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Manual Design Strategies for Multicontaminant Water-Using Networks in Batch Processes

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Supporting Information

ABSTRACT: Simple design heuristics are developed in this work to manually generate batch water-using networks with multiple contaminants. The performance indices used for analyzing the continuous systems, i.e., *concentration potential of demand* (CPD) and *concentration potential of source* (CPS), are adopted to guide the synthesis steps. Specifically, if the batch plant is operated in cyclic mode, these concentration indices are treated as the primary criteria and the time priority as a secondary issue to match the water demands and sources sequentially. On the other hand, the precedence order of the concentration and time considerations is reversed if it is only necessary to schedule a single campaign. Both the required capacities and the number of buffer tanks in storage facilities can also be determined with the proposed procedures. Finally, two examples are presented at the end of this paper to demonstrate the effectiveness of the proposed manual approach.

1. INTRODUCTION

Water integration in batch chemical processes has gained increased attention recently.[1] The available network synthesis strategies can be divided into two general classes, i.e., (1) the manual methods[2−6] and (2) the model-based methods.[7−9] The first group can be further classified into the pinch-based[2−4] and graphic-based[5,6] approaches. The main feature of the former is a design target, i.e., the minimum amount of freshwater, that must be determined before network synthesis. With a graphic-based approach,[5,6] the design task can be performed directly without the targeting step, while the minimum freshwater consumption and the maximum water recovery is ensured by following the necessary condition of optimality[10] and the nearest neighbors algorithm.[11] It is important to note that, although the existing manual methods can be implemented easily, they are applicable only to the single-contaminant systems. On the other hand, it is also clear that the material balance constraints of any multicontaminant system can be easily incorporated in a mathematical programming model. Since, generally, the time constraints on unmatched operation periods may be the primary barriers for resource integration in batch processes, storage facilities are often needed to enhance the opportunities for water recovery. As a result, solving the corresponding NLP or MINLP model usually requires considerable computation resources and a good initial guess is almost always needed to start the search process.[7,12]

A simple manual strategy is presented in this paper to synthesize multicontaminant water networks in cyclic or in single-campaign processes. By considering two types of water-using operations, i.e., the fixed load units and the fixed quantity units, this design strategy is essentially an improved version of the aforementioned graphic-based approach.[5] The extension of existing method to the multicontaminant systems is facilitated mainly with two concentration indices, i.e., concentration potential of demand (CPD) and concentration potential of source (CPS), which can be utilized to rank the contamination levels of water demands and sources, respectively.[13] For the purpose of reducing the overall operating and capital costs, the specific aims of the proposed strategy are to minimize the freshwater usage, the total number of storage tanks and also their required capacities.[5] If a periodic process is under consideration, the concentration based constraints should be treated as the primary criteria (while the schedule based constraints should be of secondary concerns) for matching the demands and sources and also for configuring the needed storage facilities. On the other hand, the priority of these two types of criteria should be reversed if the batch water network is operated in a single-campaign mode.

It should be noted from the outset that the aforementioned strategy does not guarantee a global/local optimal solution for the corresponding mathematical programming problem. If necessary, these solutions can be further considered as suitable initial guesses in the formal optimization runs. The main benefits of the proposed manual approach can be summarized as follows:

- Since only simple hand calculations are needed to implement the design steps, the convergence problems usually encountered in the programming-based approach can be avoided;

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- Realistic and more-operable designs can be produced on the basis of practical considerations that cannot be incorporated in the mathematical models.

The remaining paper is organized as follows. The problem statement is first given in the next section. The basic concepts and important design heuristics are then described to facilitate the subsequent presentation of the proposed design procedures. Two application examples are provided next to demonstrate of effectiveness of these procedures and, also, to show the benefits of choosing such a manual approach over the programming-based strategies. Finally, conclusions are drawn and some future works are discussed at the end of this paper.

2. PROBLEM STATEMENT

Let us assume that, in a given batch process, the water-using operations can be divided into two distinct types, i.e., the fixed load units and fixed quantity units (see the Appendix). These units are characterized by the following process parameters:

- For every contaminant in a fixed load unit, the mass load and the upper bounds of input and output concentrations are available in advance, and its outlet concentrations are assumed to be kept at constant levels during the discharging period.
- The total amounts of water fed to and withdrawn from a fixed quantity unit can be determined a priori. The concentration of every contaminant in the outgoing water is given, while a fixed upper bound is imposed on the corresponding concentration in the incoming water.

In addition, the charging and discharging periods of each water-using operation should be specified before implementing the proposed design procedure. It is also assumed that

- Any number of buffer tanks may be installed to facilitate water integration. There are no capacity constraints.
- An unlimited amount of freshwater is available at any time.
- For the cyclic operations, sufficient reusable waters of suitable qualities are also available to start the first cycle.

The ultimate design goals are to conserve freshwater as much as possible and, at the same time, to minimize the overall capital cost of storage system. To achieve these purposes, the following design specifications are selected with the proposed strategies:

(1) the total amounts of freshwater consumed and wastewater produced during a production cycle or campaign,
(2) the number and capacities of buffer tanks, and
(3) the network structure.

3. CONCENTRATION POTENTIALS

To facilitate clear illustration of the important ideas given in the sequel, it is necessary to define the concepts of water *sources* and *demands* first. Specifically, these terms are used in the present paper to respectively represent the waters discharged from and fed into the water-using units.[11] For water conservation purpose, it is beneficial not to supply freshwater to a demand as long as other usable sources are available. The match between source and demand should be selected according to their concentrations. In the single-contaminant systems, the potential for a demand to consume wastewater is relatively low if a stringent upper bound is imposed upon its concentration. On the other hand, a low-concentration source obviously represents a good chance for reuse by the existing demands. The same rationale can be used to analyze the multicontaminant systems.

The well-established concept of concentration potential[13,14] is adopted in the present work to evaluate the reusability of a source or the satisfiability of a demand. To realize this concept, it is necessary to first consider the maximum amount of water supplied by source S_i that can be used to fulfill 1 ton of demand D_j for every supply demand pair. Specifically, this *allocation index* ($R_{i,j}$) for the pair (S_i,D_j) can be expressed as

$$R_{i,j} = \min_{k \in K} \left(\frac{C_{D_j,k}^{\max}}{C_{S_i,k}} \right) \tag{1}$$

where the subscripts i and j are used to denote the ith source and the jth demand, respectively; subscript k is associated with the kth contaminant; $C_{D_j,k}^{\max}$ is the maximum allowable concentration of contaminant k in demand D_j; $C_{S_i,k}$ is the concentration of contaminant k in source S_i. Note that $R_{i,j}$ approaches infinity as $C_{S_i,k}$ approaches zero, which is an unreachable condition in practice.

Thus, the concentration potential of demand D_j is defined accordingly as

$$\mathrm{CPD}(D_j) = \sum_{\substack{i=1 \\ i \neq j}}^{NS} R_{i,j} \tag{2}$$

and, similarly, the concentration potential of source S_i is defined as

$$\mathrm{CPS}(S_i) = \Big(\sum_{\substack{j=1 \\ j \neq i}}^{ND} R_{i,j}\Big)^{-1} \tag{3}$$

where NS and ND represent the total numbers of sources and demands, respectively. Clearly, the magnitude of $\mathrm{CPD}(D_j)$ reflects the overall possibility for demand D_j to make use of waters discharged by the sources. It can also be inferred that the value of $\mathrm{CPS}(S_i)$ generally represents the capability of source S_i to provide reusable water. Finally, note that the above definitions are formulated under the assumptions that (1) every water-using process has one feed and one product only and (2) the demand and source associated with the same operation are labeled with the same number. Therefore, the constraint $i \neq j$ (or $j \neq i$) is imposed to avoid recycling water to the process where it is produced. For the multi-input multi-output (MIMO) systems, this constraint should be modified on a case-by-case basis, according to the assigned labels.

