A CONCEPTUAL ANALYSIS FOR RESOURCE OPTIMIZATION IN VARIABLE TIME MULTIPURPOSE BATCH PLANTS

by

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Publications

Below is a list of journal and conference papers presented in this dissertation.

Journal papers

Li, Z. and Majozi, T., 2019. Optimal Design of Batch Water Network with a Flexible Scheduling Framework. Industrial & Engineering Chemistry Research, 58(22): 9500-9511.

Li, Z. and Majozi, T., 2018. Optimal Synthesis of Batch Water Networks Using Dynamic Programming. Process Integration and Optimization for Sustainability, 2(4), 391-412.

Conference papers

Li, Z. and Majozi, T., 2018. Optimal Synthesis of Batch Water Networks with a Flexible Scheduling Framework Using Dynamic Programming. Computer Aided Chemical Engineering, 44, 205-210

Li, Z. and Majozi, T., 2017. Dynamic Programming for Optimal Synthesis of Water Networks in Batch Processes. Computer Aided Chemical Engineering, 40, 919-924.

Li, Z. and Majozi, T., 2017. Optimal Design of Batch Water Network with a Flexible Scheduling Framework. Chemical Engineering Transactions, 61, 139-144

Synopsis

Batch processing has been embraced by numerous chemical industries, such as the food, beverage, specialty chemical, and pharmaceutical industries because of its flexibility of accommodating changes in demand and responding effectively to uncertainties in market and supply chains. On the other hand, wastewater generated by batch processes depends on the specific tasks. Thus, the methods of wastewater minimization developed for continuous processes do not apply to batch processes. Few studies based on insight-based techniques have been reported to address wastewater recovery issues for flexible batch processes. The flexible batch process refers to that in which the durations of batch operations are treated as variables, not parameters. Therefore, a conceptual analysis was performed in this work to address the wastewater minimization in batch plants with flexible scheduling.

A dynamic programming approach was first proposed to design a batch water network based on predefined scheduling. Insight from these results could assist the designer in rescheduling operations to maximize water recovery through direct water reuse. However, the extent of performance improvement is limited because the rescheduling process only involves a few operations, not all of the water operations. Thus, the dynamic programming method was extended to flexible batch processes in which only durations of batch operations are given. The difference is that in the former method, the stage is determined by the timings of water operations, while for the latter approach, the stages are identified based on the inlet concentration of water operations.

Although dynamic programing approach, as an algebraic method, could provide a graphical representation of the targeting process, it is difficult to find the optimal solution when faced with complex problems. A match ranking matrix approach was proposed to prioritize matches between water sources and sinks. Batch water network could be synthesized by choosing optimal matches between water sources and sinks. Besides, a hybrid method of combing water pinch analysis and match ranking matrix method was presented to design batch water network, which takes advantages of graphical representation of pinch analysis and insight for the design of batch water network from match ranking matrix method.

Finally, the main conclusions and future work are summarized. These conceptual methods in this work could be used to address the wastewater minimization in flexible batch plants.

Content

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List of Acronyms

CIS	Common intermediate storage
DP	Dynamic programming
FIS	Finite intermediate storage
HQR	Higher quality region
LP	Linear Programming
LQR	Lower quality region
MEN	Mass Exchange Network
MINLP	Mixed integer nonlinear programming
MILP	Mixed integer linear programming
NLP	Non-linear programming
NIS	No intermediate storage
RTN	Resource task network
S-graph	Schedule-graph
SK	Water sink
SR	Water source
SSN	State sequence network
STN	State task network
TWN	Total water network
UIS	Unlimited intermediate storage
WSD	Water source diagram

1

INTRODUCTION

1.1 Background

Water scarcity is becoming a threat to sustainable development all over the world due to increasing water demands and the effects of the degradation of water quality caused by human activities. According to the report, about four billion people are suffering from water scarcity at least one month of the year, as shown in Figure 1.1. About half a billion people all over the world suffer from severe water scarcity all year round (Mekonnen and Hoekstra, 2016). South Africa is a water-scarce country in which only 13% of the land is arable, and the population experiences significant disparities in access to clean water (Gulati *et al*., 2013). Cape Town is the second-most populous city in South Africa. In 2018, the government of the city estimated that it could become the first major city in the world to have no water supply (Maxmen, 2018). Finally, the real "Day Zero" did not happen because of the coming of the rainy season. Although it was a false alarm, it has affected the lives of residents and the regular operation of industries due to water shortage. It also indicates that water crisis is not just a concept perceived in mind, but a reality.

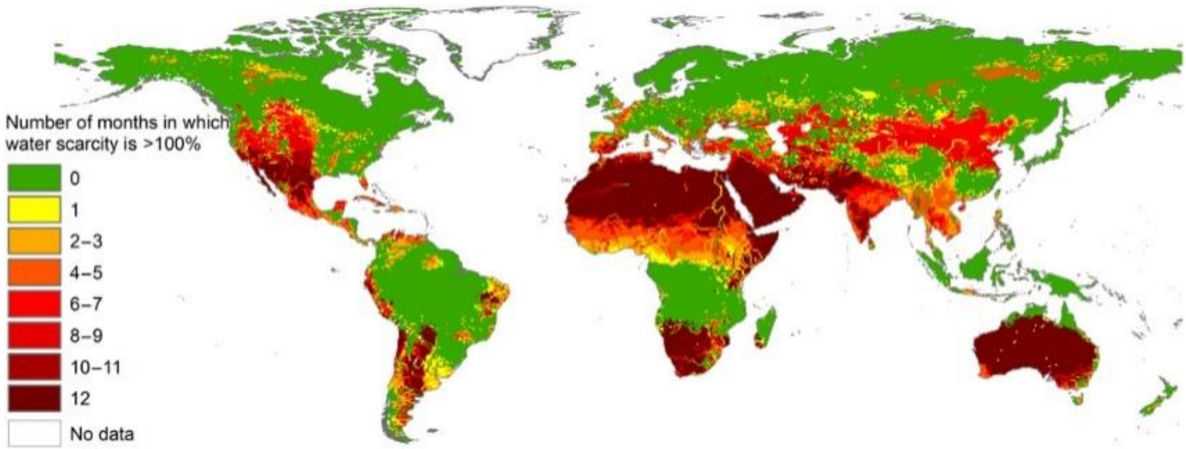

Figure 1.1 The distribution of water scarcity area (*Mekonnen and Hoekstra, 2016)*

The increasing climate variability and uncertainties caused by global warming are contributing to reducing the sustainability of water resources. Furthermore, the water scarcity will have significant impacts on the food provision and energy supply due to the water-energy-food nexus. It is projected that annual precipitation in southern Africa will be decreased by as much as 20% by the 2080s (Conway *et al*., 2015). According to results of the evaluation of water-energy-food nexus for BRICS countries, i.e., Brazil, the Russian Federation, India, China, and South Africa, the relationship between carbon dioxide emissions and economic growth for Brazil, India, and South Africa can confirm the Environmental Kuznets curve hypothesis (Panayotou, 1993). These countries should construct an adequate water resource management to enhance agricultural productivity (Ozturk, 2015). The chemical industry is the largest of the manufacturing industries in the world and is central to the economic growth of South Africa. It contributes around 5% to the GDP of South Africa and nearly 25% of manufacturing sales in 2016/17 (SA Year Book 2016/17). Though the chemical industry provides a common commodity for the people, it also consumes huge quantities of energy and water and discharges wastewater to the environment. Also, stringent regulations and social pressures have created the need for improving the efficiency of water utilization in the chemical industry and preventing the deterioration of the water system via wastewater minimization.

In general, according to the products, two different processing modes are used in the chemical industry, i.e., continuous and batch processes (Rippin, 1993). For continuous processes, raw materials and products are operated continuously at known flowrates. The states of the plant and operating conditions for the continuous processes are not changing along the time horizon. Therefore, continuous processes are usually used to produce typical products on a large scale, such as petroleum refineries, natural gas processing plants. However, in batch processes, materials are treated in finite quantities. Raw materials are feeding the vessel and then react for a given duration until physical properties of the production is achieved. Finally, the production is then discharged to the storage tank for delivery. Thus, batch processes are widely used to process low volume, high value-added products, such as agrochemical, pharmaceuticals, specialty chemicals, and cosmetics. In general, new products are initially manufactured in batch processing mode and then evolved to a continuous process because of upgrading technologies and market acceptance. Hence, this work focuses on wastewater recovery for batch process.

There are two categories of batch processes, i.e., multiproduct and multipurpose batch process. In the multiproduct batch plant, all of the batches are handled in the same way, and processing sequences of batches in each unit are identical. In multipurpose batch plants, on the other hand, the same unit could process different products and the processing paths of the batches may be different. For multipurpose batch processes, various tasks can be performed in the same unit, resulting in the problem of how to allocate the unit optimally to the tasks. Thus, most of the research focuses on multipurpose batch process as compared to multiproduct batch processes, and the industry pays more attention to multipurpose batch processes. In this work, conceptual analysis is performed to maximize water recovery for multipurpose batch processes by rescheduling the batch operations.

1.2 **Motivation**

The first motivation behind this work is that in the chemical industry, most industrial plants are processing through continuous operations because it is suitable to produce products on a large scale. Batch processing is also adopted in the chemical industry due to its ability to adjust to changing market conditions and capability of producing high value-added and small quantity products. In general, consumers prefer tailor-made products, rather than the generic products. This trend provides an opportunity for expanding the batch processing model in the industry.

In batch processes, freshwater is usually used to wash the units after production. Thus, the composition of the contaminant in wastewater is complex and changing all the time. Also, the discrete nature of batch operations makes wastewater treatment uneconomical as compared to the continuous process. Industrial activities not only consume freshwater resources but also discharge wastewater into the environment. This results in the fact that water ecosystem is unable to maintain its natural, original state. Furthermore, stringent legislation on industrial wastewater has led to an increase in effluent treatment costs. Thus, development of a systematic tool to maximize water recovery, reduce freshwater intake and to minimize wastewater discharge from industrial plants is necessary.

The final motivation for this work is that most work on the synthesis of batch water networks focuses on predefined scheduling. In batch processes, the recipe of production is always changing to adjust to the demand of the market, resulting in a change in the water network. Therefore, it is required to develop a systematic method of considering water recovery and process scheduling simultaneously.

1.3 **Problem statement**

The problem to be addressed by this research can be stated as follows.

Given:

- Production scheduling data, such as mean processing time, and the relationship between different productions, i.e. recipe,
- Limiting water data, including water quantity and water quality constraints of operations,
- the maximum capacity of the storage vessel,
- the performance of the regeneration units, such as removal ratio or outlet concentration and
- Time horizon of interest

The objective is to find an optimal production schedule that achieves the minimum amount of freshwater consumption by employing water reuse/recycling and regeneration scheme.

1.4 Research objectives

The objectives of this research are summarized as follows. It is to present a general conceptual approach that could be used to optimize water utilization in variable time multipurpose batch plants. In the analysis, variable time refers to the scenario that the duration of each batch process is given, rather than the starting and ending times of operations. Consequently, starting and ending times become optimization variables, hence the name ‘variable time’. Freshwater could be minimized through water reuse/recycling and regeneration by rescheduling the process operations. Most of the work in published literature in the area of water optimization in multipurpose batch plants tends to be steeped in mathematical modeling, with very limited conceptual analysis. This results in models that are very difficult to solve at best and almost impossible to solve at worst. The main contribution, therefore, is the development of models that are solvable in real-time or reasonable time.

