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Optimal Design of Batch Water Network with a Flexible Scheduling Framework

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The rising cost of freshwater and wastewater treatment drives the development of systematic methods for water integration in batch plants. In addition, in batch processes, production rescheduling can further reduce freshwater consumption and wastewater generation. In this work, a design procedure for the synthesis of batch water networks, based on a flexible scheduling framework, is presented. Within the procedure a match ranking matrix is utilized to prioritize the matches between water sources and sinks. Based on the ranking, batch water networks can be designed while considering the time-dependent nature of batch processes. The design of a batch water network and a production schedule can be obtained simultaneously with the objective of minimizing freshwater consumption. In this work two examples are considered to demonstrate the feasibility of the proposed method. In the first example a regenerator with a fixed outlet concentration is incorporated to treat wastewater for further reuse. In the second example a batch plant with multiple contaminants is presented, in which a fixed removal ratio regenerator is employed. The results of these two examples demonstrate that the proposed method is a simple, effective approach for the design of batch water network with a flexible scheduling framework.

1. Introduction

Water is an important resource for normal operation of batch processes. Efficient use of water not only reduces the cost involved, but also minimizes the adverse environmental impact due to wastewater discharge. Graphical methods and mathematical programming have been effectively utilized to minimize freshwater consumption in batch processes. Many efforts have been devoted to water integration for fixed schedule batch processes (Majozi et al., 2015). However, results obtained from these studies could be suboptimal. Adekola and Majozi (2011) pointed out that if the duration of batch processes is treated as variables, the optimal product schedule can result in a further reduction of freshwater consumption.

Recently, wastewater minimization and optimal production scheduling has been considered simultaneously. The formulations could determine the minimum freshwater consumption together with the corresponding production schedule. Chen and Chang (2007) proposed a general mixed integer nonlinear programming (MINLP) model to synthesize water networks in batch processes. Zhou et al. (2009) developed a systematic design methodology to optimize batch process scheduling and water allocation networks simultaneously. Li et al. (2010) used the mathematical technique to deal with single- and multiple-contaminant batch water allocation networks. A flexible scheduling model was presented by integrating batch production scheduling and water allocation networks. Adekola and Majozi (2011) addressed the problem of wastewater minimization with a flexible product schedule. Results showed that the proposed model can achieve a wastewater reduction of 19.2 % and 26 % for the two case studies considered. Chen et al. (2011) developed a mathematical model based on resource-task network representation for simultaneous scheduling and water minimization in multipurpose batch plants. The objective function is to maximize the profit by taking into account the net income from production and water-related costs. Chaturvedi and Bandyopadhyay (2014) proposed a mathematical formulation to minimize the operational cost of water allocation networks in a flexible schedule plant by utilizing multiple freshwater resources. The results of two examples showed that compared with the use of a single freshwater source, reductions of 17 % and 32 % in operating costs are observed when multiple water resources are used. Chaturvedi et al. (2016) analysed

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the effect of multiple water resources in a flexible schedule water network. The findings indicated that once the optimum schedule for a single resource that results in the minimum operating cost is obtained, the same schedule can be applied for problems involving multiple resources. Lee and Foo (2017) considered simultaneous process scheduling and water minimization based on pinch-based automated targeting model (ATM) and a state-task network (STN) based discrete-time scheduling model. Some progress of simultaneous optimization of water/energy integration and production scheduling is presented in the text book (Majozi et al., 2017).

These methods are all based on mathematical programming. However, there exists no insight-based method to deal with these issues. The envisioned contribution of this work is to consider the optimization of water utilization in flexible batch processes based on match ranking matrix method. By including a variable time dimension in scheduling problems, this research aims to investigate the opportunity to further reduce freshwater consumption.

2. Problem statement

This work addresses the problem of optimizing water resources for flexible schedule batch processes. The problem can be stated as follows.

Given:

(i) the production recipe for each product, including mean processing times in each unit operation,

(ii) the contaminant mass load of each contaminant,

(iii) water requirement and the cleaning duration for each unit to achieve the required cleanliness

(iv) maximum inlet and outlet concentrations of each contaminant,

(v) the performance of the regenerator and

(vi) the time horizon of interest

Determine the production schedule that achieves the minimum freshwater consumption by exploring recycle and reuse opportunities in the presence of a central storage vessel and a wastewater regenerator.

