CHEMICAL ENGINEERING TRANSACTIONS, Volume 12, 2007
Edited by Jiri Klemeš
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Synthesis of Water-Using Networks with Central Reusable Storage in Batch Processes

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With predefined schedule, this paper presents a mathematical formulation for synthesis of water-using networks in batch plants with a central reservoir for targeting freshwater consumption. A superstructure that considers all water reuse/recycle possibilities is presented for modeling the time-dependent water-using network. The proposed superstructure-based representation for synthesis of batch water-using networks is formulated as a nonlinear program (NLP), if used water can be reused and recycled, and a mixed-integer nonlinear program (MINLP), when water recycle is prohibited. Typical representative examples are supplied to demonstrate the good expectation of proposed superstructure-based NLP and MINLP formulations. Supported by the results, the network superstructure and its design scheme can effectively accomplish the goal of unraveling design problem of the water-using network with central reservoir(s) in batch plants.

Keywords: Batch plant, Reuse/recycle, Water-using network, Superstructure, Nonlinear program (NLP), Mixed-integer nonlinear program (MINLP)

1. Introduction

In contrast to the enormous progresses and tremendous practical applications of heat integration techniques in process industry, only limited investigations can be found in the area of water minimization. Furthermore, methods appeared in literature on water minimization usually address continuous processes (Majozi, 2005). However, since batch water-using operations have become ordinary works in the production of specialty chemicals of high commercial values, the study of systematic methodologies for water minimization in batch plants appeals to academics and practicians. One major difficulty of water minimization in batch plants is that streams in batch plants are time-dependent. Even a fixed optimal production schedule is predefined, the opportunities of water reuse and/or recycle are limited due to different operating periods for streams. A graphical technique has been proposed by Wang and Smith (1995a,1995b) to study the use of a central reservoir for water minimization in batch plants. A storage tank can collect used water during surplus periods, and then release accumulated water for latter operations. However, the graphical technique can only be applied to processes characterized by single contaminant (Majozi, 2005). Recently, a mathematical formulation is presented to study the role of central reservoir in bypassing the time dimension for water minimization in batch plants (Majozi, 2005,2006). The processes can be characterized by multiple contaminants, and the optimal scheduling sequences can be considered simultaneously if necessary.

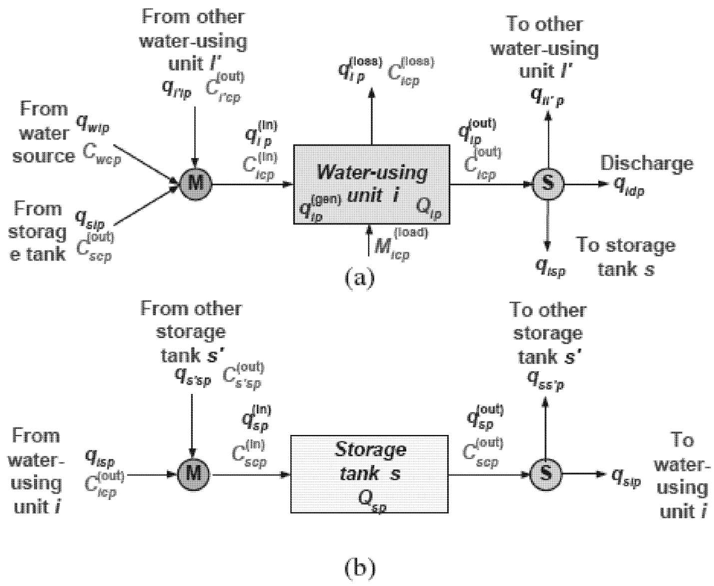

Figure 1: Superstructure of water-using units (a) and storage tanks (b)

Though water reuse/recycle can dramatically reduce the freshwater consumption in industrial processes, and a central reservoir can enhance the possibilities of water reuse/recycle and to resolve the limitation of time-dependent operations in batch plants, the subject of forbidding water recycle for pollution prevention is not systematically examined in fact. This article aims at proposing a mathematical formulation to handle the case that allows water reuse by other operations but forbids used water to return the same unit that generates the waste water.

2. Problem Statement

The batch water-using network synthesis problem addressed in this paper can be stated as follows: Givens are a set of water-using units in which some transferable components with known mass loads are to be removed away; a set of water supplies with specific concentrations，where some of them supply freshwater；a set of reservoirs for temporary storage of used water for later reuse. Also specified are the start and ending times of each water-using operation. Givens also are the maximum permissible input and output concentrations for each operation．The objective then is to determine the time-dependent operational strategy of the water-using network which targets the freshwater expenditure.