1.5 Scope of work

The main objective of this research is to develop a general framework for the synthesis of the water network in a flexible batch plant. This work proposes a dynamic programming approach for the design of a batch water network based on predefined scheduling. Insights from these results could assist in rescheduling operations to maximize water recovery through direct water reuse. However, the improvement of targets is limited because rescheduling only involves a few operations and, as a consequence, inherently entails fewer degrees of freedom compared to a complete scheduling problem. Thus, the dynamic programming method is also extended to flexible batch processes in which only duration of operations is given. Although dynamic programing approach as an algebraic method could provide a graphical representation of the results, insights from the analysis are sometimes not obvious, depending on the complexity of the problem. A match ranking matrix approach is then proposed to prioritize matches between water sources and sinks. Based on the ranking of matches, batch water networks could be synthesized by considering the time nature of batch processes. Besides, a hybrid method of combing water pinch analysis and match ranking matrix is presented to design batch water networks. This hybrid method takes advantages of graphical representation and conceptual nature of pinch analysis. Finally, the main conclusions and future work are summarized.

1.6 **Thesis structure**

The outline of this thesis is arranged as below.

Chapter 2 gives a comprehensive survey of the literature related to this work, including the topic about production scheduling, water minimization of continuous and batch processes, as well as simultaneous optimization of production scheduling and water utilization. Literature is also given on the different techniques of water minimization problems, such as insight-based methods and mathematical model-based optimization methods.

In ***Chapter 3***, a dynamic programming method is used to design an optimal batch water network with a predefined schedule. Four examples adapted from literature are demonstrated to illustrate the proposed method. Furthermore, rescheduling is then performed to maximize direct reuse and to reduce water storage.

Chapter 4 shows the extension of Chapter 3. It introduces how to use dynamic programming to design optimal batch water network with flexible production scheduling.

In ***Chapter 5***, a matrix matching method is developed to design the optimal batch water network with flexible production scheduling framework.

Pinch analysis is widely recognized as an efficient method of water recovery in continuous processes. In ***Chapter 6***, conventional pinch analysis is combined with match ranking matrix method to design optimal batch water network with flexible production scheduling.

Chapter 7 gives conclusions and recommendations for future work.

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2

LITERATURE REVIEW

In this chapter, a literature review is summarized to explain the progress of production scheduling and water minimization techniques in chemical processes. In Section 2.1, the operational philosophy for batch processes is introduced. Section 2.2 describes the techniques of production scheduling. In Section 2.3, it has briefly introduced the synthesis of water network and different water reuse schemes. Since the existing insight-based methods for the synthesis of water network mainly focus on continuous processes, water integration techniques for continuous and batch processes are reviewed in Sections 2.4 and 2.5, respectively. Section 2.6 summarizes the challenges of synthesis of water networks and future research.

2.1 Operational philosophy

The flexibility in batch processes arises mainly because of the availability of intermediate storage between processing stages in a batch plant. According to the nature of intermediate storage, there are four main operational philosophies, i.e., unlimited intermediate storage (UIS), finite intermediate storage (FIS), no intermediate storage (NIS), and common intermediate storage (CIS) (Majozi, 2010; Romero *et al*., 2004).

In general, a batch chemical process is broadly categorized into a single stage or multistage processes. For a single stage process, each stage may consist of a single unit or multiple parallel units based on the structure of processing networks. For the multistage process, it can be classified into multiproduct and multipurpose batch plants (Majozi *et al*., 2017; Reklaitis *et al*., 1996). Short-term scheduling in batch processes addresses the problems of allocating production resources to meet the product demand and managing the material transfer from one operation to another in a coordinated time. In chemical batch plants, short-term scheduling is similar to the general job-shop problems in operations research. However, there are some differences between these two activities. In chemical batch plants, additional constraints, such as the storage policy, the physical property of materials, should be considered in the production scheduling (Sanmartí *et al*. 2002). On the other hand, multiproduct batch processes follow the same sequence of unit operations. However, each batch does not have to produce the same product. The processing time of tasks corresponding to different products could be different. In contrast to multiproduct plants, multipurpose batch production does not require common processing sequences between the products (Majozi, 2010; Reklaitis *et al*., 1996).

2.2 Production scheduling

Batch processes are a widely accepted procedure in the chemical industry because of the flexibility in changing production recipe and the suitability of producing small-quantity products. The competitive pressure calls for an improved design of batch plants and better use of existing facilities. An effective production schedule must optimally allocate limited resources to tasks achieving the goal of either maximizing throughput or minimizing the total cost. There have been reported four scheduling methods for chemical processes in literature, i.e., Schedule-graph (S-graph), State task network (STN), State sequence network (SSN), Resource task network (RTN).

2.2.1 Schedule-graph (S-graph)

Most of the research in production scheduling focuses on developing general mathematical formulations. However, this general-purpose approach has limitations in its application to large-scale industrial problems in terms of computational time involved (Mokashi and Kokossis, 2002). Therefore, a few researches tried to explore the opportunities of using graph theory to solve scheduling problems.

Wu *et al*. (1999) proposed a graph-theoretic approach to determine job-shop scheduling problems. The results obtained by this graphical approach are more robust as compared to the existing mathematical methods. Mokashi and Kokossis (2002) proposed an efficient algorithm called the maximum order tree to address the product distribution problem. This graph-based method can reduce the CPU time dramatically compared to conventional methods without compromising on the quality of the solution. These graph-theoretic approaches can be used to solve scheduling problems. However, it is only applicable to job-shop problems with UIS policy.

In the chemical industry, production scheduling is different from that in job-shop problems. For example, there are many storage policies due to the characteristics of intermediate materials. Sanmartí *et al*. (1998; 2002) proposed the S-graph method to deal with scheduling problems with NIS policy. In the S-graph method, the graph nodes are the tasks of operations, while the arcs connecting different nodes are the precedence relationship of tasks. Both NIS and UIS policies can be represented by choosing the appropriate precedence relationships. Besides, other algorithms, such as branch-and-bound method can be easily incorporated into the S-graph to solve the problem.

The most widely utilized mathematical programming methods for tackling the scheduling problem are expensive in terms of computational time. Because S-graph is flexible in considering various production structures and having advantages of graph theory, it has been used to perform production scheduling in the batch plant. For example, Holczinger *et al*. (2002) applied the S-graph to solve the scheduling problem in multipurpose batch processes. An acceleration algorithm was developed to increase computational efficiency to find the optimal solutions for significant scheduling problems. Hegyháti and Friedler (2011) listed several combinatorial algorithms that can be combined with S-graph to address the scheduling problem of batch processes, which can be used to solve practical problems with additional requirements. Romero *et al.* (2004) modified the existing S-graph representation by introducing a new type of node for representing CIS policy. A set of rationales is defined to accelerate the solution strategy by reducing the searching space. In the work of Majozi and Friedler (2006), S-graph was used to optimize the production schedule for a multipurpose batch plant by maximizing the throughput. A guided search algorithm is proposed to ensure that the results are the global optimum. However, their paper only considered the non-intermediate storage policy. Hegyháti *et al*. (2009) considered scheduling problems with complicated recipes based on S-graph. NIS, ZW, and CIS policies are taken into account in their paper. Compared to mathematical programming, S-graph can avoid the occurrences of cross-transfer, which can lead to a real optimum (Hegyháti *et al*., 2009). Furthermore, S-graph can deal with production scheduling with uncertainty. Laínez *et al*. (2010) considered the uncertainties caused by exogenous factors in the scheduling process for a batch process based on the S-graph approach.

2.2.2 State task network (STN)

Kondili *et al*. (1993) proposed the STN representation to capture the characteristics of production scheduling in batch plants. In the representation, two types of nodes are defined, i.e., task nodes that represent individual batch operations and state nodes that indicate raw material, intermediate and final products. The binary variables in the formulation imply whether the tasks are implemented in a specific piece of equipment at a specific event point or not. This representation can consider the general production operation, involving stream mixing and splitting, material reuse and recycling, storage policies, and so on. The scheduling problem is formulated as a mixed-integer linear programming (MILP) model because of the deployment of binary variables. However, in the work of Kondili *et al*. (1993), a discrete-time representation was employed where the time horizon is partitioned into many intervals with equal duration. It usually leads to a large model and results in sub-optimal solutions (Floudas and Lin, 2004). Bose and Bhattacharya (2009) proposed a discrete-time STN model to deal with the scheduling in multi-stage multi-product continuous facilities. Because discrete-time representation usually leads to a large model, various specific techniques were developed by Shah *et al*. (1993) to enhance computational efficiency.

Although significant improvements have been made on the discrete-time model, the assumption of constant processing times force operations occurring at the start or end of a specific time interval, preventing its full application in the industry. Therefore, the continuous-time STN formulation was developed to overcome the limitations of discrete-time models. Compared with general discrete-time STN formulations, continuous-time STN model is faster in CPU time (Maravelias and Grossmann, 2003a, 2003b, 2006).

2.2.3 State sequence network (SSN)

SSN was proposed by Majozi and Zhu (2001) to perform short-term scheduling for batch plants in order to reduce the model size. In the representation, only state nodes are required because the tasks and units can be eliminated without any loss of accuracy. Thus, the SSN based model requires fewer binary variables (Majozi, 2010). Based on SSN representation, resource allocation model was incorporated into the overall plant model to exploit resource conservation and optimal scheduling (Zhu and Majozi, 2001). Because the SSN representation has fewer binary variables, it has been used as a cornerstone for the optimization of batch process scheduling in wastewater minimization, and heat integration (Majozi, 2010; Majozi, 2017).

2.2.4 Resource task network (RTN)

To describe all resources in a unified manner, Pantelides (1994) proposed a unified mathematical formulation to represent production scheduling for batch plants. It is to model a mixed production facility as a collection of facilities performing a variety of tasks which consume some resources and generate others. The resources can be feeds, intermediates, products, utilities, equipment, storage facilities, workforce, etc.

Zhang and Sargent (1996) extended concepts of the RTN to a mixed production facility and determined the optimal operating conditions. In the work of Castro *et al*. (2003), discrete- and continuous-time were used to determine optimal cyclic operations for a batch plant based on

RTN. Results show that discrete-time formulation is more accessible to solve to optimality than the continuous-time counterpart. Chen and Chang (2009) modified the work of Castro *et al*. (2003) and proposed an integrated formulation for multipurpose batch processes, which considers production scheduling and heat recovery problems. Furthermore, Chen *et al*. (2011) presented an integrated model for multipurpose batch plants by simultaneously considering scheduling and water recovery based on RTN approach. Castro *et al*. (2013) provide a generic modeling framework for production scheduling under energy constraints based on RTN. Castro and Grossmann (2014) addressed the modeling of crude oil operations in refineries based on RTN representation.

