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Synthesis of Property-Based Water-Using Networks in Batch Process Industries

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This paper aims to develop a mathematical formulation for the synthesis of property-based batch water networks. Different from most of the previous works on composition-based water networks, the design problem in the present study is extended to consider a number of non-conserved properties of the process streams. The objective of this work is to obtain an optimum operating strategy with the minimum total annual cost (TAC) for a property-based batch water network. The design problem is formulated as a mixed-integer nonlinear program (MINLP), and a case study is presented to demonstrate the validity of the proposed formulation.

Introduction

The growing public awareness towards environmental and economic aspects associated with waste treatment and discharge has encouraged process industries to find alternative and competitive ways to achieve the effective usage of resources and reduce the waste generation. For such purpose, water reuse is regarded as an important strategy for simultaneously reducing freshwater consumption and wastewater production. In consequence, the research area of water network synthesis has received considerable attention over the past decade and numerous research contributions have been made for both continuous and batch processes (Wang and Smith, 1994, 1995; Gunaratnam et al, 2005; Foo et al. 2005; Chen and Lee, 2008; Kim and Smith, 2004; Li and Chang, 2006).
However, the research efforts as mentioned above have been limited to "chemo-centric" or "composition-based" process systems in which the characterization of water sources and the constraints on water demands are described by the composition of pollutants. In practice, besides pollutant composition, other stream properties are also important, e.g. pH, conductivity, turbidity, etc. In order to cope with the problems governed by properties, the framework of property integration was recently proposed for continuous (Shel-

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ley and El-Halwagi, 2000; El-Halwagi et al., 2004; Kazantzi and El-Halwagi, 2005) and batch processes (Ng et al., 2008).

The aim of this paper is to extend the seminal work of Ng et al. (2008) in developing a general mathematical formulation for the synthesis of property-based batch water networks, with the inclusion of effluent treatment. All relevant parts within the process system, including water sources, water demands, storage tanks and interception units, are well formulated on the basis of their corresponding superstructure representations. The objective of design is to search for an optimal operating strategy with the minimum (TAC). A case study is used to demonstrate the adequacy of the proposed formulation.

Problem Statement

The problem to be addressed can be stated as follows. Consider a cyclic batch process with a set of water source, each has a given flow rate and is characterized by a set of properties with given property values; a set of water demands, each requires a feed with given flow rate and acceptable property values. Available for service are a set of freshwaters with known qualities, and purchased at different costs. A set of storage tanks are needed for providing temporary storage of reusable water to enhance water reuse potential. A set of interception units are added to the process system to adjust the stream properties for further reuse and/or for effluent treatment for environmental discharge. A mixing rule is important to define all possible mixing patterns among the individual properties when different water streams are mixed, given in Equation (1):

$$\overline{F} \times \psi\left(\overline{p}\right) = \sum_{n} F_n \times \psi\left(p_n\right) \tag{1}$$

where (p_n) and $\psi\left(\overline{p}\right)$ are property operators on property p_n and mixture property $\overline{p}$, respectively, and $\overline{F}$ is the total mixture flow rate. The objective is to determine the optimal operating strategy which achieves the minimum TAC for the network.

Problem Formulation

The mathematical model to be presented mainly comprises the material balances around water sources, water demands, storage tanks and interception units. Furthermore, some operational constraints are also imposed to make sure the design specifications. Based on the superstructures in Figure 1, Equations (2) and (3) define the flow rate balances at the mixing of water demands; and at the splitting of water sources, respectively.

$$F_j Y_{jt}^{\text{in}} = \sum_{i \in I} f_{ijt} + \sum_{s \in S} f_{sjt} + \sum_{k \in K} f_{kjt} + \sum_{r \in R} f_{rjt} \quad \forall j \in J \;\; , t \in T \tag{2}$$

$$F_i Y_{it}^{\text{out}} = \sum_{j \in J} f_{ijt} + \sum_{s \in S} f_{ist} + \sum_{k \in K} f_{ikt} + \sum_{e \in E} f_{iet} \quad \forall i \in I \;\; , t \in T \tag{3}$$

Equation (4) is the property operator balance at the mixing of water demands. Equation (5) specifies the constraints on acceptable property values to all the water demands.

