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Simultaneous Synthesis of Property-Based Water Reuse/Recycle and Interceptions Networks for Batch Processes

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As industry endeavors to prevent pollution and conserve resources, there is an increasing emphasis given to the optimal management of water usage and wastewater discharge. In this context, recycle/reuse strategies play an instrumental role. Water may be directly reused/recycled or purified then recycled to reduce both fresh water and wastewater. The objective of this paper is to introduce a systematic technique for the synthesis of cost-effective batch water networks. Using the new concept of property integration, a property-based approach is adopted. The water streams (sources) are characterized by a number of key properties. Additionally, constraints on the feed to water-using units (sinks) are given in terms of bounds on properties. The procedure will also consider a number of interception devices that can be used to modify the properties of the streams. A source-interception-sink representation is developed. Storage tanks are used throughout the network to enable mixing and scheduling. The procedure is supported by an optimization formulation whose solution identifies optimal allocation of sources to tanks, interception devices, and sinks. The solution also determines an optimal policy for scheduling and operating the water network. A case study is solved to illustrate the important aspects of the devised procedure.

1. Introduction

The area of synthesizing water recycle/reuse networks has received considerable research interest. Examples of such research efforts can be found in literature (e.g., Wang and Smith, 1994; Almató, 1997, 1999; Savelski and Bagajewicz, 2000; Hallale, 2002; El-Halwagi et al., 2003; Manan et al., 2004; Foo et al., 2005; Majozi, 2005; El-Halwagi, 2006). Most of the recycle/reuse work used composition-based characterization of the streams and constraints for the sinks. However, in addition to composition of pollutants, there are many applications that require the consideration of properties. For instance, the use and discharge of water streams may be dependent on various characteristics such as pH, conductivity, turbidity, toxicity, theoretical oxygen demand, and color. In order to address design problems that are governed by functionalities and properties, the framework of property integration has been recently introduced, which may be defined as “a functionality-based, holistic approach to the allocation and manipulation of streams and processing units, which is based on the tracking, adjustment, assignment, and matching of functionalities throughout the process" (El-Halwagi et al., 2004). Shelley and El-Halwagi (2000) developed the concept of property-based clusters to enable the conserved tracking of properties. Subsequently, graphical, algebraic, and optimization techniques have been developed for property-based recycle/reuse (Kazantzi and El-Halwagi, 2005; Foo et al., 2006; Qin et al., 2004). It is worth noting that these research efforts have been limited to steady-state problems. With numerous batch processes using and discharging water, it is necessary to develop systematic techniques for the synthesis of batch water networks with property-based constraints. This is the objective of this paper. A structural representation of the problem is introduced to embed potential configurations of interest. An optimization formulation is developed and its solution provides optimal allocation of sources, storage, interception, network configuration, and scheduling.

1.1 Problem Statement

The problem definition of a property-based batch water network are stated as follows: Given is a batch process with a cycle time (τ). It is characterized by the following:

- A set of water sources: SOURCES = $\{i \mid i = 1,2, \ldots, N_{\text{sources}}\}$ composed of process water streams that may be recycled or discharged. Each source has a flowrate, f_i (t) and is characterized by a set of properties: PROPERTIES = $\{p \mid p = 1,2, \ldots, N_{\text{p}}\}$. The properties of the sources are designated by $p_{i,p}$ (t), and t is the time from the beginning of the cycle ($0 \le t \le \tau$).
- A set of process sinks (units): SINKS = $\{j \mid j = 1,2, \ldots, N_{\text{sinks}}\}$. Sinks are process units that can accept the sources. Each sink requires a flowrate, g_j (t) and property values, $p_{j,p}(t)$, that satisfy the following constraints:

  $$p_{j,p}^{\min} \le p_{j,p} \le p_{j,p}^{\max} \qquad j \in \text{SINKS}, p \in \text{PROPERTIES} \tag{1}$$

  where $p_{j,p}^{\min}$ and $p_{j,p}^{\max}$ are lower and upper bounds on acceptable properties to unit j.
- A set of interception units: INTERCEPTORS = $\{k \mid k = 1,2, \ldots, N_{\text{Int}}\}$. Interception devices are units that may be added to the process to change the source properties. The interceptors are operated dynamically with the following performance:

  $$p_{k,p}^{\text{int}} = f\left(p_{i,p}^{\text{in}}, z_k, r_k, t\right) \tag{2}$$

  where $p_{k,p}^{\text{int}}$ (t) is the value of the intercepted property leaving interceptor k, z_k and r_k are design and operating variables of interceptor k, and t is time of operation.