2.3 Synthesis of Water Networks

Rudd (1968) proposed a system principle to instruct the chemical engineer how to combine different processes to achieve the assigned task. This concept is the initial definition of *process synthesis*. This definition has evolved over the past few decades. The commonly accepted definition of *process synthesis* is discrete decision-making activities of choosing some available elements to obtain an optimal solution for a given design problem from a systematic perspective (El-Halwagi, 1997). There are two crucial areas in process synthesis, i.e., mass exchanger network synthesis (mass integration) and heat exchanger network synthesis (heat integration). Within the framework of mass integration, water integration serves as a special case. This review focuses on water integration for the continuous and batch processes.

In the synthesis of water networks, there are three subclasses: (1) water reuse/recycle; (2) water regeneration; (3) total water network synthesis. In the total water network, water reuse subsystem, regeneration unit, and wastewater treatment unit are integrated from a systematic perspective. The description of these subclasses is described below.

2.3.1 Water reuse/recycle

Figure 2.1 depicts a water reuse network for the process industry. It allows water to be directly or indirect reused in other processes where the contaminant levels of reusable water are within the process limits. In Figure 2.1 (a), the reusable water is directly reused in other processes, while in Figure 2.1 (b) the reusable water is first sent to the storage and then reused by other processes. Indirect reuse is a typical case in batch processes because of the time constraint. In a water reuse network, reusable water can be blended with freshwater or reusable water from other processes to meet the contaminant levels of water-receiving processes.

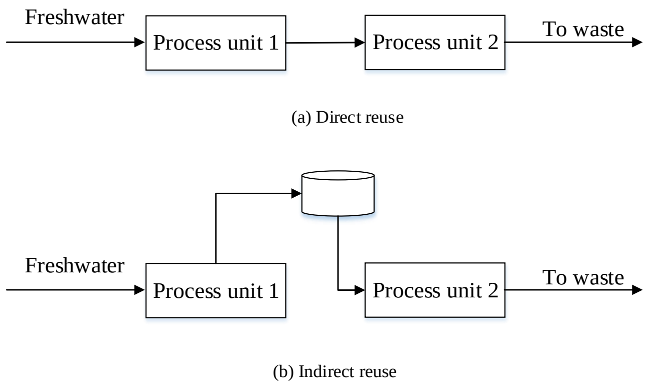

Figure 2.1 Batch water network with reuse scheme

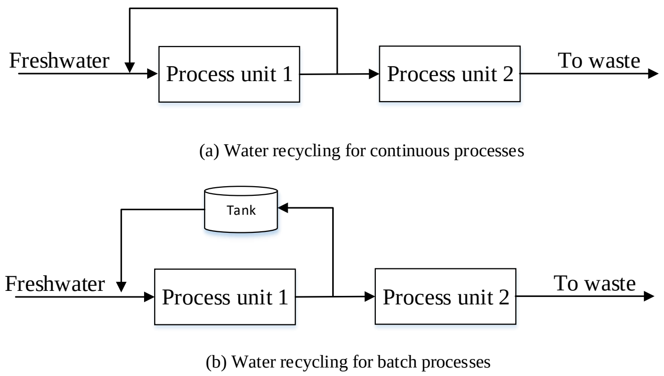

Figure 2.2 Batch water network with direct water recycling scheme

Figure 2.2 shows the water recycling scenario where reusable water is reused in the same process. In the direct recycling scenario, wastewater from the process is partially treated and then sent back to the system. Freshwater is usually used to mix this reusable water to meet the contaminant limits of water-receiving processes. Because water recycling can bring in contaminant accumulation and demand more freshwater, this scheme is thus not used in industrial activities. Figure 2.2(a) represents the water recycling scenario for continuous processes, while in Figure 2.2(b) the reusable water is first sent to the tank and then mixed with freshwater to feed the water-using operation.

2.3.2 Regeneration reuse/recycle

Figure 2.3 presents the regeneration reuse scenario where wastewater is treated to remove the contaminants and then reused in other processes (Wang and Smith, 1994a). The regenerated water might be directly reused in other operations or mixed with wastewater from other processes and freshwater to feed water-using operations. In regeneration reuse scenario, the regenerated water is not allowed to reenter the processes where the regeneration water comes from to prevent the accumulation of harmful contaminants in the activities of water cascade utilization. However, sometimes the regenerated water can reenter the process where this water is previously reused before regeneration; this refers to a different scenario of wastewater minimization, as shown in Figure 2.4.

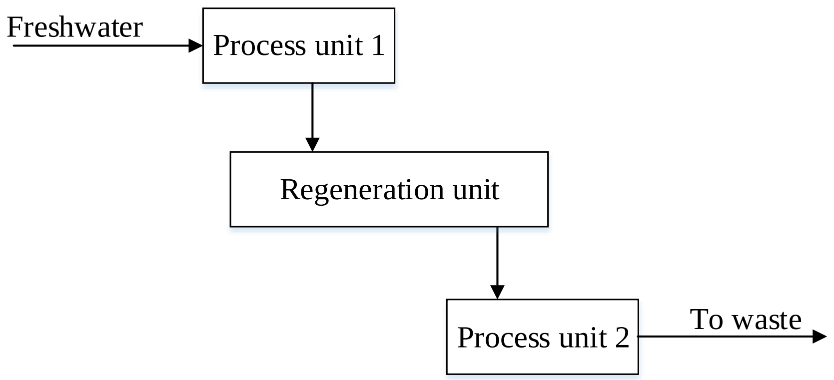

Figure 2.3 Water network with regeneration reuse

Regeneration recycling refers to the situation where wastewater is partially treated and recycled in process units where it was generated (Wang and Smith, 1994a). Although regeneration can, to some extent, reduce wastewater generation, it might not be allowed in practice due to the accumulation of contaminants. In practice, two or more methods are combined to achieve the target of wastewater minimization. Although the description above explains how to reduce freshwater requirement, systematic approaches are still required to determine the target. The water integration techniques of combining the schemes above are introduced in the following section.

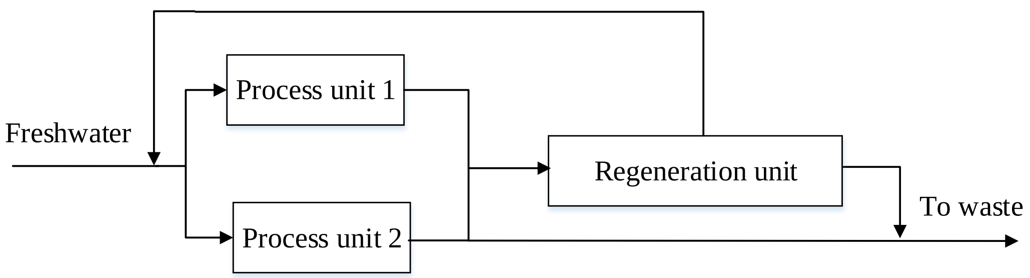

Figure 2.4 Water network with regeneration recycling

2.3.3 Total water network

In previous subsections, direct reuse/recycling and regeneration reuse/recycling are introduced. Here, the concept of total water network (TWN) is introduced by integrating direct reuse/recycling and regeneration reuse/recycling in the same water system. Kuo and Smith (1998a) proposed the concept of TWN for fixed load problems. As shown in Figure 2.5, the TWN includes three subsystems, i.e., direct reuse/recycle, regeneration, and waste treatment.

Because these water schemes consider water utilization from different views, it is necessary to treat them as an overall framework. If the potential of water recovery is maximized through water reuse/recycle scheme, employing a regeneration unit for partial purification of the wastewater could lead to further reduction of freshwater consumption. In some cases, the industrial plants utilize freshwater to dilute the wastewater to meet the emission standard. Because of the increasing cost of freshwater and stringent regulation on the environment, wastewater treatments are employed to treat the effluent to protect the environment and reduce freshwater consumption.

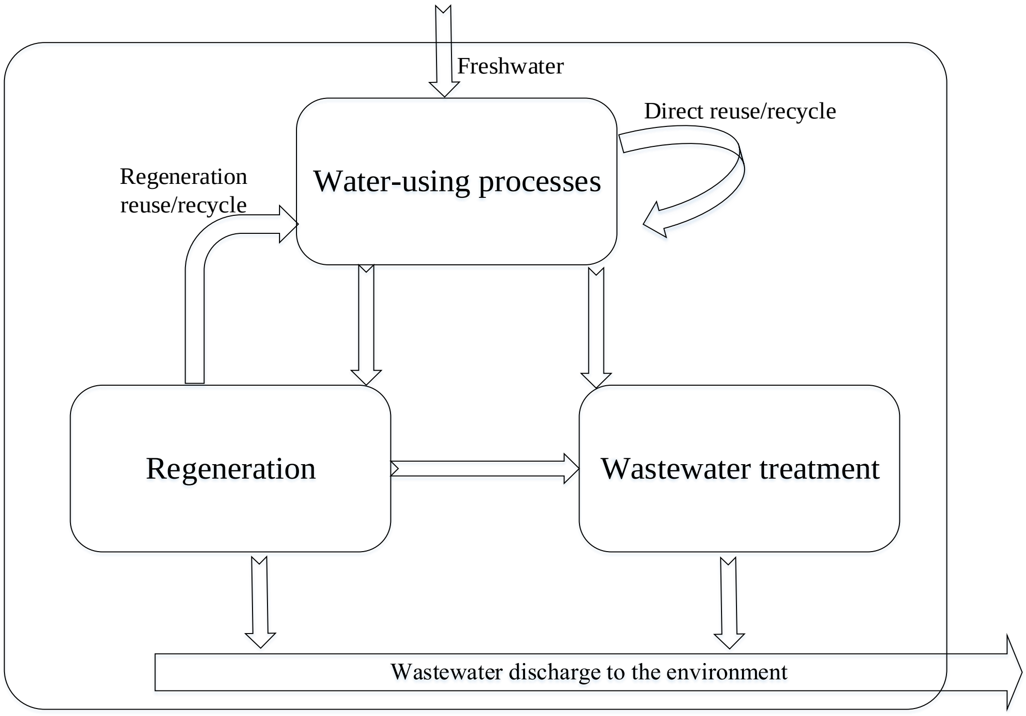

Figure 2.5 Schematic of the total water network

2.4 Water integration techniques for continuous processes

Mass integration, as a branch of process integration, provides a systematic methodology for optimizing the mass flow within a process based on setting performance targets by splitting, mixing different streams and species (El-Halwagi, 1998; Klemeš *et al.*, 2013). El-Halwagi and Manousiouthakis (1989) proposed a graphically based approach to maximize mass exchange between different mass transfer operations, such as absorbers, extractors. Water integration is a specific application of mass integration in water systems. Many methods for the synthesis of water networks have been reported in the literature. These approaches can be divided into two groups, i.e., insight-based techniques and mathematical programming methods.

2.4.1 Insight-based techniques

2.4.1.1 Graphical methods

Graphical methods provide a systematic view of determining the performance target of the system without detailed design. Besides, the physical insights provided by the graphical representation could assist chemical engineers to implement the detailed design in practice, while mathematical programming only provides the results without giving more details of the computation processes. The development of graphical methods has two stages. In the first stage, the development mainly focuses on the composite curve of Wang and Smith (1994a) to cope with fixed mass load problems. In the second period, many techniques are proposed to deal with the design of the water network. These methods are no longer limited to fixed load problems, but fixed load and fixed flowrate problems.