4. KEY CONTAMINANTS

In performing the proposed design steps, it is also important to identify two types of key contaminants.[13] A brief description of these ideas is provided in the sequel for illustration clarity:

(1) In a unit that consumes water, the concentration of every contaminant in feed (which is viewed as a demand in this study) must be kept below a specific upper bound. When the water from a source (for example, S_i) is allocated to satisfy 1 ton of a demand (for example, D_j) as much as possible, the contaminant whose concentration reaching the upper limit in D_j is referred to as the *reuse key contaminant*, or RKC, for match (S_i,D_j). Therefore, this RKC is uniquely associated with the allocation index $R_{i,j}$ defined previously in eq 1.

(2) When only freshwater is used in a fixed load process, it is beneficial to make the output concentration of one or more contaminant attain the maximum allowable value. This is due to the fact that the freshwater usage can be minimized under such conditions. Specifically, the minimum amount of freshwater (F_{fresh}^{min}) can be calculated according to the following formula:

$$F_{fresh}^{min} = \max_{k \in K}\left[\frac{m_k^{load}}{C_{out,k}^{max}}\right] \tag{4}$$

where m_k^{load} is the mass load of contaminant k and $C_{out,k}^{max}$ is the limiting output concentration of contaminant k. The contaminant corresponding to F_{fresh}^{min} is referred to as the *freshwater key contaminant* (or FKC).

5. ALLOCATION HEURISTICS

The design tasks at hand are basically concerned with allocating sources to satisfy demands. A proper source−demand match should be identified by considering contaminant and water balances, concentration constraints and also scheduling limitations. A total of 10 allocation heuristics are adopted in this work. They are listed below sequentially, in which the first 6 can be considered as *the concentration-based rules* and the rest are *the schedule-based rules*.

(1) If the amount of source S_i is sufficient for demand D_j and $R_{i,j} \leq 1$, the allocated amount of S_i should be maximized to drive the concentration of corresponding RKC to reach its upper bound at D_j.

(2) If more than one source is available, then the selection should be made on the basis of their allocation indices ($R_{i,j}$). Specifically,
- If all allocation indices are less than one, then select the source with largest $R_{i,j}$ first to reduce the freshwater usage. The allocated amount should be determined according to rule 1.
- If at least one index is larger than or equal to one, then select the source which can provide the largest amount (or not less than the required amount) to reduce the number the connecting pipelines.
- If several candidate sources can be found and their allocation indices are exactly the same, the source with the highest CPS should be reused first to reduce freshwater consumption of the downstream process.

(3) After source S_i is selected to satisfy demand D_j according to rule 2, additional checks should be performed on the output concentrations of the water-using unit associated with D_j. In particular, if the corresponding RKC for the match (S_i,D_j) is the same as FKC and also the RKC concentration in the source is higher than the maximum allowable RKC concentration in the discharged water of a fixed-load process, then it is necessary to disregard S_i, since freshwater consumption cannot be reduced with such a selection.

(4) If a demand cannot be totally satisfied by a single primary source selected according to rules 2 and 3, a secondary source should be identified on the basis of a fictitious *remainder demand*, i.e.,
- The contaminant mass loads of the fictitious demand can be determined by subtracting the mass loads of the primary source from those of the original demand. In this case, the so-called "mass load" for a particular contaminant is defined in this study as the product of its concentration and the corresponding water flow rate. This special definition is applicable only to the sources and demands, which is not the same as that of the regular mass load of a fixed-load unit.
- The limiting throughput of the fictitious demand can be calculated by subtracting the allocated amount of the primary source from the limiting throughput of the original demand.
- The allowable maximum concentration of every contaminant of the remainder demand can be calculated by dividing the mass load by the limiting throughput of the fictitious unit.

Rules 2 and 3 can be used again to allocate additional water from the secondary source for the remainder demand.

Finally, the present allocation procedure (rule 4) should be repeated until the concentration of one or more contaminant reaches the upper bound or the limiting throughput of the remainder demand becomes zero.

(5) If only freshwater can be used for a water-using unit, then the allocated amount should be determined according to the following principles:
- The output concentration of at least one contaminant should reach the maximum allowable value for a fixed-load operation.
- The amount of freshwater should be set at the limiting throughput of a fixed-quantity operation.

(6) After fixing the water qualities of a demand by following rule 2 and possibly rule 4, the contaminant concentrations in the corresponding source should be set either
- according to the given mass loads of a fixed-load process to satisfy mass balances, or
- according to the given output concentrations of a fixed-quantity process.

Note that this rule is not applicable for operations with only sources or only demands.

(7) No buffer tanks are needed when the allocated source and demand are corresponding to two distinct processes with identical discharging and charging periods. Otherwise, a buffer tank should be introduced to facilitate the chosen match.

(8) If demand D_j is due to a type-A or type-D operation (see the Appendix), the discharging period of its allocated source S_i should end before the charging period of D_j ends.

(9) If demand D_j is due to a type-B or type-C operation (see the Appendix), the aforementioned rule 8 should still hold. In addition, the discharging period of source S_i must start before the charging period of D_j begins.

(10) Although the self-recycle configuration is realizable in a type-B single-campaign operation or in any cyclic operation, the match (S_i,D_i) should not be allowed if there are other alternatives. This is primarily due to the facts that
- additional trace components in sources may accumulate in the network and, consequently, cause unforeseen operational difficulties, and,

- for cyclic operations, the water provided by S_i may have to be stored for an entire cycle before its reuse by D_j.

6. DESIGN PROCEDURES

For a batch plant operated in cyclic mode, rules 8 and 9 may be relaxed within the same cycle, since storage tanks can always be installed to render the allocated source−demand match feasible in any two consecutive cycles. On the other hand, these rules should be strictly followed if there is only a single campaign.

Let us first consider the cyclic mode. Generally speaking, every network design can be evolved by following the proposed manual procedure, according to the feed concentrations of all water-using processes. This procedure will be referred to as Procedure I throughout this paper, and its flowchart is shown in Figure 1. The steps in this procedure are explained below:

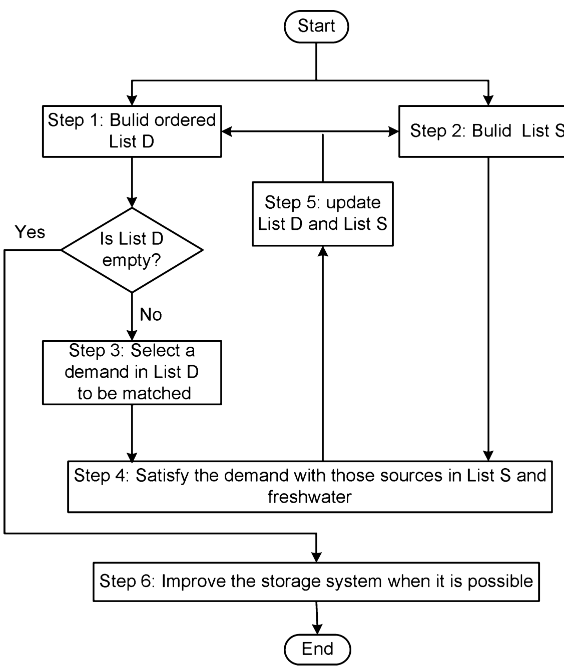

Figure 1. Flowchart of Procedure I.