A general mixing rule is needed to define all possible mixing patterns among these individual properties. One such form for mixing is the following equations (e.g. Shelley and El-Halwagi, 2000):

$$\psi(\bar{p}) = \sum_i x_i \psi(p_i) \tag{3}$$

where $\psi(p_i)$ and $\psi(\bar{p}_i)$ are operators on property p_i and mixture property $\bar{p}_i$ respectively; x_i is the fractional contribution of source i of the total mixture flowrate, i.e.

$$x_i = \frac{f_i}{\sum_i f_i} \tag{4}$$

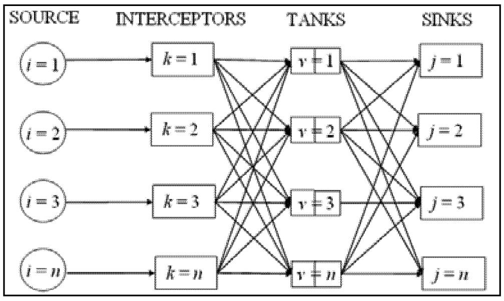

Figure 1 Source -interception-tank-sink representation

The problem can be schematically represented by a source-interception-tank-sink allocation, as shown in Figure 1. According to this representation, each source i, is fed to an interception unit k. The intercepted sources are then sent to *tank* v where they are stored and finally dispatch to the appropriate sink j.

1.2 Approach

The following approach will be used to synthesize an optimal batch water network of minimum total annualized cost:

1. Each source is assigned to an interception unit.
2. For a given size and model of an interception unit, the outlet intercepted source property $p_{i,p}^{\text{int}}$ (t) will vary with time according to the following model.
3. Reformulation of intercepted sources and sinks into discrete events.
4. Determine the minimum total annualized cost of the network.
5. Synthesize a direct-recycle water network that's meets the min TAC using storage and dispatch tanks.
6. Schedule an optimum operating scheme.

The main objective of this work is to synthesize and schedule an optimal batch network which meets the minimum total annualized cost and meets all process constraints. Hence the objective function can be expressed as:

$$\text{Minimize total cost} = \sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{sink}} C_r f_{r,j} + \sum_{k=1}^{N_{Int}} C_k I_k + 2\sum_{l=1}^{N_{Tanks}} C_v I_v \tag{5}$$

where C_r is the cost coefficient of the fresh resources, $f_{r,j}$ is the fresh resources that feds into the j^{th} sink (mass per batch cycle, τ), C_k is the cost coefficient associated with interception device k. C_k is a function of flowrate, inlet and outlet composition, system design as well as operating variable. C_v is the cost coefficient of the storage and dispatch tanks. I_k and I_v are binary integers that take the value of 0 or 1 designating the absence or presence of an interception device and tanks respectively. From Equation 5, it is noted that the number of tanks is double than the tanks required. This is because the role of each set of the tanks will alternate after each cycle. One set of tanks will first be used for collection of water sources while the other set dispatches the stored water. In the subsequent cycle, their roles are reversed. The objective function is formulated to minimise the total annualized cost that is subject to the following constraints:

Splitting of sources to respective interception device and waste treatment:

$$F_i = \sum_{i=1}^{N_{Sources}} \left(w_{i,k} + w_{i,waste} \right) \qquad i = 1, 2, \ldots, N_{\text{Sources}} \qquad (6)$$

Property operator of interception devices $\psi_{k,p}^{\text{int}}$ are driven by interception device models:

$$\psi_{k,p}^{\text{int}} = f\left(\psi_{u,p}, z_k, r_k, t \right) \qquad k = 1, 2, \ldots, N_{\text{Int}} \,; p = 1, 2, \ldots, N_{\text{P}} \qquad (7)$$

Splitting of sources from interception devices k to all pairs of tanks v for storage:

$$w_k = \sum_{k=1}^{N_{Int}} w_{k,v} \qquad k = 1, 2, \ldots, N_{\text{Int}} \qquad (8)$$