Wang and Smith (1994a) proposed the water pinch analysis to minimize wastewater generation in process industries. In their method, concentration is analogous to temperature, while the mass load is analogous to enthalpy. The limiting composite curve is constructed by combing all the segments of the processes on concentration vs. mass load diagram. A water supply line is drawn from the origin and rotates in an anticlockwise direction until it touches the limiting composite curve. The target of minimum freshwater flowrate is determined by the reciprocal of the slope of the water supply line (Wang and Smith, 1994a). The bottleneck of water recovery for the system can be determined from pinch point. However, the limitation is that the assumption of mass transfer is not always applicable to some non-mass transfer processes. Many processes, such as reactors, boilers, and cooling towers, do not have mass transfer phenomena. Therefore, another method was developed by Dhole *et al*. (1996) to determine the freshwater targets, which consists of supply composite and demand composite curves.

Although their method can identify the target graphically, the results depend on the mixing of different sources, which could lead to inaccurate solutions. The limitation is that there exist many local pinch points in the approach of Dhole *et al*. (1996). This observation could obscure the physical meaning of the pinch point and cannot provides precise information to assist the designer in designing an optimal water network. In the method of Dhole *et al*. (1996), the operations of water splitting, and mixing are not considered, which could reduce the potential of water recovery. A Load Table method was developed by Olesen and Polley (1997), in which the penalty of freshwater caused by splitting can be determined. Furthermore, Olesen and Polley (1996) considered water transfer between different plants based on the Load Table.

Sorin and Bédard (1999) proposed a two-stage approach to design water reuse networks. In the first step of their method, the target and the pinch point can be determined using the Evolutionary Table. In the second step, some special rules are defined to guide the mixing operation of water sources above and below pinch point in the network design process.

In order to avoid confusing representation of water operations, Castro *et al*. (1999) presented a simultaneous targeting-design algorithm called *water source diagram* (WSD) to attain minimum flowrate. However, this method is unable to determine the targets in regeneration scenario separately. Gómez *et al*. (2001) proposed a concentration grid method for the synthesis of water-using networks. The concentration grid is similar to WSD in Castro *et al*. (1999). But it represents the water sources in a different manner. Gomes *et al*. (2007) made some improvements for the WSD method, and thus, the modified WSD is more general for minimizing wastewater in process industries. Because WSD offers a dynamic and flexible framework for water management, Ulson de Souza *et al*. (2009) extended the WSD method to a petroleum refinery. The scenarios of maximum water reuse, regenerative end-of-pipe treatment, and differentiated regeneration were studied. Ulson de Souza *et al*. (2010) modified the WSD method and applied to a textile plant to reduce water requirement through water reuse scheme. A reduction of as much as 64% of water can be reduced compared to the scenario without water reuse. Gomes *et al*. (2013), and Calixto *et al*. (2015) also applied the WSD method to multiple contaminants systems. Besides, WSD can be applied to the hybrid systems with both mass transfer and non-mass transfer operations, as well as water gain/loss operations (da Silva Francisco *et al*., 2015; Francisco *et al*., 2018).

By the analogy between the transfer of mass and heat, El-Halwagi and Manousiouthakis (1989) developed a systematic procedure for the synthesis of cost-effective mass-exchange networks (MENs). First, pinch points are identified based on the thermodynamic analysis, which limits the extent of mass exchange between the rich and the lean streams. Next, the network which is designed based on the insights from the first step is evolved to be practical by considering more constraints. In their subsequent paper, an automatic approach was developed to generate cost-effective MENs (El-Halwagi and Manousiouthakis, 1990). The automatic method is based on a two-stage procedure. First, thermodynamic constraints are formulated as an LP problem. Next, binary variables are employed to choose the suitable match between the rich and lean streams to achieve the targets in the first step and to minimize the number of mass-exchange units.

In industrial processes, not all water-using operations involve mass transfer phenomena. In some cases, some operations only have water intake or waste discharge. Therefore, the problem of water usage and discharge can be presented by a source and a sink. Although Dhole *et al*. (1996) employed water demand and supply composite curves, pinch points defined in their method cannot represent the bottleneck of the problem. Some pinch points could be eliminated by mixing some water streams. To overcome these limitations, a *material recovery pinch diagram* was developed by El-Halwagi *et al*. (2003) to target the minimum flowrate of the fresh resource. It provides a systematic, and graphical method for the targeting and can yield the results without tedious iterations. Some important information, such as the maximum of resource recovery, and the number of unused materials, can be attained from the diagram. The same method was proposed separately by Prakash and Shenoy (2005b) almost at the same time. Prakash and Shenoy (2005b) also proposed a new design procedure for the synthesis of water networks based on nearest neighbors principle. For a specific water demand, the water sources to be chosen to feed this demand should be the nearest available neighbors in terms of concentration. A concept of source shifts was introduced by Prakash and Shenoy (2005a) to yield simpler networks. It could assist the designer in evolving these alternative networks systematically with fewer connections at the expense of a freshwater penalty.

Dunn and Wenzel (2001) introduced a source-sink mapping diagram to determine the water reuse and recycling network. It is convenient to design a simple water network using the source-sink mapping diagram, while for complex processes, the design of the piping network is complicated. Feng and Seider (2001) employed the water main to simplify the piping system. Also, internal water main was employed when designing multi-contaminant water network for water reuse scheme (Wang *et al*., 2003) and regeneration recycling scheme (Cao *et al*., 2004).

These methods mentioned above provide a systematic view for targeting the minimum freshwater requirement based on the limiting composite curve. Except for the graphical representation of Wang and Smith (1994a), different graphical techniques were also proposed. Bandyopadhyay *et al*. (2006) developed a *source composite diagram* to minimize wastewater generation for water systems with fixed-mass load and fixed-flowrate operations. In addition to the target of freshwater, some critical factors, such as the minimum effluent flowrate for treatment, the minimum contaminant removal ratio, and the minimum number of treatment units can be determined. In the work of Bandyopadhyay *et al*. (2006), graphical representation of the method, as well as its analytical algorithms, were presented in detail to explain how to attain these targets. This graphical approach has been applied to water management, hydrogen management (Bandyopadhyay, 2006). Also, Bandyopadhyay and Cormos (2008) applied the *source composite diagram* to water systems with a regeneration unit. However, this graphical approach has the same limitation as to other graphical methods. It only applies to water systems with a single contaminant. Shenoy and Bandyopadhyay (2007) extended the method to a water-using system which was supplied by multiple resources. They found that maximizing the utilization of resources with the least unit cost does not lead to the optimal water network with the minimum operating cost.

Except for these graphical methods for water allocation network, some approaches for wastewater treatment have also been developed. Wang and Smith (1994b) proposed a graphical approach for the synthesis of a distributed wastewater treatment network. If cost decreases continuously for decreasing flowrate, the proposed method can determine the minimum cost required to be treated wastewater. A treatment process network can be designed to achieve the flowrate targets with the minimum total treatment costs according to the design rules. For example, streams having a concentration higher than pinch point are fully treated. Those having the concentration equal to pinch point are partially treated, and partially bypass treatment and those starting below the pinch completely bypass treatment. The limitation of this work is that sometimes the minimum flowrate does not lead to the minimum treatment costs. This is because the relationship between wastewater flowrate and treatment cost is not linear. Also, the design for multiple treatment processes was not addressed clearly. Furthermore, it is assumed that there is no water loss for the flowrate in the treatment process. This assumption is not true for some wastewater treatment processes, such as the membrane technologies.

Hence, Kuo and Smith (1997) considered the synthesis of effluent treatment networks with multiple treatment processes. In the targeting processes, some treatment lines are allowed to cross the composite effluent curve on an individual basis, while the composite treatment curve must not cross the composite effluent curve. They also extended the method to retrofit cases. However, for a water system with multiple contaminants, their method cannot guarantee that the minimum flowrate is obtained because the designed network is achieved by iterative procedures of targeting and network design. In their subsequent paper, Kuo and Smith (1998a) introduced a new method to explore the regeneration opportunities. In their method, two different groups were defined, i.e., one group only requires freshwater, and the other requires freshwater and regenerated water. A few rules are set to migrate the water transfer between these two groups. The target of freshwater consumption, regenerated water, as well the number of regeneration unit, can be determined.

Kuo and Smith (1998b) proposed a graphical method which considers water-using subsystem and wastewater treatment subsystems as a whole. Their method offers insights to quantify the trade-off between water minimization and treatment systems. Wang and Smith (1994a) pointed out that the regeneration process must be put in the right place. Otherwise, it leads to an increase in the flowrate of regeneration.

In general, the regeneration concentration is located at the pinch point. If not, the complexity increases, making targeting more complex. Feng et al. (2007) analyzed the effect of different regeneration concentration on the targets of freshwater and regenerated flowrate. In their method, sequential optimization strategy was adopted to obtain targets of freshwater consumption, minimum regenerated water flowrate, and optimal generation concentration. First, the outlet concentration of the regeneration unit is fixed. Next, a sensitivity analysis was carried out to evaluate the effect of the outlet concentration on these targets. Based on this method, Bai *et al*. (2007) considered the total regeneration and partial regeneration scenarios. Furthermore, an improved mass problem table was introduced to identify targets of freshwater, regeneration water, and regeneration concentration.

Tan and Manan (2006) considered the retrofit of regeneration water networks. First, optimization schemes were chosen based on the insight provided by the targeting process. Next, an economic analysis of these process changes was performed to find the optimal solution with the minimum total cost. In their subsequent work, this method was applied to retrofit of water networks with regeneration for a papermaking process (Tan *et al*., 2007). In the work of Wang and Smith (1994a), mass load decomposition, and concentration decomposition were used to determine freshwater requirements of water-using processes. Bai et al. (2010) summarized some decomposition rules and combined with the mathematical model to optimize water system with regeneration reuse. Although process decomposition leads to the reduction of freshwater to some extent, it complicates network structure and results in infeasible solutions about economic concerns.

In water pinch analysis, the composite curve is first drawn. Next, the water supply line with the steepest slope is chosen as the desired objective. Finally, the target of freshwater requirement is determined by reversing the slope of the desired water supply line. The targeting process is partially automated. Some efforts have been made to implement pinch analysis automatically. For example, Jacob *et al*. (2002) formulated the pinch analysis as an LP model. The targeting process is fully automated and can cope with significant size problems. It is helpful for the application of pinch analysis in practice. On the other hand, most of the paper based on graphical techniques focused on the utility targets, rather than costs. It thus does not necessarily lead to the minimum capital cost for the network with the minimum freshwater consumption.

A graphical method was proposed by Hallale and Fraser (1998) for targeting the minimum cost before detailed design. In their method, the minimum number of trays for a network of absorption columns was initially determined. Next, the capital cost compatible with this target was accounted for through the trade-off analysis between operating and capital costs. Sujak *et al*. (2017) presented a cost-effective method to design optimal water networks that consider economic factors while exploring all of the water minimization options. The advantage of this method lies in the simultaneous consideration of water management at all hierarchical levels and the economic analysis of water minimization schemes that achieve the minimum target of freshwater to attain a maximum net profit.

2.4.2 Algebraic methods

Graphical methods, such as composite curves are helpful for chemical engineers because they provide physical insights for the overall potentials of resource recovery. However, the targeting process will be cumbersome if the size of the problem is significant. Hence, numerical targeting tools have been proposed because of the advantages of graphical methods in the view of accuracy and speed (Manan *et al*., 2004).