Step 1: Calculate CPD(D_j) by substituting the limiting concentrations of D_j and those of all sources into eq 2 for j = 1, 2,..., ND. Arrange the resulting concentration potentials in ascending order and place the corresponding demands in an ordered list. This ordered list is referred to as List D.

Step 2 : Identify the available sources according to problem specifications and place them in another unordered list called List S. The source concentrations should be temporarily set at their upper bounds.

Step 3: Identify the demand with the lowest inlet concentration potential from List D. If multiple candidates are available, select the one corresponding to the lowest CPS, to increase reuse opportunities downstream.

Step 4: Satisfy the identified demand with source(s) in List S and/or freshwater by performing the calculations suggested in rules 1−5 and 10. If necessary, a storage facility may be introduced according to rule 7.

Step 5: Determine the actual output concentrations of the process corresponding to the identified demand on the basis of rule 6 and, also, update *all* source and demand concentrations. In addition, remove the satisfied demand and the used-up source(s) from List D and List S, respectively. If the resulting List D is empty, go to step 6. If not, go to step 3.

Step 6: Improve the preliminary storage system obtained in the previous steps by
- utilizing the inherent storage capacity of one or more batch operation to reduce capital cost,[3] or
- merging several tanks into a single one at the cost of additional freshwater.

In the former case, the storage capacity required by a match, say (S_i,D_j), may be reduced or even eliminated if S_i can be kept in unit i after the specified discharging period and reused during the charging period of D_j in the present or next cycle or, conversely, if D_j can be charged at a time earlier than the specified starting time. On the other hand, the latter approach is feasible only when the wastewaters stored in the individual tanks are of similar qualities. The required storage capacity of the combined tank can be set according to the peak point on the inventory-versus-time profile.

For a batch plant operated in single-campaign mode, it is obvious that higher priorities should be given to the schedule-related constraints. Consequently, the corresponding network designs must be developed in a different procedure (referred to as Procedure II, and its flowchart is provided in Figure 2). Procedure II can be applied primarily on the basis of the charging and discharging periods of water-using processes and its main steps are explained below:

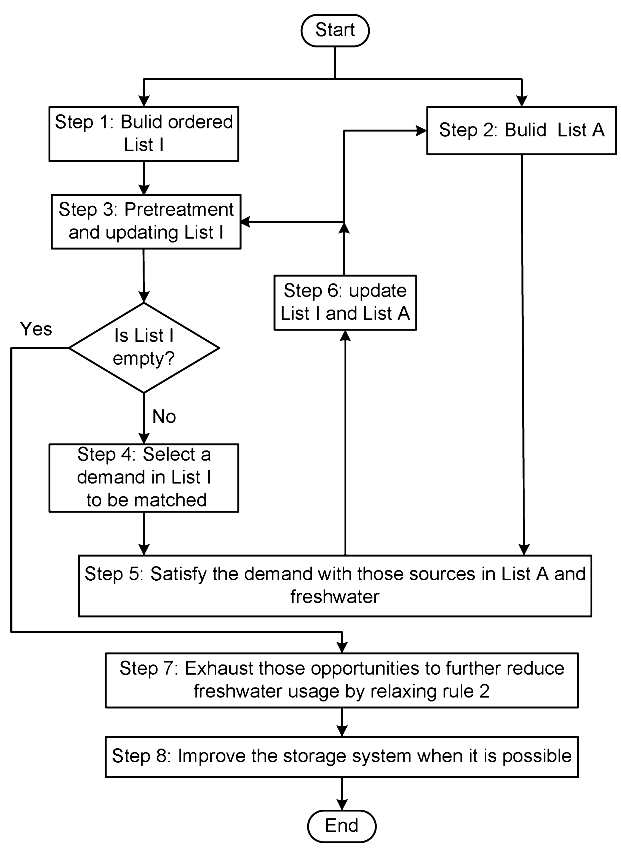

Figure 2. Flowchart of Procedure II.

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Step 1: Set the incipient time of every water demand as the instance when

- the charging period of a type-A or type-D operation ends, or
- the charging period of a type-B or type-C operation begins.

Rank these demand incipient times in ascending order and place the corresponding processes in a list called List I.

Step 2: Set the available time of every water source as the instance when

- the discharging period of a type-A or type-C operation begins, or
- the discharging period of a a type-B or type-D operation ends.

Rank these source available times in ascending order and place the corresponding processes in another list called List A.

Step 3: If the incipient time of the first process in List I is earlier than all available times in List A, then satisfy the corresponding demand by freshwater according to rule 5 and determine the output concentrations of this process according to rule 6. Remove the first process from List I and repeat the present step until the first incipient time in the updated List I is later than at least one available time in List A.

Step 4: Identify the process (or processes) with the earliest demand incipient time from the updated List I.

Step 5: Satisfy the demand corresponding to the identified process with source(s) in List A by performing the calculations suggested in rules 1−6 and 8−10. If necessary, a storage facility can be introduced according to rule 7.

Step 6: Remove the processes corresponding to the satisfied demand and the used-up source(s) from List I and List A, respectively. If the resulting List I is not empty, then go to step 4.

Step 7: Identify a fixed-load process with the earliest source available time from the updated List A. Try to explore additional opportunities to further reduce freshwater usage by relaxing rule 2 in one or more allocated match at an earlier time, to eliminate the water effluent to the environment due to this unused source. Repeat the present step until all possibilities are exhausted.

Step 8: Improve the preliminary storage system according to step 6 in Procedure I.

7. APPLICATIONS

7.1. Example 1. To illustrate the implementation steps of the aforementioned design procedures in further details, a hypothetical example is first presented here. The process data under consideration can be found in Table 1. Operations 1, 2, and 4 in this table can be regarded as fixed-load processes, while operations 3 and 5 are the fixed-quantity processes. The Gantt chart of these water-using operations is shown in Figure 3, where the duration of each batch process is expressed with a peach-colored bar and the charging and discharging periods are respectively indicated by the shaded and blank bars.

Prior to exploring water reuse opportunities in this system, let us first consider a base case in which all demands are satisfied with freshwater. For operations 1, 2, and 4, the amounts of required waters can be found to be 30, 55, and 15 tons, respectively according to eq 4. Notice that the sets of FKCs for these three operations are {A,B,C}, {A}, and {C}, respectively. On the other hand, since a water requirement of 40 tons is specified for both operations 3 and 5, the total amount of water consumed in the base case should be 30 + 55 + 15 + 40 + 40 = 180 tons in a single period (8.5 h).

