Δh_t denotes a time interval. The batch units operate at fixed time points. The end of the cycle is regarded as the beginning of the next cycle.

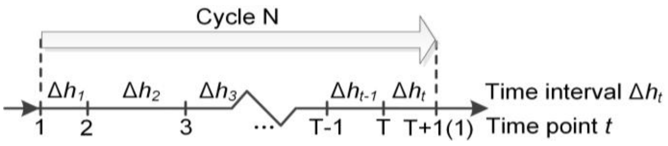

Figure 1: The representation of time points and time intervals in cycle N

Figure 2 shows the superstructure for the water integration scheme containing intermediate storage tanks and centralized treatment in multiple production lines.

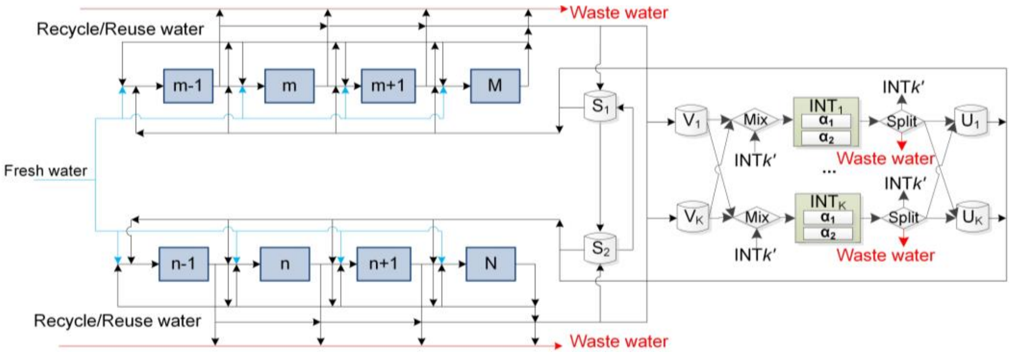

Figure 2: Superstructure of property-based batch water network in multiple production lines

The operating time of batch sources and sinks is fixed but different, so there are potential connections among batch production lines and it is necessary to utilize tanks to perform the water allocation in-line and inter-line. The sources can be directly reused when they meet the time and property requirement of the sinks. Otherwise, they must be reused indirectly through the intermediate storage tanks S in each line to eliminate the time limits, or sent to the pre-storage tanks V. The water allocation across different lines must go through tanks S. The sources and sinks in batch operation from all lines cannot be directly regenerated as property interceptors in this paper are operating in semi-continuous manner. Two groups of tanks V and U are set before and after the interceptors. The pre-storage tanks V are set to store the streams that need to be treated and the post-storage tanks U are to store the streams that have been treated. Then, the post-storage tanks distribute streams to sinks in any production line. The interceptors are arranged in mixed connection with tanks V and U to consider all connection potential and streams that have been treated can enter other interceptors for further treatment, but they are not allowed to return into the former one. Unlike the batch operation which feeds instantaneously at the time point, or the continuous operation which feeds continuously through the entire time horizon, the semi-continuous operation can feed continuously at certain time intervals. The wastewater from process sources can be discharged to the environment directly if they meet the environmental constraints. Otherwise, they need to be treated by interceptors before discharge. Noted that the streams that have been intercepted cannot be stored in the tanks U if they need to be discharged so that the capacity of tanks can be reduced.

3.2 Model formulation

The indices and the sets used in modelling are defined before the model presentation: $l \in L$, the batch production line; $i \in I$, the water sources; $j \in J$, the water sinks; $v \in V$, the pre-storage tanks; $u \in U$, the post-storage tanks; $s \in S$, the intermediate storage tanks; $p \in P$, the properties; $k \in K$, the interceptors; $x \in X$, the options of conversion factor; ψ, property operator.

3.2.1 Mass and property balance

The fresh sources can feed to the batch sinks in different lines directly, where FR is the total mass flow from the fresh source. $FRLJ_{l,j,t}$ is the mass flow from the fresh source to the batch sink j, as shown in Eq(1):

$$FR = \sum_{t \in T} \sum_{l \in L} \sum_{j \in J} FRLJ_{l,j,t} \tag{1}$$

The stream of batch process source in each line, at mass flowrate $FLI^{out}_{l,i,t}$, can be directly reused to the sinks in the same line, at $FLIJ_{j,l,i,t}$, when they meet the time and property requirement, otherwise they will be sent to the tank s at $FLIS_{s,l,i,t}$, tanks V before interceptors at $FLIV_{v,l,i,t}$ and the environment at $FLIW_{l,i,t}$. Binary parameters are used to indicate the operating time of batch sources but not listed for simplicity. The equation is shown in Eq(2):

$$FLI^{out}_{l,i,t} = \sum_{j \in J} FLIJ_{j,l,i,t} + \sum_{s \in S} FLIS_{s,l,i,t} + \sum_{v \in V} FLIV_{v,l,i,t} + FLIW_{l,i,t} \quad \forall l \in L, i \in I, t \in T \tag{2}$$