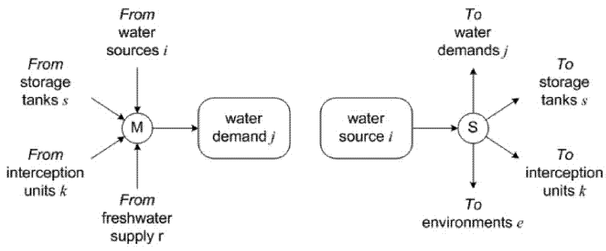


Figure 1 Superstructures for a water demand and water source

$$F_j Y_{jt}^{\text{in}} \psi_{jpt}^{\text{in}} = \sum_{i \in I} f_{ijt} \Psi_{ip} + \sum_{s \in S} f_{sjt} \psi_{spt}^{\text{out}} + \sum_{k \in K} f_{kjt} \psi_{kpt}^{\text{out}} + \sum_{r \in R} f_{rjt} \Psi_{rp} \quad \forall j \in J \ , p \in P \ , t \in T \quad (4)$$

$$\Psi_{jp}^{\text{in,min}} \le \psi_{jpt}^{\text{in}} \le \Psi_{jp}^{\text{in,max}} \quad \forall j \in J \ , p \in P \ , t \in T \quad (5)$$

Based on the superstructure for storage tank in Figure 2(a), Equations (6) and (7) are the flow rate balances at the mixing point of the storage tanks and at the splitting point of the storage tanks, respectively. Equation (8) is an overall flow balance for all storage tanks to calculate the amount of cumulative mass in the storage tank. Note that Equation (9) is used to forbid the input and output streams of a storage tank occurring in the same time intervals, so as to make sure the well-mixing of the mixture in the storage tank with all the properties achieving the constant values before being dispatched. Equations (10) and (11) make sure that the amounts of input flow and cumulative mass for each storage tank do not exceed the capacity of the storage tank at any time.

$$f_{st}^{\text{in}} = \sum_{i \in I} f_{ist} + \sum_{s' \in S} f_{s'st} + \sum_{k \in K} f_{kst} \quad \forall s \in S \ , t \in T \quad (6)$$

$$f_{st}^{\text{out}} = \sum_{j \in J} f_{sjt} + \sum_{s' \in S} f_{ss't} + \sum_{k \in K} f_{skt} + \sum_{e \in E} f_{set} \quad \forall s \in S \ , t \in T \quad (7)$$

$$q_{st} = q_{s,T} \big|_{t=1} + q_{s,t-1} \big|_{t>1} + \left(f_{st}^{\text{in}} - f_{st}^{\text{out}} \right) \Delta_t \quad \forall s \in S \ , t \in T \quad (8)$$

$$f_{st}^{\text{in}} \times f_{st}^{\text{out}} = 0 \quad \forall s \in S \ , t \in T \quad (9)$$

$$f_{st}^{\text{in}} \Delta_t \le q_s^{\max} \quad \forall s \in S \ , t \in T \quad (10)$$

$$q_{st} \le q_s^{\max} \quad \forall s \in S \ , t \in T \quad (11)$$

Equations (12) and (13) are the property operator balances at the mixing of storage tanks; and for calculating the cumulative property loads within the tanks, respectively.

$$f_{st}^{\text{in}} \psi_{spt}^{\text{in}} = \sum_{i \in I} f_{ist} \Psi_{ip} + \sum_{s' \in S} f_{s'st} \psi_{s'pt}^{\text{out}} + \sum_{k \in K} f_{kst} \psi_{kpt}^{\text{out}} \quad \forall p \in P \ , s \in S \ , t \in T \quad (12)$$

$$q_{st} \psi_{spt}^{\text{out}} = q_{s,T} \psi_{sp,T}^{\text{out}} \big|_{t=1} + q_{s,t-1} \psi_{sp,t-1}^{\text{out}} \big|_{t>1} + \left(f_{st}^{\text{in}} \psi_{spt}^{\text{in}} - f_{st}^{\text{out}} \psi_{spt}^{\text{out}} \right) \Delta_t \quad \forall p \in P \ , s \in S \ , t \in T \quad (13)$$

Based on the superstructure in Figure 2(b), Equations (14) and (15) are the flow rate balances at the mixing point into all the interception units and at the splitting of interception units, respectively. Equation (16) is used to make sure the throughput of each interception unit will not exceed its capacity. Equation (17) shows that the output flow rate of an interception unit is a function of the input flow rate.