3. Superstructure for Batch Water-Using Network Synthesis

A periodically partitioned method is proposed to overcome the different starting and ending times of various operating processes in a batch water-using network. For any operating period, Fig. 1 illustrates typical superstructures for water processing units and reservoirs. Therein the water processing unit and reservoir consider all possible water sources and all water reuse possibilities. All possible sinks are also taken into account.

4. Superstructure Modeling and Problem Formulation

In order to model the generic superstructures for synthesis of a batch water processing network, some relevant notations are shown in Fig. 1. The main objective in this work is to minimize the consumption of freshwater. The design problem can be formulated as a nonlinear program (NLP) when there is no restraint for water reuse/recycle, as stated in **P1**.

$$\textbf{P1:}\quad \min_{\boldsymbol{x}_1 \in \boldsymbol{\Omega}_1} J_1 = \sum_{\forall w \in \mathcal{F}} \sum_{\forall i \in \mathcal{I}} \sum_{\forall p \in \mathcal{P}^+} q_{wip} \tag{1}$$

Where design variables and feasible searching space comprising all restraints are given below,

$$\boldsymbol{x}_1 \equiv \left\{ \begin{array}{c} q_{wip}, q_{sip}, q_{ii'p}; q_{ip}^{(\text{in})}, q_{ip}^{(\text{out})}; q_{sp}^{(\text{in})}, q_{sp}^{(\text{out})}; \\ Q_{ip}, Q_{sp};\ C_{icp}^{(\text{in})}, C_{icp}^{(\text{out})}; C_{scp}^{(\text{in})}, C_{scp}^{(\text{out})}; \\ \forall w \in \mathcal{W},\ i, i' \in \mathcal{I},\ s \in \mathcal{S},\ c \in \mathcal{C},\ p \in \mathcal{P}^+ \end{array} \right\} \tag{2}$$

$$\boldsymbol{\Omega}_1 = \left\{ \boldsymbol{x} \left| \begin{array}{r} \left. \begin{array}{r} q_{ip}^{(\text{in})} = \sum_{\forall i' \in \mathcal{I}} q_{i'ip} + \sum_{\forall w \in \mathcal{W}} q_{wip} + \sum_{\forall s \in \mathcal{S}} q_{sip} \\ q_{ip}^{(\text{out})} = \sum_{\forall i' \in \mathcal{I}} q_{ii'p} + \sum_{\forall d \in \mathcal{D}} q_{idp} + \sum_{\forall s \in \mathcal{S}} q_{isp} \\ Q_i^{\min} y_{ip}^{(\text{in})} \le q_{ip}^{(\text{in})} \le Q_i^{\max} y_{ip}^{(\text{in})} \\ Q_i^{\min} y_{ip}^{(\text{out})} \le q_{ip}^{(\text{out})} \le Q_i^{\max} y_{ip}^{(\text{out})} \\ q_{ip'}^{(\text{out})} = y_{ip}^{(\text{out})} Q_{i,p'-1} \\ Q_{ip'} = Q_{i,p'-1} + q_{ip'}^{(\text{in})} - q_{ip'}^{(\text{out})} \\ Q_{i1} = q_{i1}^{(\text{in})} - q_{i1}^{(\text{out})} \end{array} \right\} \begin{array}{l} \text{water} \\ \text{balance} \\ \text{for each} \\ \text{operation} \end{array} \\ \left. \begin{array}{r} q_{ip}^{(\text{in})} C_{icp}^{(\text{in})} = \sum_{\forall i' \in \mathcal{I}} q_{i'ip} C_{i'cp}^{(\text{out})} + \sum_{\forall w \in \mathcal{W}} q_{wip} C_{wc} \\ + \sum_{\forall s \in \mathcal{S}} q_{sip} C_{scp}^{(\text{out})} \\ Q_{ip'} C_{icp'}^{(\text{out})} = q_{ip'}^{(\text{in})} C_{icp'}^{(\text{in})} - q_{ip'}^{(\text{out})} C_{ic,p'-1}^{(\text{out})} + M_{ic}^{(\text{load})} y_{ip'}^{(\text{in})} \\ + Q_{i,p'-1} C_{ic,p'-1}^{(\text{out})} \\ Q_{i1} C_{ic1}^{(\text{out})} = q_{i1}^{(\text{in})} C_{ic1}^{(\text{in})} + M_{ic}^{(\text{load})} y_{i1}^{(\text{in})} \\ C_{icp}^{(\text{in})} \le C_{ic,\max}^{(\text{in})} \qquad C_{icp}^{(\text{out})} \le C_{ic,\max}^{(\text{out})} \end{array} \right\} \begin{array}{l} \text{contaminant} \\ \text{balance} \\ \text{for each} \\ \text{operation} \end{array} \\ \left. \begin{array}{r} q_{sp}^{(\text{in})} = \sum_{\forall i \in \mathcal{I}} q_{isp} + \sum_{\forall s' \in \mathcal{S}} q_{s'sp} \\ q_{sp}^{(\text{out})} = \sum_{\forall i \in \mathcal{I}} q_{sip} + \sum_{\forall s' \in \mathcal{S}} q_{ss'p} \\ Q_{sp'} = Q_{s,p'-1} + q_{sp'}^{(\text{in})} - q_{sp'}^{(\text{out})} \\ Q_{s1} = Q_{s,P+1} Z^{(\text{cyc})} + q_{s1}^{(\text{in})} - q_{s1}^{(\text{out})} \\ Q_{sp} \le Q_s^{\max} \end{array} \right\} \begin{array}{l} \text{water} \\ \text{balance} \\ \text{for each} \\ \text{reservoir} \end{array} \\ \left. \begin{array}{r} q_{sp}^{(\text{in})} C_{scp}^{(\text{in})} = \sum_{\forall i \in \mathcal{I}} q_{isp} C_{icp}^{(\text{out})} + \sum_{\forall s' \in \mathcal{S}} q_{s'sp} C_{s'cp}^{(\text{out})} \\ Q_{sp'} C_{scp'}^{(\text{out})} = Q_{sc,p'-1} C_{sc,p'-1}^{(\text{out})} + q_{sp'}^{(\text{in})} C_{scp'}^{(\text{in})} - q_{sp'}^{(\text{out})} C_{scp'}^{(\text{out})} \\ Q_{s1} C_{sc1}^{(\text{out})} = Q_{sc,P+1} C_{sc,P+1}^{(\text{out})} Z^{(\text{cyc})} + q_{s1}^{(\text{in})} C_{sc1}^{(\text{in})} - q_{s1}^{(\text{out})} C_{sc1}^{(\text{out})} \end{array} \right\} \begin{array}{l} \text{contaminant} \\ \text{balance} \\ \text{for each} \\ \text{reservoir} \end{array} \\ \forall i, i' \in \mathcal{I}, s \in \mathcal{S}, p \in \mathcal{P}^+, p' \in \mathcal{P}^-, c \in \mathcal{C} \end{array} \right. \right\} \tag{3}$$