Similarly, the streams sent to batch sink j come from each batch source i, tank s, tank v, or fresh source. The mass balance and property constraints can be obtained in Eqs(3)-(5), where $\psi^{max,L,J}_{l,j,p}$ and $\psi^{min,L,J}_{l,j,p}$ are upper and lower property constraint of sink j:

$$FLJ^{in}_{l,j,t} = \sum_{i \in I} FILJ_{i,l,j,t} + \sum_{s \in S} FSLJ_{s,l,j,t} + \sum_{u \in U} FULJ_{u,l,j,t} + FRLJ_{l,j,t} \quad \forall l \in L, j \in J, t \in T \tag{3}$$

$$FLJ^{in}_{l,j,t} \psi^{in,L,J}_{l,j,t,p} = \sum_{i \in I} FILJ_{i,l,j,t} \psi^{out,L,I}_{l,i,p} + \sum_{s \in S} FSLJ_{s,l,j,t} \psi^{out,S}_{s,t,p} + \sum_{u \in U} FULJ_{u,l,j,t} \psi^{out,U}_{u,t,p} + FRLJ_{l,j,t} \psi^{R}_{p} \quad \forall l \in L, j \in J, t \in T, p \in P \tag{4}$$

$$\psi^{\min,L,J}_{l,j,p} \le \psi^{in,L,J}_{l,j,t,p} \le \psi^{\max,L,J}_{l,j,p} \quad \forall l \in L, j \in J, t \in T, p \in P \tag{5}$$

As shown in Eq(6)-Eq(8), the streams into the tank v at time t are from the batch sources. The outlet streams from the tank v can feed to interceptor k at time interval Δh_t. The rest water stored at time point t is $FV_{v,t}$. QV_v is the maximum volume of the tank v during the cycle, where yv_v means whether it exists.

$$FV_{v,t} = FV_{v,t-1} + \sum_{l \in L} \sum_{i \in I} FLIV_{v,l,i,t} - \sum_{k \in K} fVK_{v,k,t-1} \cdot \Delta h_{t-1} \quad \forall v \in V, t \in T, t > 1 \tag{6}$$

$$\psi^{out,V}_{v,t,p} \cdot FV_{v,t} = \psi^{out,V}_{v,t-1,p} \cdot FV_{v,t-1} + \sum_{l \in L} \sum_{i \in I} \psi^{out,L,I}_{l,i,p} \cdot FLIV_{v,l,i,t} - \sum_{k \in K} \psi^{out,V}_{v,t-1,p} \cdot fVK_{v,k,t-1} \cdot \Delta h_{t-1} \quad \forall v \in V, t \in T, t > 1, p \in P \tag{7}$$

$$FV_{v,t} \le QV_v \le QV^{\max} \cdot yv_v \quad \forall v \in V, t \in T \tag{8}$$

The stream balance of the interceptors K is shown in Eq(9). Eqs(10)-(11) indicate the mixed stream property before the interceptor k. While the outlet property is treated by corresponding interceptor k by multiplying conversion factor $\alpha_{k,x}$, shown in Eq(12), which is relevant to the treatment cost of interceptors. The non-corresponding property cannot be treated and any interceptor k only use one kind of conversion factor.

$$\sum_{v\in V} fVK_{v,k,t} + \sum_{k'\in K} fKK_{k',k,t} = \sum_{u\in U} fKU_{k,u,t} + \sum_{k'\in K} fKK_{k,k',t} + fKW_{k,t} \quad \forall k \in K, k' \in K, t \in T, k \neq k' \tag{9}$$

$$\psi_{k,t,p}^{in,K} \cdot fK_{k,t}^{in} = \sum_{v\in V} \psi_{v,t,p}^{out,V} \cdot fVK_{v,k,t} + \sum_{k'\in K} \psi_{k',t,p}^{out,K} \cdot fKK_{k',k,t} \quad \forall k \in K, k' \in K, t \in T, p \in P, k \neq k' \tag{10}$$

$$fK_{k,t}^{in} = \sum_{v\in V} fVK_{v,k,t} + \sum_{k'\in K} fKK_{k',k,t} \quad \forall k \in K, k' \in K, t \in T, k \neq k' \tag{11}$$

$$\psi_{k,t,p}^{out,K} = \sum_{x\in X} y_{k,x} \cdot \alpha_{k,x} \cdot \psi_{k,t,p}^{in,K} \qquad \forall k \in K, t \in T \tag{12}$$