3. Match ranking matrix

The match ranking matrix is proposed to design batch water network. The dimension of the match matrix depends on the number of water streams. Every column of the matrix represents a water sink and every row represents a water source (including freshwater). Before the water network synthesis begins, an $n \times m$ matrix is set up where n is the number of water sources and m is the number of water sinks. Note that in some cases the water using processes are not transformed into sources and sinks, as shown in the following examples. The water-using processes can be seen as water sinks and sources. Next, it is to fill the matrix with the results of freshwater consumption and reuse water quantity by Eq(1) and (2). Note that this example focuses on a single contaminant problem. For the multiple contaminant problems (Example 2 in Case study), firstly it is required to determine the freshwater consumption of a specific process for each contaminant. Next the maximum value of the results for all the contaminants is selected as potential freshwater consumption of this process. To create the ranking of the matches, their freshwater consumption potentials are primarily sorted in ascending order. However, the final rank of matches not only depends on the position in the sorted list about freshwater consumption, but is also subject to the availability of reuse water and the possibility of reduction of storage tanks.

$$F_{i,j}^{Re} + F_j^{Fw} = F_j \tag{1}$$

$$F_{i,j}^{Re} c_i^{out} + F_j^{Fw} c_{Fw} = F_j c_j^{\max,in} \tag{2}$$

Where $F_{i,j}^{Re}$ is the quantity of reused water from process i to j. F_j^{Fw} is the freshwater consumption of process j. F_j is the water requirement of process j. c_i^{out} is outlet concentration of process i. c_{Fw} is the concentration of freshwater. $c_j^{\max,in}$ is the maximum allowable inlet concentration of process j.

4. Procedures of design for flexible batch water network

The design procedure for batch water network is shown in Figure 1. In order to illustrate the design procedure for batch water network, a hypothetical example with only reuse scheme from Liu et al. (2009) is explained in detail in Section 5.1. The water limiting data is shown in Table 1.

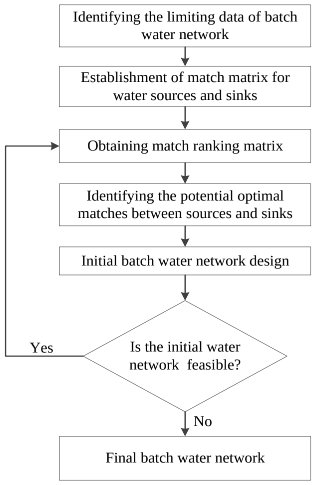

Figure 1: The design procedure for batch water network

5. Illustrative examples

5.1 Example 1 (reuse scenario)

A 6 × 5 matrix is first set up as source-sink match matrix, as shown in Table 2. The values in the cell represent the maximum potential of water reused and freshwater consumption. For example, (7.5, 22.5) in the second row denotes process B can reuse 7.5 t of water from water source A, and it requires 22.5 t of freshwater to dilute the wastewater to the allowable inlet concentration. In column 2 of Table 2, the quantity of reused water for all the water sources are zero, implying process A can be only fed by freshwater. Note that the diagonal value of the matrix is set as zero, implying it is not allowed to reuse water to the same unit.

Table 1: Water data for the illustrative Example 1 (reuse)

Operation	Quantity/t	$C_j^{in,\max} / \left(ug.g^{-1}\right)$	$C_j^{out,\max} / \left(ug.g^{-1}\right)$	Duration/h	M/kg
A	50	0	400	2	20
B	30	100	400	1	9
C	10	200	500	3	3
D	24	350	600	4	6
E	40	450	700	2.5	10

Table 2: The match matrix for the illustrative Example 1 (reuse) (unit: t)