When water reuse is encouraged but water recycle is not allowed for anti-pollution reason, some additional binary variables and constraints should be appended in previous design variables and searching space, and the network synthesis can be formulated as a mixed-integer nonlinear program (MINLP).

$$\textbf{P2:} \quad \min_{\boldsymbol{x}_2 \in \boldsymbol{\Omega}_2} J_1 = \sum_{\forall w \in \mathcal{F}} \sum_{\forall i \in \mathcal{I}} \sum_{\forall p \in \mathcal{P}^+} q_{wip} \tag{4}$$

Where new design variables and constraint space are,

$$\boldsymbol{x}_2 \equiv \boldsymbol{x}_1 \cup \left\{ \begin{array}{c} Z_{i'i}, Z_{wi}, Z_{si}; Z_{is}, Z_{id}; ZR_i, ZS_i; \\ \forall w \in \mathcal{W},\ i, i' \in \mathcal{I},\ s \in \mathcal{S},\ d \in \mathcal{D} \end{array} \right\} \tag{5}$$

$$\boldsymbol{\Omega}_2 = \boldsymbol{\Omega}_1 \cap \{Eq.(7)\} \tag{6}$$

and

$$\left.\begin{array}{lcll} ZR_i & \leq & \sum_{\forall i' \in \mathcal{I}} ZR_{i'} Z_{i'i} + \sum_{\forall s \in \mathcal{S}} Z_{si} & \\ ZR_i & \geq & Z_{si} & \forall s \in \mathcal{S} \\ ZR_i & \geq & ZR_{i'} Z_{i'i} & \forall i' \in \mathcal{I} \\ ZS_i & \leq & \sum_{\forall i' \in \mathcal{I}} ZS_{i'} Z_{ii'} + \sum_{\forall s \in \mathcal{S}} Z_{is} & \\ ZS_i & \geq & Z_{is} & \forall s \in \mathcal{S} \\ ZS_i & \geq & ZS_{i'} Z_{ii'} & \forall i' \in \mathcal{I} \\ ZR_i & + & ZS_i \ \leq\ 1 & \end{array}\right\} \forall i \in \mathcal{I} \tag{7}$$