Table 1. Problem Specification of Example 1

Time (h) intake	Time (h) discharge	contaminant	$C_{in,k}^{max}$ (ppm)	$C_{out,k}^{max}$ (ppm)	m^{load} (kg)	F^{lim} (ton)
		Operation 1				
		A	0	100	3.0	
0.0−1.0	4.0−5.0	B	0	90	2.7	30
		C	0	50	1.5	
		Operation 2				
		A	40	150	8.25	
0.0−0.5	4.5−5.0	B	60	80	1.5	75
		C	20	70	3.75	
		Operation 3				
		A	170	170	0	
5.0−6.5	5.0−6.5	B	120	120	0	40
		C	100	100	0	
		Operation 4				
		A	110	210	3.0	
2.0−2.5	6.5−7.0	B	135	200	1.95	30
		C	60	120	1.8	
		Operation 5				
		A	170	170	0	
7.0−8.5	7.0−8.5	B	120	120	0	40
		C	100	100	0	

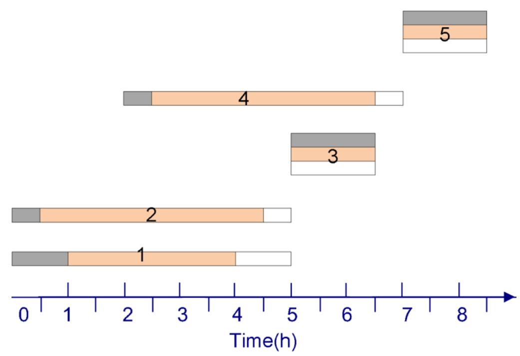

Figure 3. Gantt chart of Example 1.

7.1.1. Design for Repeated Cycles. Procedure I should be adopted in this case. The application steps are summarized below:

Steps 1 and 2: Based on the limiting data in Table 1, the concentration potentials of demands can be calculated, and they are listed in Table 2. It is clear that the *ordered* demand list is

$$\text{List D} = (D_1, D_2, D_4, D_3/D_5)$$

and the *unordered* source list is

$$\text{List S} = (S_1, S_2, S_3, S_4, S_5)$$

Step 3a: List D is not empty and Demand D_1 should be considered first.

Step 4a: Since the maximum allowable concentrations of D_1 are all zero, it can be decided (based on rules 2 and 3) that only freshwater can be used to satisfy this water demand. According

Table 2. Concentration Potentials of Demands (D_j) in Example 1

	D_1	D_2	D_3	D_4	D_5
CPD(D_j)	0	0.967	4.067	3.033	4.067
order	1	2	4	3	4

to allocation rules 5 and 6, the needed amount of freshwater is the same as the limiting throughput, i.e., 30 tons, and the output concentrations of unit 1 should be those at the limiting values, i.e., 100 ppm (A), 90 ppm (B), and 50 ppm (C).

Step 5a: Since freshwater is used to satisfy D_1, List S remains unchanged and the updated demand list becomes

$$\text{List D} = (D_2, D_4, D_3/D_5)$$

Step 3b: The updated List D is not empty and Demand D_2 should be considered next.

Step 4b: According to rules 2 and 3, S_1 should be chosen to match D_2. From the definition of allocation index given in eq 1, it can be determined that $R_{1,2} = 0.4$ and the corresponding RKCs are contaminants A and C. The amount of water supplied by source S_1 for match (S_1,D_2) should be $75 \times R_{1,2} = 75 \times 0.4 = 30$ tons. Since the limiting throughput of D_2 is 75 tons, the required amount of freshwater is $75 - 30 = 40$ tons. Based on the fact that the time durations of S_1 and D_2 are not overlapping, a storage tank is needed to facilitate this match. The resulting intermediate network for operations 1 and 2 is provided in Figure 4, in which the charging and discharging periods of the storage tank are marked with angled solid lines and the actual contaminant concentrations are given in square brackets.

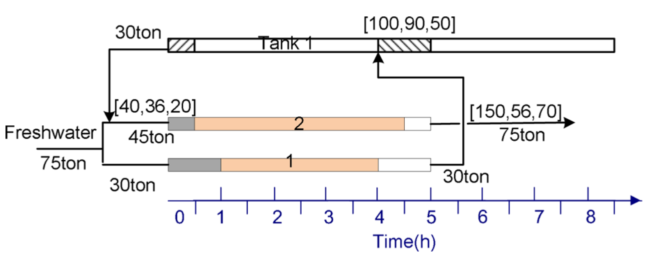

Figure 4. Network configuration of operations 1 and 2 of Example 1 in cyclic mode.

Step 5b: Since source S_1 has been used up, the updated source list becomes

$$\text{List S} = (S_2, S_3, S_4, S_5)$$

and the demand list can also be updated:

$$\text{List D} = (D_4, D_3/D_5)$$

Step 3c: List D is not empty and Demand D_4 should be considered next.

Step 4c: According to rule 2, S_2 should be chosen first to match D_4. The allocation index $R_{2,4} = 0.733$ can be calculated according to eq 1 and the corresponding RKC is contaminant A (which is not the same as the FKC of contaminant C). The amount of S_2 to be used for match (S_2,D_4) is $30 \times R_{2,4} = 30 \times 0.733 = 22$ tons. Therefore, source S_2 is still capable of providing $75 - 22 = 53$ tons of water for other reuse opportunities and $30 - 22 = 8$ tons of freshwater are needed to satisfy demand D_4. Based on the component balances, the actual feed and product concentrations of unit 4 can be easily determined to be (110, 41.07, 51.33) and (210, 106.07, 111.33), respectively. Finally, another storage tank is introduced for this match, and the resulting network configuration is given in Figure 5.

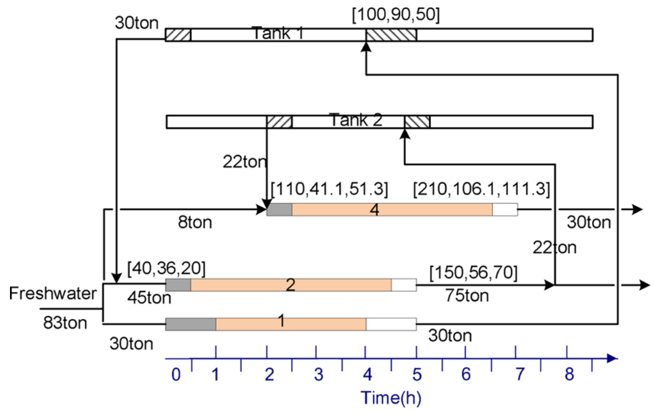

Figure 5. Network configuration of operations 1, 2, and 4 of Example 1 in cyclic mode.

Step 5c: Since S_2 has not been completely consumed in matching D_4, the source list remains the same, i.e.,

$$\text{List S} = (S_2, S_3, S_4, S_5)$$

Since D_4 is satisfied, the updated demand list is

$$\text{List D} = (D_3/D_5)$$

Step 3d: The updated List D is not empty and D_3 and D_5 should be simultaneously considered next. Since these two demands have the same maximum inlet concentrations and flow rates, they can be viewed as an artificially combined demand and, therefore, both should go through the same allocation steps.