	A	B	C	D	E
A	(0,0)	(7.5, 22.5)	(5, 5)	(21, 3)	(33.33, 0)
B	(0, 50)	(0,0)	(5, 5)	(21, 3)	(33.33, 0)
C	(0, 50)	(6, 24)	(0,0)	(16.8, 7.2)	(36, 4)
D	(0, 50)	(5, 25)	(3.33, 6.67)	(0,0)	(30, 10)
E	(0, 50)	(4.29, 29.71)	(2.86, 7.14)	(12, 12)	(0,0)
Fr	(0, 50)	(0, 22.5)	(0, 6)	(0, 10)	(0, 14.28)

Table 3: The ranking matrix for the Example 1 (reuse)

	A	B	C	D	E
A	-	2	1	1	1
B	2	-	1	1	1
C	2	3	-	2	2
D	2	4	3	-	3
E	2	5	4	4	-
Fr	1	1	2	3	4

Next, the freshwater requirements of all the source-sink matches are sorted in ascending order to receive the match ranking matrix, as shown in Table 3. The ranking for stream matching can be extracted from source-sink match matrix. During the ranking processes, if a few matches have the same ranking based on freshwater consumption, the ranking should be checked again by considering it from a holistic perspective. For example, for process B (column 3 of Table 2), the matches of A-B and Fr-B have the same quantity of freshwater, while quantity of reused water for match A-B is 7.5 t. In columns 3, 4 and 5 of Table 2, wastewater produced from process A has a high quality so that it can be reused to processes C, D, E (Rank 1). The match of Fr-B is ranking as 1 and A-B is ranking as 2. It is worth noting that (0, 0) is not including in the ranking matrix, because in this work water recycling in the same process is not allowed. Also in column 2 of Table 2, the quantity of reuse water from all the sources to process A (column 2) is zero, indicating that process A can only be fed by freshwater. The match Fr-A should be at rank 1 and other matches are at Rank 2. The same procedure is repeated for the remaining processes. The results of all the rankings are shown in Table 4.

Table 4: The potential optimal matches between sources and sinks for Example 1(reuse)

	A	B	C	D	E
1	Fr-A	Fr-B	A-C; B-C	A-D; B-D	A-E; B-E
2			Fr-C	C-D	C-E

The next step is to identify the potential optimal matches between sources and sinks based on the match ranking matrix. The insight obtained could be used to make preparation for the design of batch water network. The results of this example are shown in Table 4. For process A, the potential optimal match is Fr-A. Because freshwater supply is infinite, the other matches are omitted. For process C, D, E, there are two potential optimal matches. The match at rank 2 is regenerated in the matrix in case the quantity of reuse water is insufficient to meet the requirement.

The initial water network is obtained by Table 4. During initial water network synthesis, the match ranking matrix is used for match prioritization applying the following procedure: For every water sink, the match with rank 1 is implemented. After the streams representing rank 1 are used, if the sink is not satisfied, the stream representing rank 2 is matched. This procedure is continued to the last rank until the requirement is met. During the process of design, the time constraints for these processes are considered. In this example, process A can be only fed by freshwater and its wastewater has a high quality. Therefore, process A is set as the first unit for this batch operation and fed by freshwater (50 t). Compared with other processes, process E with a higher allowable inlet concentration could reuse wastewater from other processes. The end time of process E is set as the end time of interest of this batch operation, in other words, process E starts at 6 h and ends at 8.5 h. However, at this moment the freshwater consumption and reuse water quantity for process E cannot be identified. Until now the sequence of process A and E is fixed. The next step is to determine the processes B, C, D. As shown in Table 4, matches of A-C and A-D are at rank 1. Furthermore, quantity of wastewater from process A could be able to meet the total water requirement of processes C and D, while process B is insufficient.lit is assumed that processes C and D start at the end time of process A. The freshwater consumption of processes C and D is 5 t and 3 t. The quantities of reused water from process A are 5 t (process C) and 21 t (process D). The remaining water for process A is 24 t. As for process E, the potential optimal match at rank 1 is A-E and B-E. The water requirement (33.33 t) is higher than the available water from process A (24 t) and process B (22.5 t). It requires these two processes to supply wastewater to process E together. In order to reduce the storage capacity, all the wastewater from process B is sent to process E and the end time of process B coincides with the start time of process E. The stored water from process A is 10.83 t (= 33.33 t – 22.5 t). As shown in the column 3 of Table 4, the optimal match for process B is Fr-B. Process B is supplied by freshwater (22.5 t). The total freshwater consumption for entire batch process is 80.5 t (= 50 t + 3 t + 5 t + 22.5 t). The wastewater generated from each process can be obtained from simple water balance.