If the streams treated in property interceptors need to be sent to the batch sink j, they should feed into the storage tank u first. The streams which enter the storage tank u at time interval t are from interceptor k, similar to the equations about the tank v. The rest of water stored in the tank u at time t is $FU_{u,t}$, and QU_u is the maximum volume of tank u during the cycle, where yu_u means whether tank u exists, shown in Eqs(13)-(15).

$$FU_{u,t} = FU_{u,t-1} + \sum_{k\in K} fKU_{k,u,t-1} \cdot \Delta h_{t-1} - \sum_{l\in L}\sum_{j\in J} FULJ_{u,l,j,t} \quad \forall u \in U, t \in T, t > 1 \tag{13}$$

$$\psi_{u,t,p}^{out,U} \cdot FU_{u,t} = \psi_{u,t-1,p}^{out,U} \cdot FU_{u,t-1} + \sum_{k\in K} \psi_{k,t-1,p}^{out,K} \cdot fKU_{k,u,t-1} \cdot \Delta h_{t-1} - \sum_{l\in L}\sum_{j\in J} \psi_{u,t,p}^{out,U} \cdot FULJ_{u,l,j,t} \quad \forall u \in U, t \in T, t > 1 \tag{14}$$

$$FU_{u,t} + FU_{u,t}^{out} \le QU_u \le QU^{\max} \cdot yu_u \quad \forall u \in U, t \in T \tag{15}$$

In addition, this paper adds tank s to introduce water reuse inside each production line and between different lines. Eq(16) shows that the inlet streams of tank s at time t come from water source i in the same line and tank s’ in other lines. The flow into the water sink j in the same line and tank s’ in other lines. Note that water exchange between different lines cannot operate at the same time point. Eqs(17)-(18) indicate the corresponding property balance and volume constraints of storage tank s:

$$FS_{s,t} = FS_{s,t-1} + \Big(\sum_{i\in I} FLIS_{s,l,i,t} + FSS_{s',s,t}\Big) - \Big(\sum_{j\in J} FSLJ_{s,l,j,t} + FSS_{s,s',t}\Big) \quad \forall l \in L, s \in S, t \in T, t > 1, l = s \neq s' \tag{16}$$

$$\begin{aligned} \psi_{s,t,p}^{out,S} \cdot FS_{s,t} = {} & \psi_{s,t-1,p}^{out,S} \cdot FS_{s,t-1} + \Big(\sum_{i\in I} FLIS_{s,l,i,t} \psi_{l,i,p}^{out,L,I} + \sum_{s'\in S} FSS_{s',s,t} \cdot \psi_{s',t,p}^{out,S}\Big) - \psi_{s,t,p}^{out,S} \cdot \Big(\sum_{j\in J} FSLJ_{s,l,j,t} + \sum_{s'\in S} FSS_{s,s',t}\Big) \\ & \forall l \in L, s \in S, t \in T, t > 1, l = s \neq s' \end{aligned} \tag{17}$$

$$FS_{s,t} + FS_{s,t}^{out} \le QS_s \le QS^{\max} \cdot ys_s \quad \forall s \in S, t \in T \tag{18}$$

The total mass flow into the environment is the sum of all kinds of process sources and the streams from interceptors. Note that the streams directly sent to the environment cannot come from the storage tank v or u. The mass balance equations and property constraints are described by Eq(19)-Eq(21).

$$FW = \sum_{t\in T}\sum_{l\in L}\sum_{i\in I} FLIW_{l,i,t} + \sum_{k\in K}\sum_{t\in T} fKW_{k,t} \cdot \Delta h_t \tag{19}$$

$$\psi_p^W \cdot FW = \sum_{t\in T}\sum_{l\in L}\sum_{i\in I} FLIW_{l,i,t} \psi_{l,i,p}^{out,L,I} + \sum_{k\in K}\sum_{t\in T} fKW_{k,t} \cdot \Delta h_t \cdot \psi_{k,t,p}^{out,K} \quad \forall p \in P \tag{20}$$

$$\psi_p^{\min,W} \le \psi_p^W \le \psi_p^{\max,W} \quad \forall p \in P \tag{21}$$