Step 4d: On the basis of rules 2, 3, and 10, the available sources for matching D_3 and D_5 should be S_2 (53 tons) and S_4 (30 tons). Note that S_3 and S_5 are not preferred to satisfy D_3/D_5, because the water sources and demands in this case are of indistinguishable qualities and, thus, the corresponding matches should form either two self-recycles, i.e., (S_3,D_3) and (S_5,D_5), or a single loop embedded with two matches (S_3,D_5) and (S_5,D_3). According to the definition given in eq 1, the allocation indices $R_{2,3}$ and $R_{4,3}$ can be evaluated to be 1.133 and 0.81, respectively. Thus, based on allocation rule 2, it can be concluded that the water from S_2 should be reused first. From the special features associated with the corresponding matches, i.e.,

- units 3 and 5 are fixed-quantity processes and both require 40 tons of water,
- the amount of available water from S_2 is only 53 tons, and
- $R_{2,3} \geq 1$,

it is reasonable to deduce that S_2-supplied water can be evenly divided, i.e., 26.5 tons each, and allocated to D_3 and D_5, respectively. To satisfy each of these demands, an additional 13.5 tons should be supplied by S_4 and/or with freshwater. According to allocation rule 4, the limiting concentration of contaminant A in a corresponding *remainder demand* can be calculated as follows:

$$\frac{(40 \times 170) - (26.5 \times 150)}{13.5} = 209.26 \text{ ppm}$$

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Similarly, the limiting concentrations of B and C in the same remainder demand can be determined to be 245.63 and 158.89 ppm, respectively. For illustration convenience, let us denote the aforementioned remainder demands of D_3 and D_5 as $D_{3'}$ and $D_{5'}$, respectively. The corresponding allocation index $R_{4,3'}$ (or $R_{4,5'}$) can then be determined to be 0.996 and RKC is contaminant A. To satisfy $D_{3'}$, the amount of S_4-supplied water should be 13.5 × 0.996 = 13.45 tons and the required amount of freshwater is 13.5 − 13.45 = 0.05 ton. Clearly, the same arrangement should be adopted to satisfy $D_{5'}$. Notice that a third storage tank is needed to store the wastewater produced by unit 4. The resulting preliminary network is given in Figure 6, and the actual feed and product concentrations of each operation are provided in Table 3. Note that, in this table, the underlined values denote the contaminant concentrations, which are equal to the given upper bounds.

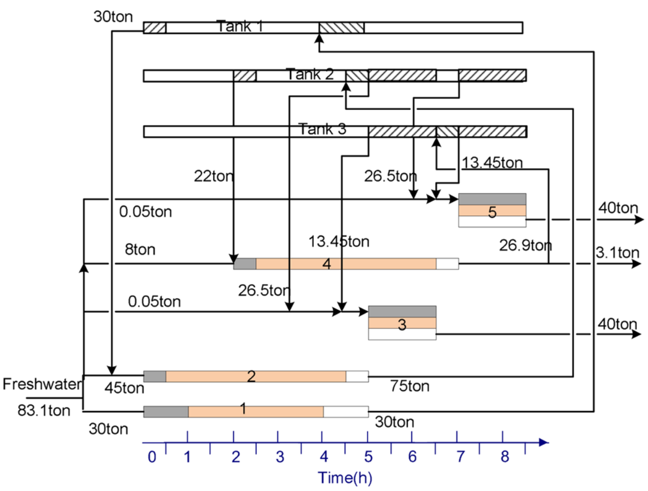

Figure 6. Preliminary network configuration of Example 1 in cyclic mode.

Step 5d: Since List D is now empty, step 6 should be performed next.

Step 6: Plot the water inventories in tanks 1−3 as functions of time (see Figure 7). Notice that the tank volumes should be chosen to accommodate the peak points of these profiles, i.e., 30, 75, and 26.9 tons. Based on allocation rules 7−9, the following decisions can be made:

- The storage capacity of unit 1 can be utilized to replace Tank 1 if 30 tons of S_1 can be kept in unit 1 until the charging of D_2 starts in the next cycle and the charging duration of D_1 can be shortened to be [0.5, 1] hour.
- The storage capacity of unit 2 can be used to store 53 tons of wastewater from S_2 of during [5, 8.5] h and supply half the amount to satisfy matches (S_2,D_3) and (S_2,D_5), respectively. The required storage capacity of tank 2 can be reduced from 75 tons to 22 tons.
- The storage capacity of unit 4 can be used to store 13.45 tons of wastewater from S_4 during (7, 8.5) h and the storage capacity of tank 3 can be reduced from 26.9 tons to 13.45 tons.
- Since the wastewaters stored in tanks 2 and 3, i.e., S_2 and S_4, are of significantly different qualities, they cannot be combined.

The final network configuration is given in Figure 8.

Table 3. Actual Inlet and Outlet Concentrations of Example 1 in Cyclic Mode

contaminant	$C_{in,k}$ (ppm)[a]	$C_{out,k}$ (ppm)[a]
	Operation 1	
A	0	100
B	0	90
C	0	50
	Operation 2	
A	40	150
B	36	56
C	20	70
	Operation 3	
A	170	170
B	72.77	72.77
C	83.81	83.81
	Operation 4	
A	110	210
B	40.07	106.07
C	51.33	111.33
	Operation 5	
A	170	170
B	72.77	72.77
C	83.81	83.81

[a]Underline indicates concentrations that reach the given upper bounds.

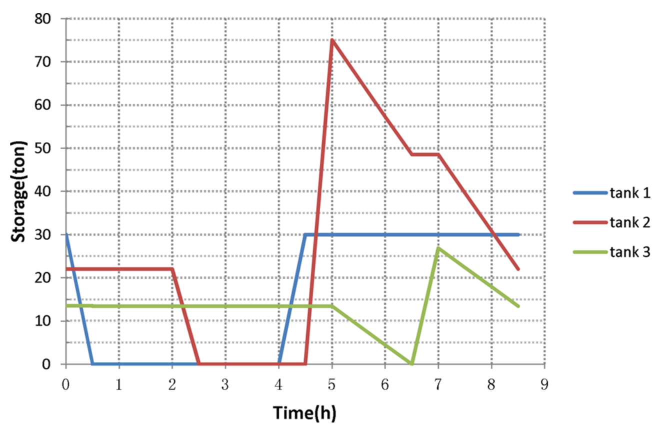

Figure 7. Storage profile of tanks of the preliminary network configuration of Example 1 in cyclic mode.

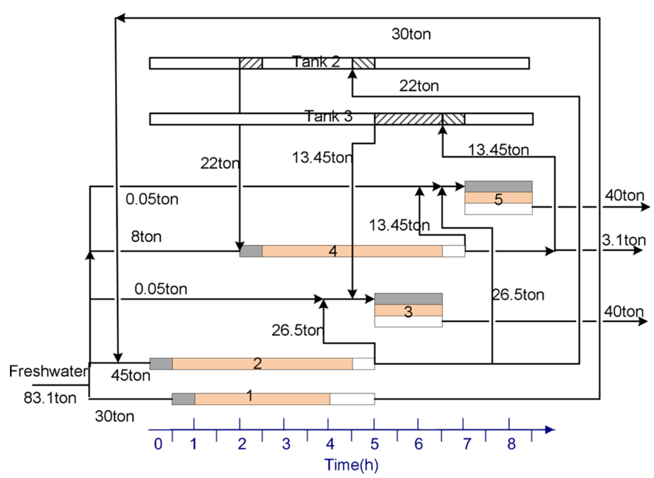

Figure 8. Final network configuration of Example 1 in cyclic mode.

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Notice that the total amount of freshwater required in the final network is 83.1 tons, which represents a 53.8% reduction from that in the base case. Let us also check the optimality of this design. For the cyclic processes with only one contaminant, Foo et al.[15] showed that the freshwater target of a batch network is exactly the same as that for a fictitious process created by treating all operations as continuous ones. Although the global minimum of the corresponding MINLP model involving more than one contaminant cannot always be obtained,[7] the lower bound of minimum freshwater consumption rate can be determined by considering each contaminant separately and solving the simplified optimization problems with any available method.[15] More specifically, this lower limit should be the maximum value among all aforementioned minimum freshwater usage levels. For the present example, the freshwater target is 80 tons for each contaminant. Thus, the amount of freshwater consumed in Figure 8 is really very close to the lower bound of true optimum and the error is merely 4%.