The composite curves presented by Wang and Smith (1994a) can find the pinch point and determine the minimum freshwater requirement before detailed design. However, in their method, only one pinch point was defined. In the paper of Dhole *et al*. (1996), many local pinch points were defined. This observation could obscure the designers and complicate the problem because the multiple pinch point can confuse the designer, which is the global pinch point. To rectify the shortcoming of these methods, a two-step procedure was proposed by Sorin and Bédard (1999). The Evolutional Table was used to identify these targets for the problem. However, Evolutionary Table failed to find the true pinch point if more than one global pinch points existed. In the work of Hallale (2002), *water surplus diagram* was proposed for the targeting process. This method is also tedious and time-consuming to plot as compared to the other forms of composite curves. Thus, a numerical equivalent form, i.e., *water cascade analysis*, was developed to simplify the targeting process (Manan *et al*., 2004). A similar cascade representation based on the *load interval diagram* was proposed by Almutlaq and El-Halwagi (2007) to identify rigorous targets for water-using systems. Aly et al. (2005) modified the *load interval diagram* and developed the *load problem table* to obtain freshwater requirement of water systems.

In water-using systems, water quality is usually characterized by the contaminant concentration. In practice, except for the concentration, the property is also used to represent the quality of streams, such as density, electric resistivity, viscosity. A property-based algebraic technique was developed by Foo *et al*. (2006) to identify the targets for material reuse network. Hortua *et al*. (2013) proposed an integrated approach for simultaneous optimization of property and mass integration. However, in their work, only water reuse and recycling were taken into account, while water regeneration was not considered, which may further reduce the total cost. An Extended Composite Table Algorithm was developed by Parand *et al*. (2014) to determine the targets of the total water network. A fixed post-regeneration concentration was set to obtain freshwater and regeneration flowrate. The trade-off analysis between freshwater and regeneration flowrate was analyzed by relaxing post-regeneration concentration.

When designing the water networks, the first step is to determine the targets by pinch analysis or algebraic methods. The designer then utilizes the insights from the targeting process to design the networks. In this process, a feasible network is attained by removing the loops created by the matching procedure. However, the loop breaking depends on the problem size and the experience of the designer. When the number of operations becomes more prominent, and the loops overlap, it is difficult to break all of the loops. Furthermore, sometimes the loop breaking could bring unrealistic splitting of operations.

Hence, Savelski and Bagajewicz (2000) introduced the necessary conditions of optimality for assisting the designer in checking the feasibility of matches. These conditions can be used as heuristic rules for the design of water allocation problems. Based on these rules, an LP model was developed by Bagajewicz and Savelski (2001) to determine the target, and a MILP formulation was proposed to choose the optimal matches. Also, Bagajewicz *et al*. (2000) incorporated the necessary conditions into the model to design the multiple-contaminant water network. Teles *et al*. (2008) developed a sequential approach for multiple-contaminant water-using networks. In their method, a superstructure was established to account for all possible connections among different water-using operations. Then, the water requirement of each operation is met in sequence from the first to the last element. Although this approach can transform NLP problems into a succession of LP problems, the interaction between different operations was not considered. Pan *et al*. (2012) presented an iterative method for the synthesis of optimal water networks with regeneration recycling. This method is capable of designing networks with known outlet concentrations and given removal ratios. Kim (2012) proposed a combined approach to assess different water schemes. They pointed out that costs associated wastewater effluent treatment are the key determinant for choosing the regeneration unit.

2.4.3 Mathematical optimization-based approaches

Although graphical and algebraic methods are powerful and straightforward, their inability to account for multiple contaminants is a common drawback which limits its application. Hence, mathematical programming has been used to cope with the synthesis of water network (Bagajewicz, 2000; Foo, 2012; Klemeš, 2012, 2013). Mathematical programming follows a general superstructure that represents all possibilities of connections for the system under consideration. The principle of the superstructure-based methods is fundamentally the same. The NLP or MINLP model formulated for the superstructure is optimized by removing its redundant constraints and then generate a final result. Thus, the desired design is automatically obtained (Hernández-Suárez *et al*., 2004).

The seminal work of addressing water allocation issues based on the superstructure was proposed by Takama *et al*. (1980), in which the superstructure was constructed to explore opportunities for possible water reuse and regeneration. Then, the model was solved to attain the optimal water network. Alva-Argáez *et al*. (1998) combined the insight provided by water pinch analysis with mathematical programming tools for the design of industrial water systems. A penalty form was added in the objective function to pursue a reduction of infeasibilities. The MINLP model was solved by decomposing into a sequence of relaxed MILP problems. In their subsequent work, a MILP formulation was presented to screen water network for multiple contaminants problem (Alva-Argáez *et al*., 1999). Huang *et al*. (1999) modified the model developed by Takama *et al*. (1980) to consider water recovery and wastewater treatment. Some useful features in realistic applications were considered, for example, multiple sources and sinks, water losses. In the solution process, the results obtained by water pinch analysis were set as the initial points, and some variables were bounded at a reasonable level.

In the work of Jödicke *et al*. (2001), except for the general costs, such as pumping costs, purchase cost of freshwater, and cost of wastewater treatment, costs of splitting and merging of pipes were also considered in the objective function. Hernández-Suárez *et al*. (2004) decomposed the complex superstructure into a series of basic superstructures. The advantage is that the problem is easy to solve. However, the reduction of complexity for the problem is accompanied by excluding some alternative solutions that may have stream recirculation and recycle. Chang *et al*. (2009) proposed a systematic procedure to improve the operational flexibility of water networks. Two scenarios were considered. One is to relax the allowed minimum freshwater requirement at normal conditions, and the other is to deploy auxiliary pipelines to eliminate existing pipelines. Results indicate bottleneck of the problem is the point where the concentration of the mixture of freshwater and reuse water approaches their upper bound, while the maximum inlet and outlet concentration reach their lower bound. This finding can give the designer information on how to carry out process changes in the retrofitting of the existing network.

In a recent paper, Jiang and Chang (2013) proposed an iterative strategy to solve the NLP model to enhance the flexibility index of the water network. Karuppiah and Grossmann (2008) considered the issues of the effects of uncertainties on the water network. The uncertainties in the problem include the amount of mass load and parameters of treatment units. Lagrangean decomposition for global optimization was used to solve the proposed model. In the process, the nonconvex problem was approximated by piecewise linear estimators, and tight lower bounds were thus attained by solving the relaxed problem.

In the above literature, water reuse/recycle scenario is mostly considered. The synthesis of total water networks is rarely addressed because of complexity (Bagajewicz, 2000). Two factors mainly affect complexity. One is the bilinear terms in the mass balance equations in the form of water flowrate multiplying water concentration. The other is the cost terms in the objective function, which cannot ensure the solution is the global optimum.

To eliminate nonconvex terms in mass balances, it is usually not allowed to mix streams before regeneration. Gabriel and El-Halwagi (2005) developed a simultaneous synthesis procedure for the design of material reuse and regeneration networks. The modeling of regeneration units was taken outside the optimization model, and several simplifying assumptions were proposed to transform the original model into a linear program. Nápoles-Rivera *et al*. (2012) extended the model to a multi-component case. The linear relationships obtained can ensure global optimality for the problem. Ahmetović and Grossmann (2011) developed a general superstructure for the synthesis of total water networks. Some additional connections were considered in their work, such as multiple sources with different quality, and hybrid operating units (mass transfer and non-mass transfer operations). Furthermore, pumping cost was also considered in the objective function, and tight bounds on the variables were added as constraints to solve the model. Boix *et al*. (2011) comprehensively considered the design of multi-contaminant water networks from the aspects of resource conservation, network complexity, and economic feasibility. A multi-criteria decision-making procedure was provided for the practitioner to choose a proper network.

Lovelady *et al*. (2009) presented a reverse model by combining the effluent of industrial processes with the watershed of the water ecosystem. The maximum allowable concentrations for the contaminants emitted from the industrial plants were determined based on the material flow analysis. These concentrations were incorporated into the water recovery model to generate the optimal design of a water network and to select a plant location. However, the limitation is that it does not optimize water recovery issues for different plants simultaneously. Lira-Barragán *et al*. (2011a) considered the location of a new plant based on an MINLP model by investigating the impacts of effluents on the surrounding watershed. The objective function is to minimize total annual cost, including wastewater treatment costs, and operating costs of the industrial plan, such as transportation of materials, land cost, and labor fees. However, wastewater recovery was not considered in the model. To overcome these limitations, Lira-Barragán *et al*. (2011b) presented an integrated model combining water recovery models for the new plant with environmental modeling of the watershed system. A few alternative locations for the new plant were considered in their work. Compared with the previous work (Lira-Barragán *et al*., 2011a), the proposed formulation can obtain more reductions in the total cost due to the consideration of mass integration inside the plant.

In the past, most papers focused on the development of complex models for water reuse and water regeneration for intra- and inter-plant water integration. The complexity of treatment processes and wastewater composition is ignored. Because the design of wastewater treatment plants not only needs to achieve the goal of contaminants removal but also is constrained by practical engineering constraints. Environmental impacts are also not considered from the perspective of the life cycle. Besides, the interactions between industrial plants, residence, and agriculture are not considered because in the past water shortage problem is not severe.

In the work of Quaglia *et al.* (2014), a practical framework was presented to address water recovery issues in the industry. Wastewater engineering knowledge and optimization method were incorporated into a computer-aided environment to find the optimal solution. It makes the method more applicable to real industrial problems. Sotelo-Pichardo *et al*. (2014) tried to design a water network with the minimum cost from the life cycle of the project. Some uncertainties such as water demand and environmental regulations are considered.

García-Montoya *et al*. (2015) proposed a model to achieve water reuse in residence through water reuse, recycling, and regenerating, as well as the rainwater recovery activities. The method applies to the scenario where water demands are changing through different hours of the day and the situation in which water requirement of different seasons of the year are not equal. Rubio-Castro *et al*. (2016) proposed a multi-period MINLP model for water reuse in the agriculture sector. Although different scenarios and conditions were considered in the proposed optimization formulation, some important parameters, such as evapotranspiration, the precipitated water, were set at a fixed value or ignored, which can affect the results.

2.5 Water integration techniques for batch processes

The time dimension introduces an additional constraint when considering water recovery opportunities in batch plants. During water recovery activities, the constraints of water quality and quantity, as well as the time feasibility of these activities should be considered simultaneously. The water integration techniques for batch processes are similar to continuous processes. These approaches can also be classified as insight-based approaches and mathematical methods (Gouws *et al*., 2008).

2.5.1 Insight-based techniques for batch processes

Wang and Smith (1995) first extended the water pinch analysis developed for continuous processes to batch processes. The approach divides the water-using processes into many concentration intervals and time intervals based on the parameters of water-using operations. Next, time is treated as the primary constraint, while concentration feasibility is considered as a secondary constraint. In other words, for each concentration subinterval, water is reused from one time subinterval to the next, and the freshwater requirement for this concentration interval is determined. The sum of freshwater consumption across all the concentration intervals is the target for the batch process. However, in their work, streams are splitting so that water can enter the operation during the course of the process, which is not allowed in completely batch plants. Furthermore, it is assumed that the operations are fixed mass transfer units.