Once initial water network is determined, it is required to check if the designed water network satisfies with the time and water reuse constraints. If it is feasible, the final water network is obtained, otherwise, some infeasible matches of sources and sinks are deleted to redesign the water network. In this case there exist other options with the same freshwater consumption. However, because the storage capacity is larger than the aforementioned choice, it is not explained in detail. The final network is shown in Figure 2.

5.2 Example 1 (regeneration scenario)

To illustrate the application of the proposed approach, the example from the Liu et al. (2009) is revisited. The reuse scenario has been addressed in Section 5.1. The total freshwater consumption is 80.5 t (Figure 2), which could match with the results of Liu et al. (2009). In this section the regeneration scenario will be considered in which a regeneration unit with fixed outlet concentration is employed. For the purpose of simplicity, the detail procedure is not explained. The freshwater consumption is 57.813 t, while the results of Liu et al. (2009) is 68.594 t (product schedule is fixed) and the results of Adekola and Majozi (2011) is 64.07 t (product schedule is flexible). Hence, this amounts to a saving of 15.7 % of water for Liu et al. (2009) and a saving of 9.8 % of water for Adekola and Majozi (2011). The final network is shown in Figure 3.

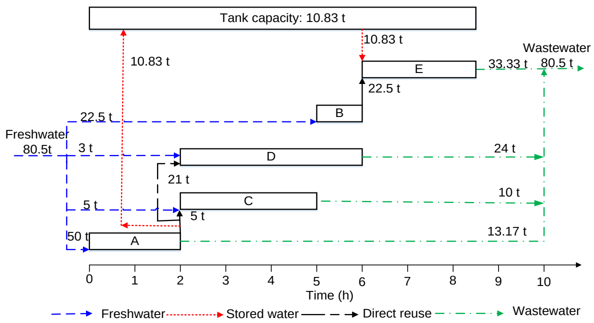

Figure 2: Water network for Example 1 (reuse)

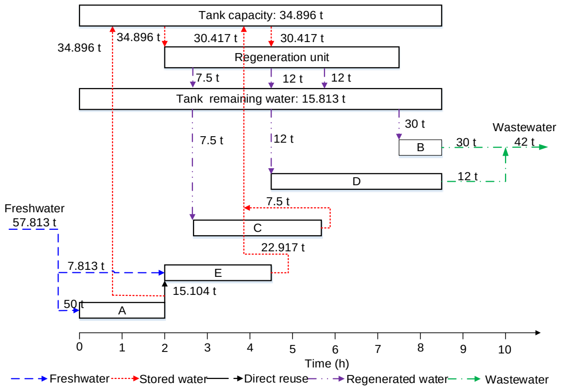

Figure 3: Water network for Example 1 (regeneration)

5.3 Example 2

This example taken from Adekola and Majozi (2011) is based on a section of a pharmaceutical production plant which produces four types of products, i.e. shampoos, deodorants, lotions and creams. 4 mixers for product mixing were available. Each product was produced by a specific mixer. Mixer 1 was dedicated to the mixing of shampoos, mixer 2 was dedicated to the mixing of deodorants, mixer 3 was dedicated to the mixing of lotions and mixer 4 was dedicated to the mixing of creams. The general production procedure is as follows. Raw material is charged to a mixer. The raw material is then mixed until the required physical characteristics are obtained. Once a product is mixed, it is removed and stored. The mixers are then washed. Since all the operations are dependent on others, freshwater consumption could be minimized by changing the sequence of batch operations.