7.1.2. Design for a Single Campaign. Procedure II should be followed to produce this design. A summary is given below:

Steps 1 and 2: According to the charging and discharging periods of each demand and source in Figure 3, one can generate two ordered lists:

$$\text{List I} = (D_2, D_1, D_4, D_3, D_5)$$

$$\text{List A} = (S_1, S_2, S_3/S_4, S_5)$$

Step 3: D_1, D_2, and D_4 should be satisfied by freshwater, because the incipient times of these three demands are earlier than any source available time. The minimum quantities of freshwater required by these three operations can be found to be 30, 55, and 15 tons, respectively, while the corresponding product concentrations are (100, 90, 50) ppm, (150, 27.27, 68.81) ppm, and (200, 130, 120) ppm. The obtained network configuration is provided in Figure 9. The updated List I is

$$\text{List I} = (D_3, D_5)$$

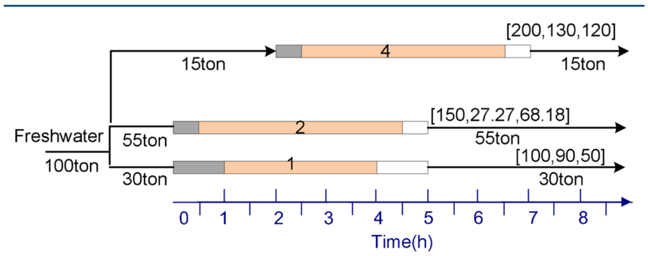

Figure 9. Network configuration of operations 1, 2, and 4 of Example 1 in a single-batch mode.

Step 4a: List I is not empty and D_3 should be considered next.

Step 5a: According to rules 8−10, only S_1 and S_2 can be chosen to satisfy D_3. The corresponding allocation indices are as follows: $R_{1,3} = 1.333, R_{2,3} = 1.133$, and their RKC(s) are B and A, respectively. Since the required amount of demand D_3 is 40 tons and there is not enough S_1, so 40 tons of S_2 is allocated and an intermediate storage tank is introduced to facilitate reuse. The outlet concentration of operation 3 can be easily determined to be (150, 27.27, 68.18) ppm.

Step 6a: Since there is still 55 − 40 = 15 tons of S_2 left after satisfying D_3, List A is unchanged. The updated list I is

$$\text{List I} = (D_5)$$

Step 4b: D_5 is the last one to be satisfied in the design process.

Step 5b: According to rules 8 and 9, the first four sources in the updated List A can be considered as possible candidates, since their available times are earlier than the incipient time of D_5. To make a proper selection, their allocation indices should be computed:

$$R_{1,5} = 1.333 \quad R_{2,5} = R_{3,5} = 1.133 \quad R_{4,5} = 0.83$$

and there are 30 tons of S_1, 15 tons of S_2, and 40 tons of S_3 available for matching 40 tons of demand D_5. According to rules 2 and 7, the best choice in this case should be S_3 and a second storage tank is needed to realize match (S_3,D_5). The obtained preliminary network is given in Figure 10.

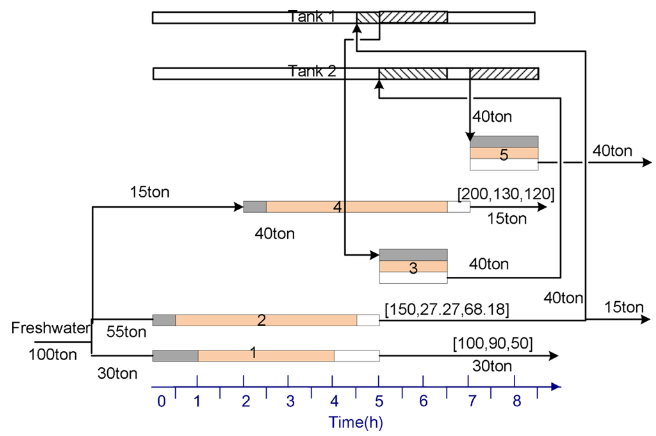

Figure 10. Preliminary network configuration of Example 1 in a single-batch mode.

Step 6b: The updated list A is

$$\text{List A} = (S_1, S_2, S_4, S_5)$$

and the updated List I is now empty, step 7 should be performed next.

Step 7: Since $R_{2,3} > 1$ and $R_{3,5} > 1$ and no freshwater is needed to facilitate either match (S_2,D_3) or match (S_3,D_5), opportunities for further reduction of freshwater usage cannot be identified here.

Step 8: Let us consider the two allocated matches in Figure 10, i.e., (S_2,D_3) and (S_3,D_5). In the former case, unit 2 can be utilized to store 40 tons of S_2 during the period [5, 6.5] h and, as a result, tank 1 can be eliminated. On the other hand, it is not possible to reduce the storage capacity required by the latter match because units 3 and 5 are both operated in semibatch mode. The final network configuration given in Figure 11 needs only one tank whose required storage capacity is 40 tons.

Notice that the freshwater usage in Figure 11 is 100 tons, which means a 44.44% savings when compared with that required in the base case. The important results of the present example are summarized in Table 4.

7.2. Example 2. Let us consider the production schedule in Figure 12, which was originally studied by Chen et al.[8] with a model-based approach. In this Gantt chart, tasks 1, 2, and 3 are repeated four, three, and five times, respectively, with durations of 2, 2.5, and 1.5 h, respectively. Note that no charging or discharging periods are marked on any of these tasks. It is

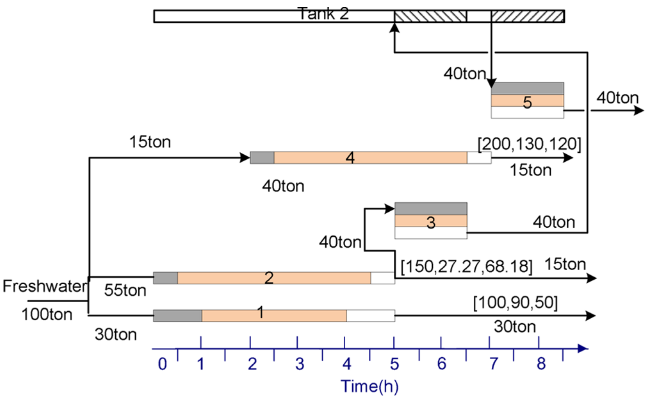

Figure 11. Final network configuration of Example 1 in a single-batch mode.

Table 4. Summary for Network Design of Example 1

	freshwater (ton)	number of tanks	capacity of storage (ton)	water recovery (%)
base case	180	0	0	0
single batch	100	1	40	44.44
cyclic batch	83.1	2	(22, 13.45)	53.83

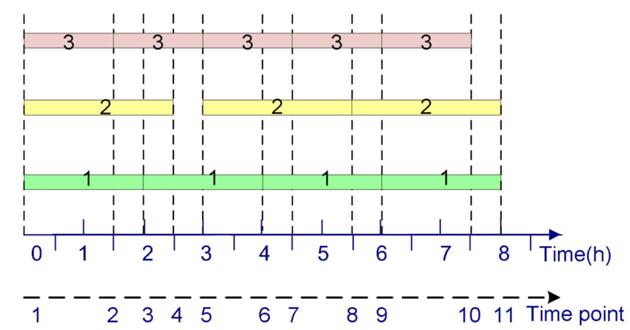

Figure 12. Gantt chart for the production schedule of Example 2.[8]

therefore assumed in this example that every task can be viewed a fixed-load batch process and, also, water can be charged to and discharged from this process almost instantaneously. The process data of all water-using operations can be found in Table 5.