To overcome these limitations, Majozi et al. (2006) reversed the priority of the constraints for water recovery activities. First, the sequence of constraints is the same as Wang and Smith (1995). Subsequently, time is treated as a primary constraint and concentration as a secondary constraint to investigate the effect of the priority on results. First sequence and cyclic operations were considered in their method. In the work of Chen and Lee (2008), a different representation of the targeting process was presented on a concentration vs. quantity diagram. This approach can be applied to a hybrid system comprising various operations (fixed load and fixed flowrate) and operating models (completely batch and semi-continuous). Some useful concepts and principles were adopted to evolve the initial network and to ensure the network meets the practical constraints. Subsequently, this graphical approach was extended fixed flow rate problems. The freshwater consumption was identified in the first step, and then some constraints were used to reduce the network complexity by removing some connections (Chen and Lee, 2010). Kim (2011) addressed water reuse issues for discontinuous water systems. First, water upper and lower bound targets for each time interval were obtained based on the water composite curve of Wang and Smith (1994a). Next, the water network was designed to achieve the lower bound target within and beyond the particular time interval, and the requirements of the storage tank were then obtained when water reuse between different time intervals occurs. Chaturvedi (2017) proposed a graphical technique to perform energy management for batch water allocation network. However, in the proposed method, opportunities for water reuse were not considered.

Foo *et al*. (2005) proposed a two-stage approach for the design of batch water networks. First, water cascade analysis (Manan *et al*., 2004) developed for continuous processes was extended to batch processes. For each time interval, water was cascaded from high-quality to low-quality streams. The sum of freshwater consumption for all the time intervals is the target of the problem. Next, the network was configured to achieve the targets in the first step. This method could be used to deal with water recovery issues for both mass transfer and non-mass transfer operations. A similar method was also proposed by Liu *et al*. (2007) to solve the water recovery problems for discontinuous or batch water systems. This method can obtain a different configuration with fewer storage tanks compared with Wang and Smith (1995). However, the network design and targeting process are performed simultaneously.

Chaturvedi and Bandyopadhyay (2012) proved that in a single batch process, the target of freshwater consumed in a batch plant could be achieved through the sequential transfer of wastewater from one time interval to the next. For cyclic operations, the targeting process is the same as continuous processes by aggregating all the time intervals into a single interval. Chaturvedi and Bandyopadhyay (2013) addressed the targeting of multiple freshwater resources with different quality in batch processes. The concept of prioritized cost developed by Shenoy and Bandyopadhyay (2007) was used as an indicator to choose the external resource by linking pinch quality, quality of freshwater, and its cost. Results show the prioritized cost of a resource mainly depends on the highest pinch quality of all the subsequent intervals, not depending on a single pinch of the interval the sources states. Chaturvedi *et al*. (2016) proposed a conceptual approach to address scheduling problems with multiple water resources. They pointed out that the optimal schedule for a single resource also applies to the scenario with multiple resources.

In the papers mentioned above, only the water reuse scheme was considered in batch processes. However, deployment of regeneration units is favorable in the synthesis of batch water networks because it further reduces the freshwater requirement. Foo *et al*. (2012) proposed a systematic procedure to design a total batch water network. It includes water reuse, water regeneration, and wastewater treatment. However, their method is only applicable to cyclic operations. In practice, the water system usually consists of multiple contaminants. Thus, in the work of Li *et al*. (2013), a manual method was presented to design batch water networks with multiple contaminants. Like most graphical techniques for continuous processes, the graphical methodologies for batch processes are restricted to the single contaminant system. More effort is required to develop novel water integration techniques for batch water systems with multiple contaminants.

2.5.2 Mathematical programming method for batch processes

Although insight-based methods can provide more insights for the engineers, the limitations of dealing with single contaminant prevent this method from full application on a large scale or for multiple contaminants. Mathematical programming exhibits its advantages in these problems. In the following subsection, progress in the optimization of water utilization for batch processes is reviewed.

2.5.2.1 Water minimization for predefined schedule

Water reuse scheme has been widely used in batch plants to reduce freshwater demand and wastewater generation, as well as energy consumption (Puigjaner *et al*., 2000). Most of the mathematical programming techniques for batch processes follow the same procedure, and the problem is formulated as the MINLP model.

Kim and Smith (2004) developed an MINLP model for water recovery in discontinuous water systems. A decomposed approach is selected to solve the MINLP problem. This design method was extended by Tokos and Pintarič (2009) to a brewery plant with discontinuous and semi-continuous water-using operations. Yao and Yuan (2000) addressed the wastewater minimization problem of optimal design of multi-purpose batch processes. A multi-objective formulation was developed to investigate the effect of conventional factors on waste emission.

It not only considered the equipment type and size selections but also considered raw material selection.

Majozi (2005a) developed a mathematical model for water integration in multipurpose batch plants. A superstructure was proposed to represent all possibilities of water reuse and recycle. In this method, it is assumed that the given production schedule is optimal for water-using operations. Furthermore, the outlet concentration of each operation is maintained at its maximum. This complies with the necessary conditions of optimal water networks for process industries, ensuring that the global optimality of the proposed model is guaranteed. Majozi (2005b) proposed a continuous-time based model for the design of a water network with and without a central reusable water storage facility. The predefined schedule was given *a prior*. Also, flexible mass transfer was considered in the proposed model. In other words, the outlet concentration and water requirement for each operation can vary simultaneously.

Li and Chang (2006) developed a general mathematical model for discontinuous water-reuse systems. To make the model more practical, additional logic constraints are incorporated into the formulation to model the relationship between water streams and pipelines. Chen *et al*. (2008) considered the synthesis of batch water-using networks with fixed production scheduling. A continuous-time based RTN formulation was proposed to model the short-term and periodical batch water system. Gouws and Majozi (2008) addressed the water recovery in a multipurpose batch plant with multiple contaminants. In the model, some vessels were dedicated to storing wastewater with specific contaminants and periodic operations were also considered by collecting the wastewater produced in one batch as a feed for subsequent batches of the same product. Results of the case study show that it is possible to achieve the goal of almost zero effluent.

Halim and Srinivasan (2011) presented a sequential methodology for simultaneous optimization of energy and water in a batch plant. A stochastic search-based procedure was used to generate alternative schedules. Based on the schedule obtained, heat recovery was performed to determine the minimum utility targets. Simultaneously, direct water integration was considered for each production schedule. Dogaru and Lavric (2011) considered the dynamic nature of the composition of water streams in water systems with predefined scheduling. In their method, it is assumed that the structure of water utilization remains unchanged at each time interval. Freshwater was utilized to meet the water demands through the reusable water stored in the tank with changing compositions, and accordingly, the wastewater flow directed to the tank was also identified based on the mass balance. Tokos *et* *al*. (2012) presented an MINLP model for a large-scale water system. However, the formulated model is huge and complex because of the changing daily production scheduling.

Due to the existence of the time gap in batch processes, the tank is usually used to store wastewater for further reuse. On the other hand, the effluent from an operation can be sent to an empty tank or mixed with the current water content of the tank. If the effluent has a relatively higher quality, the mixture operation could degrade the water quality, and some potential reusability is lost. It inevitably increases freshwater consumption. However, if each potential stream is stored in a tank, it could require more water storage tank, which will cause a higher investment cost and a more complex network. Furthermore, most batch plants are small- and medium-sized enterprises. Thus, less tank and smaller storage capacity are often desired.

Almató *et al*. (1997) presented a two-stage methodology to evaluate water reuse opportunities in a batch plant. In the first step, a heuristic procedure was applied to obtain an initial feasible solution. The optimization model was solved to determine the best tank-stream assignment to minimize freshwater consumption. However, their paper only considered water reuse opportunities. Although they considered the effect of increment of the number of tanks on freshwater reduction, the operation cost and capital investment are not considered.

Almató et al. (1999a) developed an optimization framework for water reuse in a batch plant. A superstructure representing the connections between storage tanks and water-using units was built to determine connections and flowrates between tanks and units. The formulated NLP model was solved by simulated annealing and deterministic methods. Almató *et al.* (1999b) extended the previous methodology to minimize the cost of water management activities, considering the cost associated to freshwater supply, wastewater treatment, as well as piping cost and operating cost. Results indicate for every case there is a certain number of tanks that lead to the optimal reuse network from an economic point of view.

Majozi (2006) proposed a two-stage algorithm for minimizing the capacity of water storage in a multipurpose batch plant. The target of freshwater consumption was determined under the condition of the given capacity of water storage tanks. This target was acted as a constraint in the second stage. The capacity of central water storage was optimized as a variable.

Oliver *et al*. (2008) presented an integrated method of pinch analysis and MILP to consider water recovery in batch processes. Water pinch analysis provides the target of the minimum water requirement and offers the possibility of connections between different water operations. The usage of water storage tank allows water reuse at different time points to be feasible. The information was incorporated into the MILP model to design batch water networks. Results of the formulated MILP model indicate that the freshwater reduction is greater than that obtained by water pinch analysis, but fewer storage tanks are required. Hence, the results should be determined based on the trade-off between water resources and economic performance. If the plant is in the region where the freshwater resource is scarce, the alternative network that achieves the minimum freshwater requirement, but employing more tanks will be favored by the designer. However, if the plant lacks space or has a low budget, the alternative network is chosen by considering practical conditions (Oliver *et al*., 2008).

In the work of Shoaib *et al*. (2008), a three-stage hierarchical approach was proposed for the synthesis of batch water networks. First, the target was identified by solving a linear transportation model for water recovery. Next, the formulated MINLP model was transformed into a MILP model by relaxing the bilinear terms. The target obtained in the first stage was determined *a priori* in the model, and MILP model was solved to design a batch water network with the minimum number of tanks. Finally, the network obtained in the second step was simplified by minimizing the connection of different operations.

In general, the above papers follow the same procedure. The target of freshwater consumption is determined first, and then this target is incorporated into the model to minimize the number of tanks. Freshwater consumption and storage number/size reduction are not optimized simultaneously. Thus, fuzzy mathematical programming is employed to find a compromised solution by defining a fuzzy variable. Nun *et al*. (2011) incorporated fuzzy constraints into automated targeting method to analyze the trade-off between freshwater requirement and number of storage tanks. The resulting problem can be formulated as the MILP model, which can be solved globally without significant computational difficulties.

For the synthesis of batch water networks, minimizing the number of intermediate storage tanks can decrease the operation cost to some extent. More actions can be taken to further reduce the cost by making full use of the inherent vessels. Sometimes, these operation units remain idle for most of the time horizon after other processes reuse wastewater. Thus, it is significant to arrange these idle processing units at a proper time to make full use of the equipment.

Gouws and Majozi (2009) presented a model to explore the possibilities of utilizing the idle processing units as the inherent storage vessel. Two scenarios were considered in their work. The first one is the grassroots design problem. It aims to minimize wastewater generation and the size of the central storage tank by making use of these inherent storages. However, the second case is a retrofit design problem. Wastewater generation is minimized through the utilization of the inherent storage under the constraint of the fixed capacity of the storage tank. Majozi and Gouws (2009a) analyzed the effect of usage of the tank on the batch water network. In their work, two scenarios were considered. The first scenario considered direct water reuse, implying wastewater generated from one operation is directly reused in another operation if the end time of the source coincided with the start time of the sink. Therefore, no water storage was required to store the reusable water. In the second scenario, the wastewater was temporarily be stored in a dedicated tank and then was sent to a water sink.