$$f_{kt}^{\text{in}} = \sum_{i \in I} f_{ikt} + \sum_{s \in S} f_{skt} + \sum_{k' \in K} f_{k'kt} \quad \forall k \in K, t \in T \tag{14}$$

$$f_{kt}^{\text{out}} = \sum_{j \in J} f_{kjt} + \sum_{s \in S} f_{kst} + \sum_{k' \in K} f_{kk't} + \sum_{e \in E} f_{ket} \quad \forall k \in K, t \in T \tag{15}$$

$$f_{kt}^{\text{in}} \leq f_{k}^{\max} \quad \forall k \in K, t \in T \tag{16}$$

$$f_{kt}^{\text{out}} = \mathrm{G}_k\left(f_{kt}^{\text{in}}\right) \quad \forall k \in K, t \in T \tag{17}$$

Equation (18) is the property operator balance at the mixing point into all the interception units. Equation (19) specifies the property constraints as the input confinements for all interception units. Equation (20) shows that the output property values of an interception unit are dependent on the input condition and performance of the interception unit.

$$f_{kt}^{\text{in}} \psi_{kpt}^{\text{in}} = \sum_{i \in I} f_{ikt} \Psi_{ip} + \sum_{s \in S} f_{skt} \psi_{spt}^{\text{out}} + \sum_{k' \in K} f_{k'kt} \psi_{k'pt}^{\text{out}} \quad \forall k \in K, p \in P, t \in T \tag{18}$$

$$\Psi_{kp}^{\text{in,min}} \leq \psi_{kpt}^{\text{in}} \leq \Psi_{kp}^{\text{in,max}} \quad \forall k \in K, p \in P, t \in T \tag{19}$$

$$\psi_{kpt}^{\text{out}} = \mathrm{H}_k\left(f_{kt}^{\text{in}}, \psi_{kpt}^{\text{in}}\right) \quad \forall k \in K, p \in P, t \in T \tag{20}$$

Equations (21) and (22) are the flow rate and property balances for effluent discharged to all the environments around the process system. Equation (23) specifies the property constraints as the environmental discharge limits to all the environments.

$$f_{et} = \sum_{i \in I} f_{ijt} + \sum_{s \in S} f_{sjt} + \sum_{k \in K} f_{kjt} \quad \forall e \in E, t \in T \tag{21}$$

$$f_{et} \psi_{ept} = \sum_{i \in I} f_{ijt} \Psi_{ip} + \sum_{s \in S} f_{sjt} \psi_{spt}^{\text{out}} + \sum_{k \in K} f_{kjt} \psi_{kpt}^{\text{out}} \quad \forall e \in E, p \in P, t \in T \tag{22}$$

$$\Psi_{ep}^{\text{env,min}} \leq \psi_{ept} \leq \Psi_{ep}^{\text{env,max}} \quad \forall e \in E, p \in P, t \in T \tag{23}$$

The objective function subject to all the constraints mentioned above is to minimize the total annual cost (TAC):

$$\begin{aligned} \min TAC = & \sum_{r \in R} \sum_{j \in J} \sum_{t \in T} C_r f_{rjt} \Delta_t + A \sum_{s \in S} \left[C_s^{\text{fix}} x_s + C_s^{\text{var}} \left(q_s^{\max}\right)^{\alpha_s} \right] + A \sum_{k \in K} C_k^{\text{inv}} \left(f_k^{\max}\right)^{\beta_k} \\ & + N \sum_{k \in K} \sum_{t \in T} C_k^{\text{op}} f_{kt}^{\text{in}} \Delta_t + A \sum_{* \in \Theta} \left[C_*^{\text{fix}} x_* + C_*^{\text{var}} \left(f_*^{\max}\right)^{\gamma_*} \right] \\ & \Theta = \left\{ ie, ij, ik, is, ke, kj, kk', ks, rj, se, sj, sk, ss' \right\} \end{aligned} \tag{24}$$

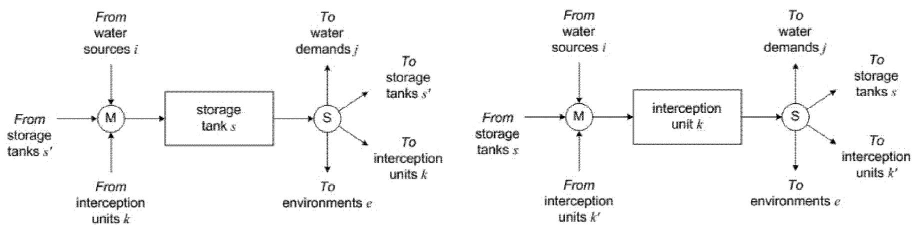
Equations (25) and (26) are used to correlate the binary variables with the continuous variables. Equation (27) can be added to eliminate uneconomically small flow rates.