Here, $Z_* = 1$, denotes the existence of the corresponding connection; ZR_i with unity value indicates that operation *i* receives, in direct or circuitous ways, used water from storage tank; Similarly, ZS_i with unity value signifies that operation *i* supplies in direct or circuitous ways, used water to reservoir. The second and third terms in Eq.(7) show the direct and indirect receiving, respectively, from storage tanks. The first term guarantees zero value for ZR_i if unit *i* does not receive used water in direct or indirect ways. The fourth to sixth terms state the conditions of supplying used water to storage tanks by unit *i*. The last term describes that one operation cannot simultaneously receive used water from storage tanks and supply water to reservoirs.

It is noted that **P1** and **P2** may result in multiple solutions. One more reasonable solution can be found by seeking a design with minimized storage tanks. This design can be formulated as the following NLP for reuse/recycle case.

$$\textbf{P3:} \quad \min_{\boldsymbol{x}_1 \in \boldsymbol{\Omega}_3} J_2 = \sum_{\forall s \in \mathcal{S}} Q_s \tag{8}$$

where some additional restraints, such as restriction on maximal permissible freshwater consumption and tank sizes Q_s, are appended in $\boldsymbol{\Omega}_3$, where ε is very small positive value, say 0.001.

$$\boldsymbol{\Omega}_3 = \boldsymbol{\Omega}_1 \cap \left\{ \sum_{\forall w \in \mathcal{F}} \sum_{\forall i \in \mathcal{I}} \sum_{\forall p \in \mathcal{P}^+} q_{wip} \leq J_1^*(1+\epsilon); Q_{sp} \leq Q_s, \forall s \in \mathcal{S}, p \in \mathcal{P}^+ \right\} \tag{9}$$

For recycle forbidden case, the problem can be formulated as a MINLP,

$$\textbf{P4:} \quad \min_{\boldsymbol{x}_2 \in \boldsymbol{\Omega}_4} J_2 = \sum_{\forall s \in \mathcal{S}} Q_s \tag{10}$$

$$\boldsymbol{\Omega}_4 = \boldsymbol{\Omega}_2 \cap \left\{ \sum_{\forall w \in \mathcal{F}} \sum_{\forall i \in \mathcal{I}} \sum_{\forall p \in \mathcal{P}^+} q_{wip} \leq J_1^*(1+\epsilon); Q_{sp} \leq Q_s, \forall s \in \mathcal{S}, p \in \mathcal{P}^+ \right\} \tag{11}$$

5. Illustrative example

In the investigated example, one cycle of this process involves two single-stage batch processes with three and six repeated operations with elapsed time of two hours

Table 1: Data for illustrative example

Unit	Function	$Q_i^{\max}$ (ton)	$C_{ic,\max}^{(\mathrm{in})}$ (kg/ton)	$C_{ic,\max}^{(\mathrm{out})}$ (kg/ton)	$M_{ic}^{(\mathrm{load})}$ (kg)	Elapsed time (h)	Repeated operations
1	Extraction	200	0.05	0.1	5	2	3
2	Extraction	200	0.1	0.4	10	1	6

and one hour, respectively. Both are liquid-liquid extraction processes using freshwater for removal of a salt byproduct (contaminant) from the organic phase. The basic data are given in Table 1. For solving the NLP and MINLP formulations, the General Algebraic Modeling System (GAMS, Brooke et al., 2003) is used as the main solution tool. The NLP and MINLP solvers are SNOPT and BARON, respectively. With predefined scheduling where processes 1 and 2 are operated in parallel, the water-using network for single-batch operation mode is shown in Fig.2(a), where all three operations of process 1 and four out of six operations of process 2 are fed with freshwater, and the third and the fifth operations of process 2 reuse the outlet water from the first and the second operations of process 1. The targeting freshwater is 250 kg within 6 hours period. It is obvious that a lot of qualified used water from process 1 are discarded as wastewater. These used water can be collected in a reservoir and reused for latter process 2, as shown in Fig. 2(b). Here, 16.67 kg outlet water from process 1 is stored for one hour in the tank and then reused by process 2 with additional 12.5 kg freshwater for dilution. By adopting one reservoir that can handle 16.67 kg used water, the freshwater depletion rate can be reduced to 225 kg. However, 50 kg qualified used water from the last operation of process 1 is still discarded in such case. This 50 kg water can be stored in tank for later reuse by the first and the second operations of process 2 in the next cycle if we adopt cyclic operation mode, as shown in Fig. 2(c). In such a case, the targeting freshwater is further reduced to 187.5 kg, but a larger tank size that can reserve 50 kg water is needed.