Similar work was done to consider water reuse in a multiple contaminant batch plant without central reusable water storage (Majozi and Gouws, 2009b). Furthermore, Nonyane and Majozi (2012) considered wastewater minimization in a flexible batch plant in which the production schedule was operated on a long-term horizon. This approach is an extension of the work published by Majozi and Gouws (2009). The difference is that the adaption of cyclic scheduling concepts was incorporated into wastewater minimization model. Zhou et al. (2016) proposed an optimization model for the design of multi-period mass exchange networks. In their method, multipurpose mass exchange refers to the streams that can be exchanged by more than one match in different periods. Results show that the proposed method not only makes mass exchange units being utilized efficiently but also reduces the cost through proper arrangement of multipurpose mass exchangers and storage devices.

Also, regeneration reuse scheme is adopted in batch processes. In the work of Liu *et al*. (2009), a water regenerator was deployed to reduce freshwater consumption in cyclic batch operations further. In their method, the batch operations were divided into a few time intervals. In each interval, mass balances can be constructed to model the water flow. Freshwater can be determined by solving these established models. Finally, the regeneration flowrate was identified by employing the freshwater obtained in the previous step as a constraint.

Except for the truly batch processes, water reuse for the hybrid system with batch processes and continuous processes is also considered. Lee *et al*. (2013) addressed the water recovery problems for hybrid water systems, including truly batch, semi-continuous, and continuous units. In their method, continuous processes are treated as a special semi-continuous process. Thus, the original problem is seen as a batch water network with a fixed schedule. In their subsequent work, Lee *et al*. (2014a) developed a two-stage approach to address the water recovery for a batch plant with continuous and batch operations. However, the difference is that all of the batch processes are treated as continuous units by employing auxiliary water tanks. This assumption makes it possible to use these methods developed for the continuous processes to minimize freshwater consumption for the batch processes. Subject to the targets determined, the water storage policy was optimized to minimize the number and the capacity of tanks. In the work of Lee *et al*. (2014b), a four-stage formulation was proposed to address water minimization for cyclic batch processes and minimize the storage capacity and inter-connections. Results indicate the addition of inter-connection constraints in the model can reduce the number of inter-connections up to 21%.

In batch processes, the property-based resource conservation network is also considered. For example, Chen *et al*. (2010) proposed a general framework for property-based resource conservation networks involving batch and continuous processes. A unified model for the hybrid system was thus established by treating the continuous process as a batch process.

2.5.2.2 Simultaneous optimization of water and product schedule in batch plants

In the above description, water integration in batch processes focused on the systems with predefined scheduling. However, when the chemical designer performed the grassroots design of batch plants, they may not pay more attention to the utility systems. For the retrofit of batch processes, the potential of water recovery is still limited due to the existing infrastructure and layout of these facilities. Therefore, simultaneous optimization of wastewater minimization and production scheduling is necessary for the sustainable development of batch plants which are located in water scarcity regions.

In the work of Majozi (2005b), water recovery model was incorporated into the scheduling framework where the starting and finishing times of water operations are treated as optimization variables. A continuous-time based formulation was developed to minimize freshwater consumption with and without a central reusable water storage facility. Cheng and Chang (2007) proposed an integrated batch water model. In their formulation, the interactions between production scheduling subsystem, water-reuse subsystem, and wastewater treatment were considered, rather than considering each subsystem individually. Similarly, Zhou *et al*. (2009) developed a comprehensive formulation representing water utilization in flexible batch plants. In this contribution, a continuous-time formulation was used to represent production scheduling. Furthermore, a hybrid strategy combining DICOPT and the genetic algorithm was employed to obtain the globally optimal solution.

Li *et al*. (2010) modified the state-time-space superstructure proposed by Zhou et al. (2009) for optimization of batch water allocation network. In their modified superstructure, the employment of mixers/splitters could rule out the streams which bypass water users without any mass exchange. Adekola and Majozi (2011) presented a continuous-time based methodology to address wastewater minimization problem by employing a regeneration unit for flexible batch processes. The resultant network can achieve the minimum wastewater generation and the optimum batch production schedule. Results show that more reductions of freshwater can be achieved through the redesign of the production scheduling compared with predefined scheduling. Chen *et al*. (2011) developed a resource-task-network based mathematical model to optimize production scheduling and wastewater recovery. In their model, both short-term and periodic scheduling were considered. A relaxation linearization was employed to solve the resultant formulation.

Adekola *et al*. (2013) extended the model of Adekola and Majozi (2011) to simultaneous optimization of energy and water in flexible batch plants. By rescheduling the operations, an improved result can be obtained in terms of water and energy saving as compared to the scenario optimizing water and energy separately. Seid and Majozi (2014) used the modified scheduling framework (Seid and Majozi, 2012) to optimize both water and energy in flexible production scheduling simultaneously. Compared to Adekola *et al*. (2013), the number of event points and usage of utility and water are also improved.

Chaturvedi and Bandyopadhyay (2014a) considered the effect of multiple external resources on the operating costs. Results of two examples show reductions of 17% and 32% in operating costs can be achieved as compared to a single freshwater source. Chaturvedi and Bandyopadhyay (2014b) proposed a multiple objective formulation to cope with the issues of minimizing freshwater requirement and maximizing production in a batch process at the same time. The optimal solution between the production and the freshwater consumption was obtained through the Pareto optimal front. Chaturvedi *et al*. (2016) optimized water utilization in a batch plant by employing multiple water resources. They pointed out that the optimal production scheduling for a single resource can also be suitable for the multiple freshwater scenario, of which operating cost could also be minimized. Dong *et al*. (2016) developed a general framework for water recovery in a flexible scheduling framework. In their work, different regeneration modules were considered in the wastewater recovery model. Adekola and Majozi (2017) considered the effect of changeover on water reduction in a flexible batch schedule. Freshwater consumption can be reduced through an appropriate arrangement of the sequence of tasks in a unit. Results show that reductions of freshwater of 33% and 48.8% were obtained in the two case studies. Lee and Foo (2017) presented a discrete-time based formulation for water network synthesis in batch plants. The automated targeting method was used to model water flows in the batch plant. Thus, the formulated MILP model is easy to solve. However, this method is only applicable to the system with a single contaminant because of the inherent limitation of automated targeting method.

Pulluru and Akkerman (2018) proposed a generic water classification to capture the composition change in water streams in variable schedules. It is more practical in the industry and can avoid the computational complexity caused by the detailed modeling of contaminations.

2.6 Water Network Synthesis Challenges

The challenges in the synthesis of batch water networks can be summarized into the following aspects, namely, (1) nonconvexity, (2) nonlinearity, and (3) uncertainty.

2.6.1 Nonconvexity

Nonconvexity is one of the major problems in the synthesis of water networks. It is usually presented as bilinear terms in mass balance equations in the formulation. Implementation of global optimization techniques is one of the viable ways to get around such problems. Some techniques have been developed to handle bilinear terms to guarantee near global/global solutions for nonconvex problems, such as reformulation linearization techniques, branch and bound algorithms, piecewise under- and over-estimators (Nápoles-Rivera *et al*., 2012).

Branch- and bound is a non-heuristic algorithm for global optimization in nonconvex problems. The procedure is described as follows. The solution space is repeatedly partitioned into smaller and smaller subsets, and upper and lower bounds are then identified for each subset. Those subsets with a bound that exceeds the upper and lower bounds are discarded. The partition continues until finding a solution better than the best one found so far (Lawler and Wood, 1966).

The reformulation-linearization technique is used to generate tight linear programming based on lower bounds. This procedure first generates valid quadratic constraints by using pairwise products of inequality constraints, or products of equality constraints with variables, and then subsequently linearizes these constraints by defining new variables. The bilinear objective term is similarly linearized to produce a lower bounding linear program (Sherali and Alameddine, 1992). When solving a non-convex MINLP, it is not easy to solve the model directly. The common way is to relax the original problem through piecewise under- and over-estimators.

One way to further relax the original problem is to replace non-convex functions with convex under-estimating functions. Another way is to define a new variable acting as a place holder for the non-convex function and to add constraints forcing the defined variable to be approximately equal to the non-convex function (Burer and Letchford, 2012).

2.6.2 Nonlinearity

Nonlinearity refers to the situations where the output variables are not simply proportional to the input variables, but instead, the relationship is dynamic and variable. In the synthesis of water networks, one of the sources of nonlinearities in the problem is the bilinear terms in mass balances, i.e., production of flowrate and concentration. In the synthesis of water networks, the deployment of the regeneration unit can enhance the potential of water recovery. Detailed design of the regeneration unit and multiple contaminants problem result in an inherently nonlinear formulation (Khor *et al.*, 2014).

Development of appropriate superstructure for water recovery problems is a useful way of alleviating the problem convergence of nonlinear formulations (Khor *et al.*, 2014). There are three approaches for superstructure representation for water network synthesis, i.e., the alternative collection techniques, the combinatorial synthesis technique, and the insight-based synthesis technique (Quaglia *et al.*, 2015).

The alternative collection techniques generate a water network by listing all known configurations based on previous experiences. However, this technique only considers known alternatives and cannot obtain innovative alternatives previously unexplored (Quaglia *et al.*, 2015).

The combinatorial synthesis techniques generate a superstructure by connecting all relevant raw materials, products, and operations. It can overcome the drawbacks of alternative collection techniques. However, the resulting model is expensive in terms of computational time.

The insight-based synthesis techniques generate a superstructure based on commercial and engineering insights (Quaglia *et al.*, 2015). These methods are capable of generating superstructures containing innovative solutions, while at the same time excluding those alternatives which are known to be infeasible or not-convenient. By eliminating infeasible and not-convenient alternatives, the computational resources needed for the solution of the formulation are reduced (Quaglia *et al.*, 2015).

2.6.3 Uncertainty

The uncertainties caused by data and parameters are also a significant challenge in wastewater minimization field. If the right data are not extracted in the process synthesis, it could result in a sub-optimal solution (Foo, 2012). Various approaches to addressing uncertainties are widely used in the synthesis of water networks. These methods include stochastic programming (Dantzig, 2011), chance-constrained optimization (Charnes and Cooper, 1959), flexible analysis (Grossmann and Sergeant, 1978), Monte Carlo simulation (Hammersly and Handscomb, 1964), and robust optimization (Ghaoui and Lebret, 1997).

Stochastic programming is an approach for modeling optimization problems in which data are uncertain (Kall *et al*., 1994). The most widely applied method in practice is the two-stage stochastic programming model. In the first stage, the decision maker takes some actions which make random events occur to represent the uncertainties. In the second stage, a recourse decision is made in response to the action in the first stage. In the work of Khor et al. (2014), a two-stage stochastic programming method was used to design the water network. In the first stage, the maximum flowrate for water reuse/recycle was determined. The effects of uncertainty on the freshwater requirement were then investigated by modifying freshwater supply and wastewater flowrate to meet the demands of the existing water network. In the work of Jeżowski et al. (2007), superstructure representation and stochastic optimization technique are combined to design heat exchanger and water networks to enhance efficiency and robustness of optimization. Results indicate the approach could obtain the same solutions matching with the literature or even better ones in some cases.