3.2.2 Objective function

The objective function of TAC includes the cost of fresh sources, the variable and fixed costs of all tanks, and the interceptors cost considering operation cost, variable and fixed investment. TAC is expressed as follows:

$$\begin{aligned} \min TAC = {} & C^R \cdot FR + \sum_{s\in S} (C_s^{fix,S} + C_s^{var,S} \cdot QS_s) AF \cdot ys_s + \sum_{u\in U} (C_u^{fix,U} + C_u^{var,U} \cdot QU_u) AF \cdot yu_u \\ & + \sum_{v\in V} (C_v^{fix,V} + C_v^{var,V} \cdot QV_v) AF \cdot yv_v + \sum_{k\in K}\sum_{t\in T}\sum_{x\in X} N \cdot C_{k,x}^{oper,K} \cdot fK_{k,t}^{in} \cdot \Delta h_t \cdot y_{k,x} \\ & + \sum_{k\in K}\sum_{x\in X} (C_{k,x}^{fix,K} + C_{k,x}^{var,K} \cdot fK_k^{in,\max}) AF \cdot y_{k,x} \end{aligned} \tag{22}$$

4. Case study

An example adapted from the work of Vázquez-Castillo (2013) is used to demonstrate the proposed strategy. There are three kinds of interceptors to dispose of components, toxicity and pH. Table 1-2 illustrate the mass flow, property value and operating time of sources and sinks. Relevant conversion factors, processing time and cost of property interceptors are listed in Table 3. There are 11 time intervals in one period and the system operating lasts for 333 periods. The unit price of fresh water is $C^{R}=0.1\$/\text{kg}$ and the annual factor AF is 0.3.

Table 1: Data of sources in different production lines for Case Study

Water sources	Period t	F/kg	Composition/ppm	Toxicity/%	pH
Process source 1 in line 1 (L1SR1)	4	1,088	0.460	0.5	4.8
Process source 2 in line 1 (L1SR2)	5	816	0.570	0.9	4.7
Process source 3 in line 1 (L1SR3)	6	1,587	0.490	0.7	5.2
Process source 1 in line 2 (L2SR1)	7	698	0.395	1.8	5.1
Process source 2 in line 2 (L2SR2)	8	1,791	0.290	1.9	5.4
Process source 3 in line 2 (L2SR3)	9	1,351	0.054	1.4	5.8
Fresh water R			0.000	0	7.0

Table 2: Data of sinks in different production lines for Case Study

Water sinks	Period t	F/kg	Comp^{Max} /ppm	Comp^{min} /ppm	Tox^{Max} /%	Tox^{Min} /%	pH^{Max}	pH^{Min}
Process sink 1 in line 1 (L1SK1)	10	544	0.15	0	2.00	0	8.0	5.3
Process sink 2 in line 1 (L1SK2)	13	1,152	0.15	0	2.00	0	7.8	5.4
Process sink 3 in line 1 (L1SK3)	15	446	0.015	0	2.00	0	8.2	5.2
Process sink 1 in line 2 (L2SK1)	17	712	0.001	0	2.00	0	7.5	5.35
Process sink 2 in line 2 (L2SK2)	19	521	0.15	0	2.00	0	8.4	5.5
Process sink 3 in line 2 (L2SK3)	21	394	0.005	0	2.00	0	9.4	5.6
Waste water W			0.2	0	0.1	0	9.0	5.2

Table 3: Data of property interceptors

Property	Interceptor	Processing time/h	Conversion factor	Operating cost /$\$\cdot\text{kg}^{-1}$	Fixed cost /\$	Variable cost /\$
Composition	COMP^1	1	0	0.0143	8,000	25
	COMP^2	1	0.1	0.0073	7,000	18
Toxicity	TOX^1	1	0	0.00216	9,000	28
	TOX^2	1	0.1	0.00165	8,200	21
pH	NEU^1	1	0.3	0.0178	5,200	16
	NEU^2	1	0.8	0.0099	4,800	14