To be able to compare the design results generated according to the proposed procedures with those reported in Chen et al.,[8]

Table 5. Process Data of Example 2

contaminant	$C^{max}_{in,k}$ (ppm)	$C^{max}_{out,k}$ (ppm)	m^{load} (g)	F^{lim} (ton)
		Task 1		
A	5	15	675	
B	0	0	0	67.5
C	0	0	0	
		Task 2		
A	0	0	0	
B	50	100	2500	50
C	0	0	0	
		Task 3		
A	120	220	5600	
B	200	450	14000	56
C	200	9500	520800	

rule 10 is relaxed among the repeated tasks shown in Figure 12 and these tasks are treated as different operations with distinct labels. For example, the four consecutive operations of task 1 are numbered sequentially as 1.1, 1.2, 1.3, and 1.4, respectively. The repeated operations of tasks 2 and 3 are named in exactly the same way. In addition, the amounts of water input and output of each water-using operation are set at the limiting values. Notice that only a single contaminant is allowed in performing tasks 1 and 2, respectively, i.e., contaminant A in the former case and contaminant B the latter. Thus, it is easy to see that (1) any operation used to implement task 1 or task 2 can only consume waters produced by operations of the same type, and (2) any operation used to carry out task 3 can consume water produced by any operation of tasks 1 and 2 whose maximum outlet concentrations are less than the maximum inlet concentration of task 3 for each contaminant.

To facilitate meaningful discussion, let us first generate a base case design. In this design, all demands are satisfied with freshwater and water reuse is not explored. The total amount of required freshwater should be $(67.5 \times 4) + (50 \times 3) + (56 \times 5) = 700$ tons. Next, Procedure I can be implemented to produce the cyclic water network design ishown n Figure 13, and the

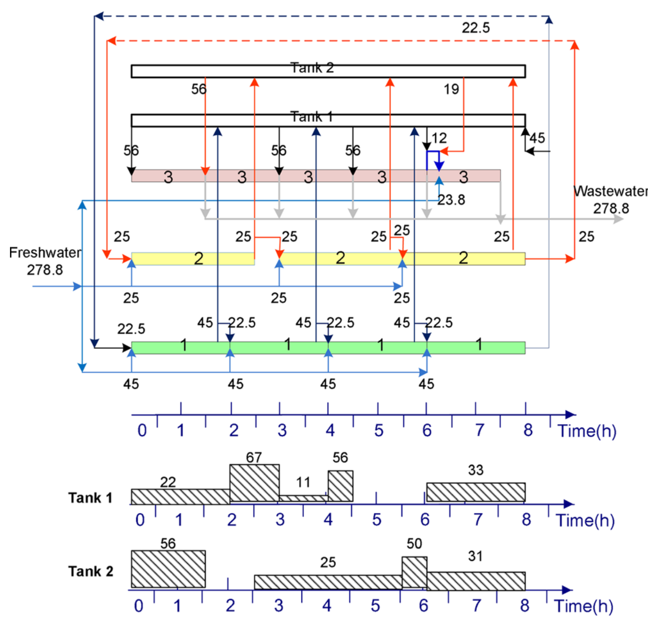

Figure 13. Final network configuration of Example 2 in cyclic mode.

detailed design steps are provided as Supporting Information. Note that 278.8 tons of freshwater are needed in this design, which represents a 60.17% reduction from the base-case level. Notice also that two storage tanks must be installed to facilitate water reuse and the required capacities are 67 and 56 tons, respectively. These results are actually very close to those obtained with a conventional mathematical programming approach.[8]

The single-campaign designs are then evaluated in the sequel. Notice that, since step 7 in Procedure II is not successfully applied in Example 1, a better illustration of this step can be provided here with the present example. Let us first carry out steps 1−6 to obtain the preliminary network in Figure 14. This design requires 407.94 tons of freshwater (which is a 41.72% savings, when compared with the base-case level) and two storage tanks with capacities for 45 and 11 tons, respectively.

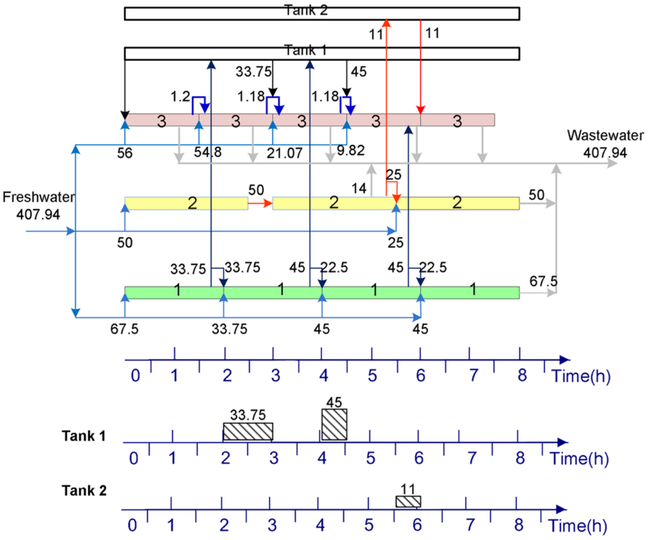

Figure 14. Preliminary network configuration of Example 2 in a single-batch mode.

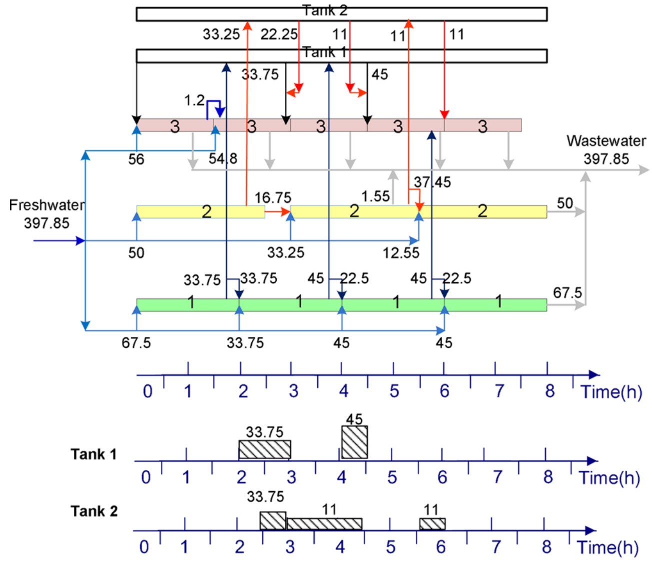

Figure 15. Final network configuration of Example 2 in a single-batch mode.

Step 7 can then be implemented to improve this preliminary network:

It should be noted that 14 tons of $S_{2,2}$ are discharged directly to the environment as wastewater. In fact, there is a good chance to introduce freshwater to partially satisfy $D_{2,2}$, to reduce the contaminant level of $S_{2,2}$ and, consequently, allow better utilization of this effluent water. Since $S_{2,1}$ is originally used to satisfy $D_{2,2}$ in the preliminary design, "additional" water should be available at the end of operation 2.1 if the suggested design change is adopted. It is obviously beneficial to replace the freshwaters consumed by $D_{3,3}$ and $D_{3,4}$ with this "new" water source. Based on the aforementioned analysis, $D_{3,3}$ and $D_{3,4}$ can be rematched under the assumption that $S_{2,1}$ is available while keeping other conditions unchanged. The resulting new matches are listed below:

- 33.75 tons of $S_{1,1}$ and 22.25 tons of $S_{2,1}$ are used to satisfy $D_{3,3}$, and
- 45 tons of $S_{1,2}$ and 11 tons of $S_{2,1}$ are used to satisfy $D_{3,4}$.