Splitting of dispatch sources from tanks v:

$$w_v = \sum_{v=1}^{N_{Tanks}} \left(g_{v,j} + g_{v,waste} \right) \qquad v = 1, 2, \ldots, N_{\text{Tank } v} \qquad (9)$$

Property operator of the storage tanks v is given by:

$$\psi_{v,p} = \frac{\sum_{k=1}^{N_{Int}} w_{k,v} \psi_{k,p}}{\sum_{k=1}^{N_{Int}} w_{k,v}} \qquad k = 1, 2, \ldots, N_{\text{Int}} \,; p = 1, 2, \ldots, N_{\text{P}} \qquad (10)$$

Overall material balance around the mixing point of the feed to the sink:

$$G_j = \sum_{r=1}^{N_{Fresh}} f_{r,j} + \sum_{v=1}^{N_{Tnaksv}} g_{v,j} \qquad r = 1, 2, \ldots, N_{\text{Fresh}} \,; v = 1, 2, \ldots, N_{\text{Tanks } v} \qquad (11)$$

Material property operator constraints around the mixing point of feed to the sink j:

$$G_j \times \psi_{j,p}^{in} = f_{r,j} \times \psi_{r,p} + \sum_{v=1}^{N_{Tanksv}} g_{v,j} \times \psi_{v,p}^{out} \qquad j = 1, 2, \ldots, N_{\text{Sinks}}; \; p = 1, 2, \ldots, N_{\text{P}} \qquad (12)$$

Sink constraints:

$$\psi_{j,p}^{\min} \le \psi_{j,p} \le \psi_{j,p}^{\max} \qquad j = 1, 2, \ldots, N_{\text{Sinks}}; \; p = 1, 2, \ldots, N_{\text{P}} \qquad (13)$$

All the unused sources flow for reuse/recycle to the process sinks are fed to the waste treatment system before discharge to the environment:

$$\text{waste} = \sum_{v=1}^{N_{Tanksv}} g_{v,waste} \qquad v = 1, 2, \ldots, N_{\text{Tanks } v} \qquad (14)$$

From the formulation described above, it is noted that the mathematic formulation is a mixed integer nonlinear program (MINLP) which can be solved to determine the minimum total annualised cost for the water network with interception units.

1.3 Case Study

A semi-batch chemical process operates with an eight-hour cycle time. The process produces two recyclable water sources and has two process sinks that require water. The feed to process sinks is constrained by criteria on flowrate, composition of a sulfur pollutant, and pH. Tables 1 and 2 provide a summary of the pertinent data for the sources and sinks.

Table 1 Data for the process sources of the case study (*t* is start time of the cycle, hr)

Source	Function for flowrate (kg/s)	Function for pollutant composition (ppm)	Function for pH	Start time (hr)	End time (hr)
1	6.0	$20 \times t + 10$	$2 \times t + 8.0$	0	1
2	2.0	30	7.7	3	4

Table 2 Data for the process sinks of the case study

Sink	Minimum flowrate demand (kg/s)	Maximum flowrate demand (kg/s)	Minimum allowable pollutant composition entering the sink (ppm)	Maximum allowable pollutant composition entering the sink (ppm)	Minimum pH entering the sink	Maximum pH entering the sink	Start time (hr)	End time (hr)
1	8.0	8.5	0	17	6.0	7.2	5	6
2	3.0	3.2	0	20	7.0	7.5	7	8

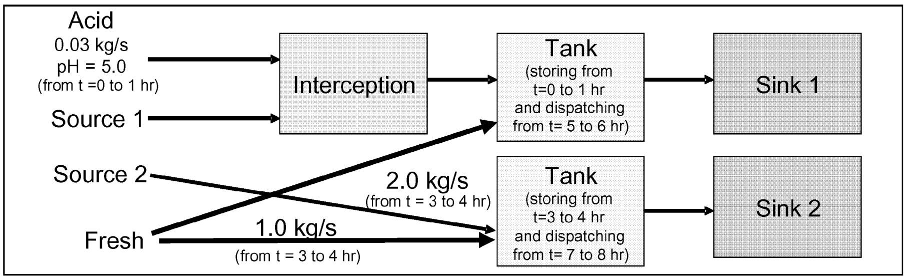

Figure 2 Optimal Solution of Case Study

To adjust the pH, neutralization units using an acid (pH = 5, cost = \$0.2/kg) or an alkali (pH = 11, cost = \$0.1/kg) may be used as interceptors. For pollutant removal, activated carbon adsorption may be used for interception (removal efficiency = 90%, cost = \$0.05/kg intercepted water). Fresh water (zero content of the pollutant and a pH of 7.0, cost = \$0.01/kg) may be used as needed. The total annualized cost of a tank (including pumping and piping) is \$20,000 per year. The mixing rule for pH is given by:

$$10^{-p\bar{H}} = \sum_i \left(x_i \times 10^{-pH_i} \right) \tag{15}$$

The objective is to synthesize a cost-effective water-recycle network. Following the proposed approach, the identified solution is shown by Fig. 2. The minimum total annualized cost of the system is \$181,912/yr.

2. Conclusion

A systematic procedure has been developed for the synthesis of batch water networks. Property-based constraints are used to determine acceptable feed to the process sinks. Also, property-based characterization of sources is used to describe the various recyclable water streams in the process. A source-interceptor-tank-sink representation was used to incorporate potential configurations of interest, which then solved by a mathematical-optimization approach. The solution of optimization determines the duty and location of each interception device, the assignment of sources to interceptors, tanks and sinks. A case study was solved to illustrate the usefulness of the approach.

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4. References

Almató, M., Sanmart, E., Espuna, A. and Puigjaner, L. 1997, Rationalizing the Water Use in the Batch Process Industry. Comp. Chem. Eng. 21: S971-976.

Almató, M., Espuña, A. and Puigjaner, L., 1999, Optimisation of Water Use in Batch Process Industries. Comp. Chem. Eng. 23: 1427-1437.

El-Halwagi, M. M., 2006, Process Integration, Elsevier Inc., San Diego, CA, USA.

El-Halwagi, M. M., Gabriel, F. and Harell, D., 2003, Rigorous Graphical Targeting for Resource Conservation via Material Recycle/Reuse Networks. Ind. Eng. Chem. Res., 42, 4319-4328.

El-Halwagi, M. M., Glasgow I. M., Eden, M. R. and Qin, X., 2004, Property Integration: Componentless Design Techniques and Visualization Tools. AIChE J., 50(8), 1854-1869 (2004).

Foo, D. C. Y., Manan, Z. A. and Tan, Y. L., 2005, Synthesis of Maximum Water Recovery Network for Batch Process Systems, J of Clean Prod. 13(15): 1381-1394.

Foo, D. C. Y., Kazantzi, V., El-Halwagi, M. M. and Manan, Z. A., 2006, Surplus Diagram and Cascade Analysis Techniques for Targeting Property-Based Material Reuse Network, *Chem. Eng. Sci*., 61, 2626-2642.

Hallale, N., 2002, A New Graphical Targeting Method for Water Minimisation. Adv. Env. Res., 6 (3), 377-390.

Kazantzi, V., El-Halwagi, M. M., 2005, Targeting Material Reuse via Property Integration. Chem. Eng. Prog. 101(8), 28-37.

Majozi, T., 2005, An effective technique for wastewater minimisation in batch processes, J of Clean Prod. 13(15): 1374-1380.

Manan, Z. A., Tan, Y. L. and Foo, D. C. Y., 2004, Targeting the Minimum Water Flowrate Using Water Cascade Analysis Technique. AIChE J, 50(12), 3169-3183.

Qin, X., Gabriel, F., Harell, D. and El-Halwagi, M. M., 2004, Algebraic Techniques for Property Integration via Componentless Design. Ind. Eng. Chem., 43, 3792-3798.

Shelley, M.D. and El-Halwagi, M.M., 2000, Componentless design of recovery and allocation systems: a functionality-based clustering approach. Comp. Chem. Eng., 24, 2081-2091.

Savelski, M., Bagajewicz, M. 2000, On the Optimality of Water Utilization Systems in Process Plants with Single Contaminant. Chem. Eng. Sci., 55, 5035-5048.

Wang, Y. P. and Smith, R., 1994, Wastewater Minimisation. Chem. Eng. Sci. 49, 981-1006.

Wang, Y. P. and Smith, R. (1995). Time pinch analysis. Trans IChemE*, Part A*. 73: 905-914.