As shown in Figure 3a, process sources 1-3 in line 2 which meet the property constraints of sinks send 4.852 kg, 866 kg and 1,351 kg water into the tank S_2, avoiding the reuse opportunity waste due to the mismatching of time. Then the tank S_2 distribute 4.852 kg water to sink 1 and 521 kg to sink 2 in its own line, as well as 544 kg to sink 1 and 1,152 kg to sink 2 in another line through S_1. The rest water sources are sent into pre-storages V_1 and V_2. Connections between tanks V, U and interceptors are shown in Figure 3a. The interceptor COMP^2 operates at the flowrate of 501.25 kg·h^{-1} in time interval 5-6 h and 2330.19 kg·h^{-1} in 6-7h. TOX^1 operates at the flowrate of 1,863.32 kg·h^{-1}, 219.85 kg·h^{-1} and 809.07 kg·h^{-1} in 6-7 h, 10-13 h and 13-15 h. NEU^1 operates at the flowrate of 2,199.72 kg·h^{-1} in 6-7 h. Correspondingly, the item in Figure 3b doesn't involve the use of storage tanks S. The source 2, 3 in line 1 and source 3 in line 2 send all their water into the pre-storage V_1 at their operating time. Then the rest water sources are sent into V_2. COMP^1 and NEU^1 both operate at the flowrate of 1,767.59 kg·h^{-1} in 6-7 h. TOX^1 operates at different flowrates in 4-5 h, 6-7 h, 9-10 h, 13-15 h, 15-17 h, 17-19 h and 19-21 h. The corresponding connections between tanks V, U and interceptors are also shown in Figure 3b. Finally, tank U_1 sends 2.229 kg water to sink 1 in line 2. Tank U_2 distributes 459.816 kg water to sink 1 in line 1 and 420.595 kg water to sink 2 in line 2. Although the use of tanks S increases the number of tanks to 5 from 4 and increases their cost slightly, the total freshwater consumption in this work is significantly reduced from 2,886 kg to 1,416 kg in one period, comparing to the situation without storage tanks S shown in Figure 3b. The results of cost comparison for each part are displayed in Table 4.

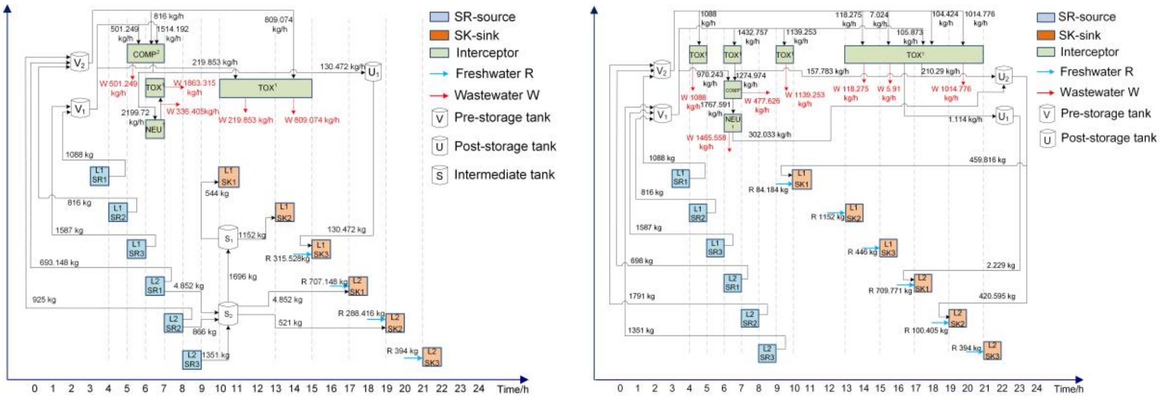

Figure 3: The final structure a) with intermediate storage tanks S, b) without intermediate storage tanks S

Table 4: Comparison of TAC

Item	interceptor cost ($•y^{-1})	storage cost ($•y^{-1})	Fresh water cost ($•y^{-1})	TAC ($•y^{-1})
Without storage tank s	69,762	15,890	96,116	181,768
With storage tank s	68,053	26,335	47,176	141,564

At the same time, the item with intermediate tanks draws the total water flow passing by the interceptors down slightly. It finally reduces the interceptor capacity, which is relevant to the interceptors' investment cost as well. It also avoids the mixing of more water in pre-storage tanks V, which allows interceptors to treat less water to meet the demand of environment or process sinks and using the components interceptor with lower conversion efficiency and interceptor treatment cost. The TAC of the item with intermediate tanks S is 141,564 $·y^{-1}, which is decreased by 21.22 %. The effectiveness of the method is proved.

5. Conclusions

This paper presents an integration approach for the property-based water network design by considering the potential interactions among batch production lines. Intermediate storage tanks are involved to perform the water allocation in-line and inter-line, as well as the reuse from property interceptors. By implementing these measures, a 22.12 % drop in TAC is achieved in the case study by comparing with the situation removing intermediate storage tanks, demonstrating the effectiveness of the method.

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