For the reuse scenario, the total freshwater consumption is 3,404.69 kg, as shown in Figure 4. Compared with the results (3,587 kg) of Adekola and Majozi (2011), a reduction of 5.1 % in freshwater consumption is achieved. For the regeneration scenario, a regenerator with given removal ratio of the various contaminant is employed. As for the detail parameter of the regeneration unit, one can refer to Adekola and Majozi (2011). The total freshwater consumption is 2,151.58 kg, which is less than that of results (2,653 kg) of Adekola and Majozi (2011). The final network is shown in Figure 5. Note that the freshwater consumption is further reduced. However, it did not consider the mass transfer in the design process.

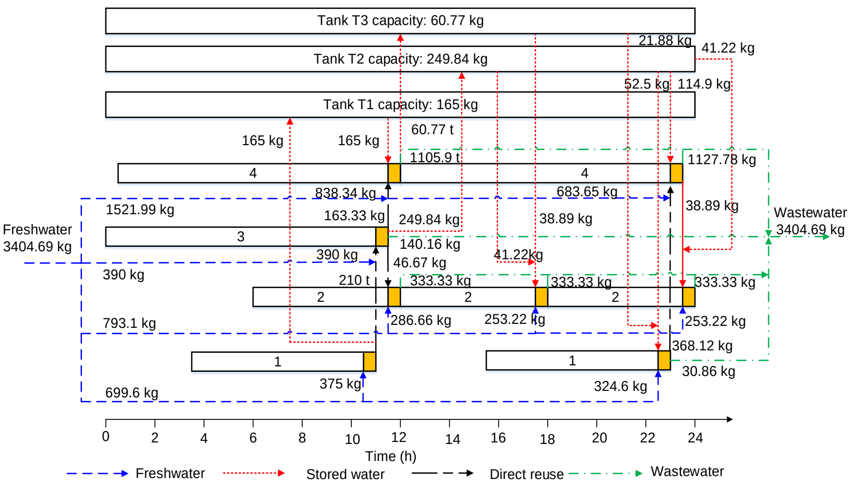

Figure 4: Water network for Example 2 (reuse)

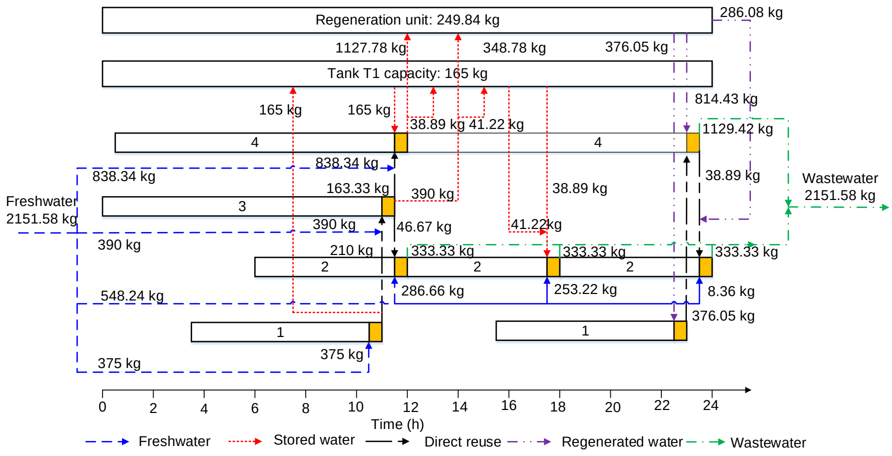

Figure 5: Water network for Example 2 (regeneration)

6. Conclusions

A design procedure of flexible batch water network is introduced in this work. During the design process, a match ranking matrix approach is proposed to identify the optimal batch water network with a flexible schedule framework. Two examples from literature are used to demonstrate the applicability of the proposed approach. The regeneration unit with fixed outlet concentration or fixed removal ratio is employed in these examples. The results show that this approach could be effective for the design of flexible batch water network, where single or multiple contaminants are involved. The limitation of the proposed method is that when the batch processes are complex, the proposed approach could result in suboptimal results. Hence, future work should focus on the combination of the proposed approach with mathematical programming to ensure that the obtained solutions are globally optimal. Furthermore, in order to obtain globally optimal results, the objective function should consider the total cost of batch water network, including capital and operation cost.

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