6. Conclusions

The time dependency of water-using operations in batch plant can be partially bypassed by implementing a central reservoir to collect surplus water from prior operations and to release used water into latter processes. With predefined schedule, this paper presents a mathematical formulation for synthesis of water-using networks in batch plants with central storage tank(s) for targeting freshwater consumption. A superstructure that considers all water reuse/recycle possibilities is presented for modeling the time-dependent water-using network. The proposed superstructure-based representation for batch water-using networks is formulated as a nonlinear program (NLP), if usedwater can be reused and recycled, and a mixed-integer nonlinear program (MINLP), when water recycle is forbidden to control possible pollution. One literature example is supplied to demonstrate the good expectation of proposed superstructure-based NLP and MINLP formulations.

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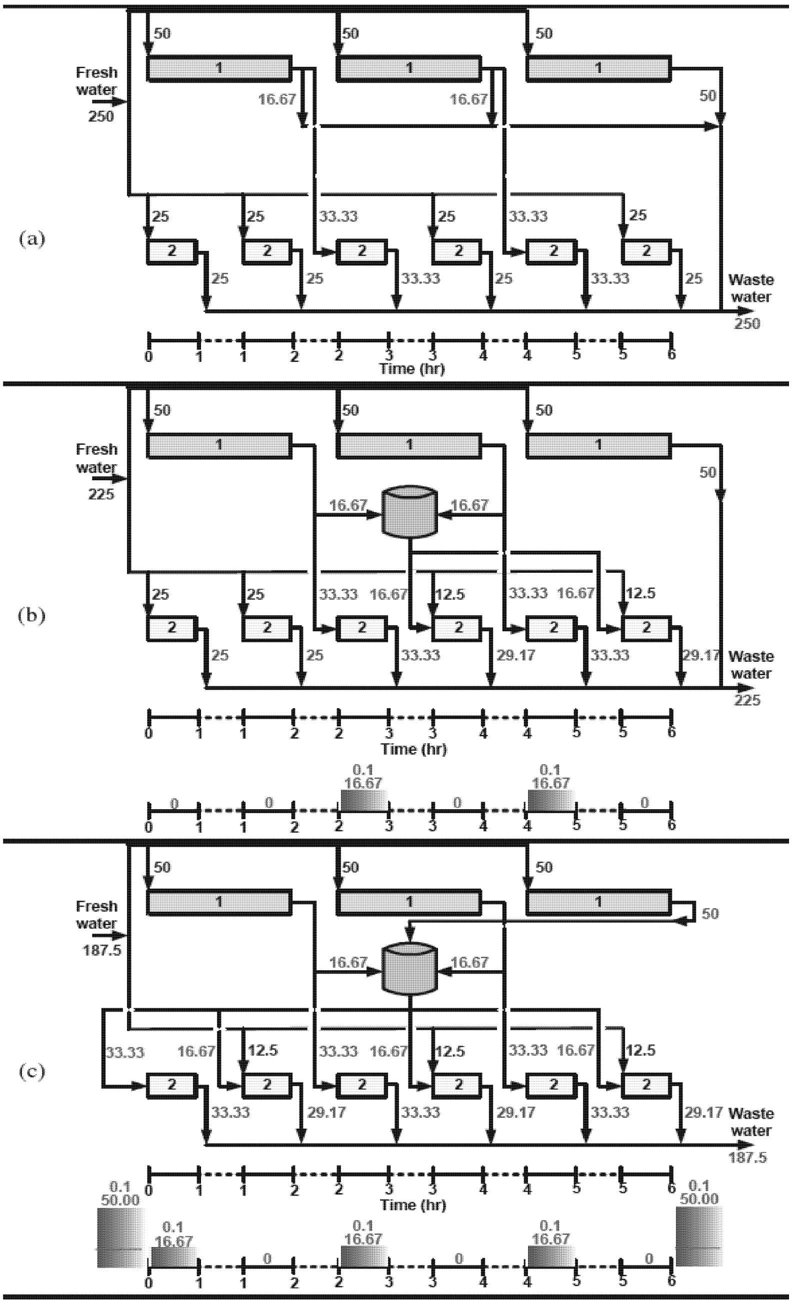

Figure 2: Water-using networks for illustrative example: single operation without (a) and with (b) reusable storage, and (c) for cyclic operation with storage