The amount of $S_{2,1}$ for $D_{2,2}$ should be reduced to 50 − 22.25 − 11 = 16.75 tons, and the effluent from $S_{2,2}$ now becomes 1.55 tons. The improved design is presented in Figure 15, in which the freshwater consumption level is decreased to 397.85 tons. Two storage tanks are still required in this network, and their needed capacities are 45 and 33.75 tons, respectively.

Finally, the key features of network designs produced with the proposed procedures and those generated by solving the conventional mathematic programming models[8] are summarized and compared in Table 6. It can be observed that, although both approaches yield similar solutions, the proposed procedures obviously require significantly less computation resources and the implementation steps are relatively easier.

Table 6. Summary and Comparison of Network Design of Example 2

	freshwater (ton)	number of tanks	capacity of storage (ton)	water recovery (%)
base case	700	0	0	0
single batch (preliminary)	407.94	2	(45, 11)	41.72
single batch (improved)	397.85	2	(45, 33.75)	43.16
cyclic batch	278.8	2	(67, 56)	60.17
single batch (Chen et al.[8])	397.88	2	(45, 47.54)	43.16
cyclic batch (Chen et al.[8])	275.26	2	(42.79, 50)	60.68

8. CONCLUSIONS

Simple manual procedures have been developed in this work for designing multicontaminant water-using networks in batch processes. The proposed design approach is essentially an improved and extended version of the graphic-based approach[5] for the single-contaminant systems. The extension to the multicontaminant cases is brought about mainly on the basis of the concept of concentration potentials.[13] The proposed design objectives are to minimize the freshwater usage, the total number of storage tanks and also their required capacities. A total of ten (10) heuristic rules are provided as design aids to allocate the source-demand matches. If a periodic process is under consideration, the concentration based rules should be followed strictly and the schedule based rules are of secondary concerns. On the other hand, the priority of these two types of allocation rules should be reversed if the batch water network is operated in a single-campaign mode. The implementation results in case studies show that this manual strategy is quite effective for producing near-optimal matches and the corresponding storage facilities.

The design results produced in this study have also been compared with the published solutions obtained by solving the mathematical programming models.[8] It can be found that very similar designs can be generated by both strategies. However, since a manual design procedure can be implemented easily and requires considerably less computation resources, the proposed methodology should be considered as a viable choice in practical applications.

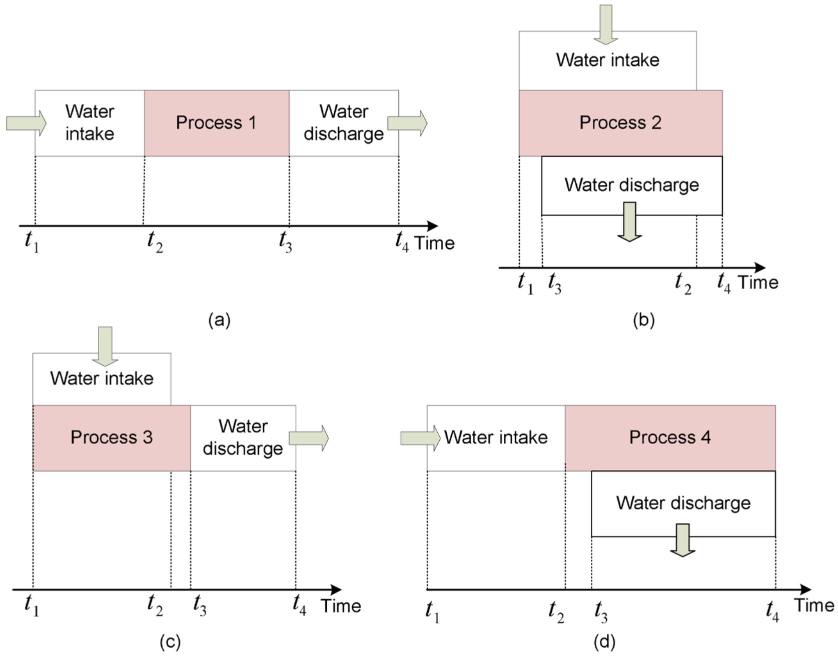

Figure A1. Types of batch processes: (a) true batch and (b–d) semibatch operations.

APPENDIX: CLASSIFICATION AND CHARACTERIZATION OF BATCH WATER-USING OPERATIONS

Similar to their counterparts in the continuous processes, the batch water-using operations can be classified to two broad categories, primarily based on the material balance and concentration constraints:[2,5,11]

- The first can be considered to be mass-transfer-based, i.e., the so-called *fixed load operation*, where water is utilized as a mass separating agent (MSA). Typical examples include the washing, extraction, and scrubbing operations. In each operation, the amounts of transferable contaminants to be picked up by water and the maximum allowable input and output concentrations are all assumed to be constants.
- A water-using operation of the second type is not mass-transfer-based, which is referenced, in this study, as the *fixed quantity operation*. For example, water could be used as a raw material and/or as a product of a batch chemical reaction. The total amounts of waters fed to and withdrawn from any such operation are assumed to be predetermined in this work and they are not necessarily equal. The outgoing water usually leaves at specific concentrations, while the incoming water is often constrained by fixed upper bounds.

In addition to the aforementioned process constraints, every batch water-using operation should be performed according to one of the time schedules presented in Figure A1. To be more specific, water is assumed to be fed to a processing unit within a given duration (t_1,t_2) and withdrawn in the interval (t_3,t_4). Although it is quite obvious that $t_1 < t_2$, $t_3 < t_4$, and $t_1 < t_4$, the precedence of t_2 and t_3 should be determined on a case-by-case basis. If water is required to be fed/withdrawn at a fixed flow rate within a predetermined time interval, the process is considered to be operated in a *semibatch* mode. Typical operation schedules of such processes can be found in Figure A1b–d. Otherwise, the water-using unit is regarded as a true *batch* process (i.e., see Figure A1a). The washing operation may be considered as an example of the former scenario. On the other hand, a typical case of the latter is the batch polymerization reaction in which water is used as a heat carrier. In this operation, freshwater is charged before the actual reaction takes place and wastewater is discharged after reaction ends. For illustration convenience, the batch and semibatch processes shown in Figure A1a–d are referenced in this paper as operations of type A, B, C, and D, respectively.

ASSOCIATED CONTENT

Supporting Information

The detailed design steps in Example 2 are provided as Supporting Information. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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NOMENCLATURE

Sets, Parameters, and Variables

D = the set of demands
K = the set of contaminants
S = the set of sources
C = concentration
CPD = concentration potential of demand

CPS = concentration potential of source
F = flow rate
M = mass load
ND = the number of elements in set D
NS = the number of elements in set S
R = allocation index
List A = the ordered list of sources according to their incipient time in ascending order
List D = the ordered list of demands according to their values of CPD in ascending order
List I = the ordered list of demands according to their incipient time in ascending order
List S = the unordered list of available sources

Superscripts

min = minimum
max = maximum
load = mass load

Subscripts

i/S_i = ith source
j/D_j = jth demand
fresh = freshwater
k = kth contaminant
out = outlet

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