$$Q_s^{\text{L}} x_s \leq q_s^{\max} \leq Q_s^{\text{U}} x_s \quad \forall s \in S \tag{25}$$

$$f_{*t} \leq f_*^{\max} \leq F_*^{\text{U}} x_* \quad \forall t \in T \tag{26}$$

$$f_{*t}\left(f_{*t} - F_*^{\text{L}}\right) \geq 0 \quad \forall t \in T, * \in \Theta \tag{27}$$

The model of the above design problem is an MINLP problem because of the bilinear terms in the property operator balances and the binary variables to identify the existence of the storage tanks and pipe lines.



(a) (b)

Figure 2 Superstructures for (a) storage tank and (b) interception unit

Case Study

A cyclically-operated batch process with an 8 hours cycle time is analyzed. This process involves two water demands (D1 and D2), two water sources (S1 and S2) and two main properties, i.e. pH and the total suspended solids (TSS). The limiting data are given in Table 1. To adjust the pH values of the sources, an acid (pH=3) and a base (pH=11) are used. Besides, to remove the TSS content, a filtration unit with an outlet of 50 ppm is used. The cost information of the case study is given in Table 2. The mixing rules of pH and TSS are given in Equations (28) and (29), respectively.

$$\bar{F} \times 10^{-p\bar{H}} = \sum_{n} F_n \times 10^{-pH_n} \Big|_{pH \le 7} - \sum_{n'} F_{n'} \times 10^{(14 - pH_{n'})} \Big|_{pH > 7} \quad (28)$$

$$\bar{F} \times \overline{TSS} = \sum_{n} F_n \times TSS_n \quad (29)$$

The unit costs for freshwater, acid and alkali are summed to \$1/ton, \$10/ton and \$6/ton. Besides, it is also assumed that 1,050 batches are operated annually with an annualization factor of 0.1. The environmental limits for pH (6.5-7.5) and TSS (<100 ppm) are used. The MINLP is solved by the General Algebraic Modeling System (GAMS) in a Core 2, 2.0 GHz processor with BARON as the solver. The model entails 645 constraints, 370 continuous variables and 32 binary variables. The optimization model results in a minimum TAC of \$143,553/yr, with the resultant network in Figure 4.

Table 1 Processing data for the case study

	Flow rate (ton/h)	pH	TSS (ppm)	Start-end times (h)
D1	25	6-7	0-200	2-6
D2	40	7-8	0-50	5-8
S1	20	5	200	0-5
S2	30	9	300	3-7
Freshwater	To be optimized	7	0	-

Table 2 Capital cost information of the case study

Storage cost	Fixed charge = $10000x_s$, variable charge = $20q_s^{max}$
Piping cost	fixed charge= $120x_*$, variable charge= $3600f_*^{max}$
Interception cost	Capital cost = $15000f_k^{max}$, operating cost= $_{t\in T}\ 0.05f_{kt}^{in}\ t$

Conclusion

A mathematical formulation has been developed for the synthesis of property-based batch water networks, on the basis of the proposed superstructures. A case study was solved to demonstrate the application of the proposed model.

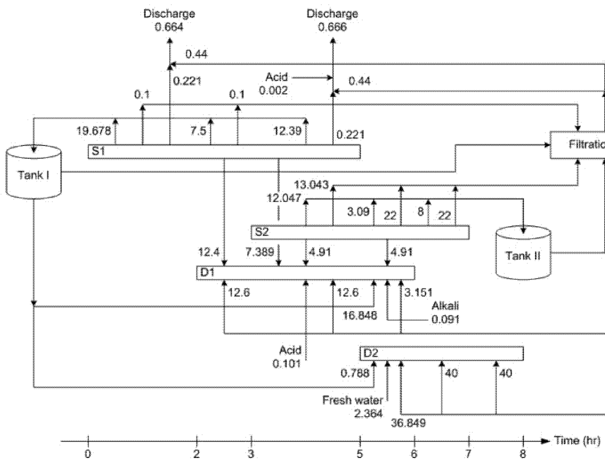


Figure 4 Resultant network for the case study

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