Robust optimization aims to optimize the problem over the entire uncertainty range to ensure that the solution quality in the worst case is still acceptable (Ghaoui and Lebret, 1997). This means that the solution obtained should remain close to the optimal solution and is almost feasible even when the worst case occurs. It provides solutions which are relatively resilient to system changes and prevents decision-maker against parameter ambiguity and stochastic uncertainty (Mulvey *et al*., 1995). There exist many ways to compute the worst case, i.e., a finite number of scenarios such as historical data, or continuous uncertainty sets such as polyhedral or ellipsoids (Gabrel *et al*., 2014). The selection of uncertain parameter sets should be based on the trade-off between system performance and protection against uncertainty. Khor *et al*. (2014) pointed out that in the synthesis of water networks, uncertain variables can be represented by a finite number of scenarios derived from historical data or expert experience.

Flexibility is to ensure the system to keep steady-state operation over a variety of operating conditions (Morari, 1983; Swaney and Grossmann, 1985). The index of flexibility is measured by the expected deviations from its nominal value in theory. The actual deviation is usually regarded as the production of the expected deviations and a common scalar variable. Two types of problems arise in the flexibility analysis of a process. One is the feasibility test to establish whether a given design is still operating normally over a specified range of uncertain parameters. The other is to evaluate the flexibility index. The objective is to determine a measure of the flexibility of a design by establishing a reasonable range that a design can tolerate for normal operations (Grossmann and Floudas, 1987).

Monte Carlo simulation is widely used to predict the statistical properties of outputs of a system based on the probability distributions of specific inputs to have a better understanding of the risk of a decision (Hammersly and Handscomb, 1964). It can be used to compare the water network based on robustness, or resistance to variations outside of design conditions. Furthermore, it is simple and can be easily implemented with computer aids. Tan *et al*. (2007) demonstrated the application of Monte Carlo simulation in the design of the water network when facing variant mass loads.

2.6.4 Future research direction for water integration

A rapidly rising global population and growing prosperity are putting more pressures on energy, water, and food resources. This situation makes countries all over the world to pay more attention to the concept of sustainable development, especially for the process industry. Recently, artificial intelligence, particularly machine learning, attracts the interests of the researchers from the academic and industrial community. It is apparent that chemical engineering is at a critical crossroad. Hence, some suggestions for future work are described as follows.

a. Extension to other resources conservation problem. The field of water integration for continuous and batch processes has been mature. This observation can be concluded from the publications in the past five years. In these papers, most of them are based on general superstructure-based mathematical programming methods. Since water integration is a special case of mass integration, targeting and design techniques developed in water network can be extended to the synthesis of other resources conservation network, such as hydrogen network, nitrogen recovery, or property-based resource recovery.

b. Inter-plant resource integration. To protect the environment while increasing business success, eco-industrial parks are set up to minimize energy and raw material use, and waste generation. It not only considers the resource conservation in its industry but also focuses on the physical exchange of resources such as materials, energy, water, and by-products between different industries. Water integration techniques, as systematic procedures for the synthesis of water networks, can be extended to the optimal design of resources cascade utilization networks in eco-industrial park. By minimizing environmental impacts, resource recycling can be maximized through these techniques in process systems engineering domain. Furthermore, some key concepts of process systems engineering could provide the systems thinking method for understanding the interactions between social, economic, and natural worlds.

c. Multi-objective optimization. Most of the studies about water integration focused on minimizing freshwater consumption or the total cost of water network systems. These objectives are relatively easy to trace mathematically. Sometimes, the reduction of freshwater consumption for a specific process does not necessarily mean that it reaches the best solution from the perspective of the life cycle. The implementation of water saving project may bring an increase in energy consumption. Thus, the evaluation of a single objective after being optimized cannot ensure that the process is still optimal for other objectives. For example, solar power is recognized as clean energy as compared to traditional fossil fuel. However, solar panel production could discharge pollutants to the environment, and the deployment of the solar panel could affect the local ecosystem. Sometimes, the water recovery project is feasible from an economic and technological perspective. However, the managers are not interested in implementing the project because of the risk of deploying new equipment. Thus, the incorporation of multiple objectives in the formulation is necessary for the designer and researchers to consider the water recovery in the industry.

2.7 Conclusions

Strict environmental regulations and social conception of environmental protection have created the need for wastewater minimization in the process chemical industries. Water integration techniques play a significant role in the wastewater minimization of chemical industries. Many techniques have been developed for the optimal synthesis of water networks in the continuous chemical processes, for example, the insight-based methods and optimization-based techniques. These methods not only assist to design water networks with water reuse scenario, but also are able to synthesize total water networks, including water reuse, water regeneration, and wastewater treatment processes.

Although many efforts have been made in the synthesis of water network in continuous processes, the water conservation problems in batch chemical processes should also be considered. Compared with continuous processes, wastewater recovery in batch processes is more complex. This is because the water quality, water quantity, and time constraints should be taken into account simultaneously. The water integration techniques in batch processes can be classified into two groups, i.e., predefined production scheduling and flexible production scheduling. The general procedures of water conservation techniques in batch processes is to integrate water reuse model with production scheduling model. This results in models that are very difficult to solve at best and almost impossible to solve at worst. Furthermore, most of the work in published literature in the area of water optimization in batch processes tends to be steeped in mathematical modeling, with very limited conceptual analysis. Therefore, the conceptual analysis of water optimization in batch processes is an important area in the future.

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3

OPTIMAL SYNTHESIS OF BATCH WATER NETWORKS BASED ON DYNAMIC PROGRAMMING

3.1 Introduction

Conservation and improvements in water resource management have been a global challenge (Bagatin *et al*. 2014). Water cascading utilization and approaches that aim to increase water efficiency further can be considered guiding principles for sustainable water resource management. The stringent regulation of environmental emissions has been driving the industry and academia to find ways of minimizing freshwater consumption and wastewater generation. Reduction of freshwater consumption could result in higher profitability and less adverse impacts on the environment. Although continuous processes have the advantage of manufacturing on a large-scale in the chemical industry, numerous chemical products still retain batch processing as their primary method of manufacture, such as pharmaceutical, agricultural, and food products. Batch processes have been widely used in the chemical industry due to their suitability for the production of small volume, high value-added products, as well as their capability of adjusting to rapid market changes. Therefore, it would be favorable to develop a systematic approach to design optimal water networks for batch processes.

Unlike continuous processes, batch operations do not only have to obey the concentration constraints, but also consider time feasibility issues. For example, wastewater generated by a process can be recovered if it obeys the inlet concentration constraint of the receiving unit and if the receiving unit is operated during or after the wastewater is generated. In the past decades, much effort has been placed on the optimal design of water-using networks in batch processes.

An overview of the developments and methodologies proposed for batch water networks was presented by Gouws *et al*. (2010). These methodologies can roughly be divided into insight-based and mathematical techniques. Insight-based techniques for batch water networks share their roots with their continuous counterparts. However, apart from concentration constraints, time constraints should be taken into account during the targeting of batch processes. Hence, batch processes tend to be more complex because of the existence of scheduling issues.

Mathematical programming techniques offer a general modeling framework in the synthesis, optimization, and planning of batch chemical processes (Majozi, 2010). Two main approaches arise when considering water integration for batch processes. One approach focuses on the minimization of water within a predefined schedule where the timings of operations are stipulated a priori. This particular approach bears many similarities to that of insight-based techniques for batch processes. The other approach involves minimization of water where the start and finishing times are not known beforehand. In this approach, only duration is specified, and the optimal schedule that achieves the minimum water targets is determined (Gouws et al., 2010).

The earliest contribution, such as Almató *et al*. (1997) and Kim and Smith (2004), utilized storage tanks to override the time gap between the finishing time of discharging task and starting time of the receiving task. In both these contributions, each storage tank is dedicated to a single reuse opportunity, resulting in a higher capital cost. Majozi (2005) circumvented the use of central storage tank to exploit opportunities for water reuse/recycle. In the subsequent work, a two-stage approach is proposed to minimize the freshwater consumption and the capacity of the reusable water storage tank (Majozi, 2006). In addition to minimization of freshwater consumption and storage capacity, Chen *et al*. (2008) considered minimizing the number of connections by formulating a mixed integer nonlinear (MINLP) program. The results from these papers indicate that freshwater can be substantially reduced through water reuse/recycle. However, wastewater treatment has not been adequately considered in water integration of batch processes. Cheng and Chang (2007) developed a general mixed-integer nonlinear programming (MINLP) model to synthesize water networks in batch processes by optimizing batch schedules, water-reuse subsystems, and wastewater treatment subsystems simultaneously. In practice, there exist processes with a mixture of continuous and batch operations, for example, breweries, sugar mills, and tire-production plants. Lee *et al*. (2013) considered the synthesis of water networks for systems consisting of truly batch, semicontinuous, and continuous units. Furthermore, in their subsequent work, inter-plant water network was synthesized in process units operated in mixed continuous and batch modes (Lee *et al*. 2014).

There are other contributions that are worthy of mention in water minimization in batch plants using a flexible schedule. For example, Adekola and Majozi (2011) addressed the problem of simultaneous production scheduling and wastewater minimization by employing a wastewater regenerator to further reduce freshwater consumption. Similarly, Chen *et al*. (2011) proposed a mathematical model for simultaneous scheduling and water minimization in multipurpose batch plants. However, in their work, the scheduling framework is based on the Resource-Task Network representation. Chaturvedi and Bandyopadhyay (2014) developed a multiple objective formulation to simultaneously target the minimization of freshwater requirement and the maximization of production in a batch process. Lee and Foo (2017) proposed an integrated technique of simultaneous targeting and scheduling in batch processing plants by combining pinch-based automated targeting model and production scheduling model based on state-task network representation.

The seminal work of insight-based approaches for the optimal design of batch water networks was proposed by Wang and Smith (1995). This approach treated time as the primary constraint and concentration feasibility as a secondary constraint. However, the authors only considered situations where batch processes consume or produce water continuously during their operation in a semi-continuous manner.

Based on this observation, Majozi *et al*. (2006) proposed a graphical technique for wastewater minimization in completely batch operations. Firstly, it took the time dimension as the primary constraint and concentration as the secondary constraint. Next, the priority of constraints was reversed to demonstrate the effect of the targeting procedure of the proposed approach on the final design. Chen and Lee (2008) presented a graphical technique to deal with a hybrid batch water system comprising fixed-mass load and fixed flowrate problems. They also considered completely batch and semi-continuous operations. Kim (2011) proposed a two-stage graphical approach to minimize freshwater consumption and wastewater generation for discontinuous water systems. In the first step, the lower and upper bound targets of the water systems are obtained by pinch analysis. In the second step, the optimal water network is designed to achieve the lower bound target.

Chaturvedi *et al*. (2016) provided a simplified conceptual approach of dealing with scheduling problems of a batch water network with multiple water resources and analyzed the effect of multiple water resources on a batch water network schedule. Furthermore, some algebraic methods have been developed to perform water reuse/recycle for batch process. Foo *et al*. (2005) developed a time-dependent water cascade analysis for the synthesis of a maximum water recovery network for a batch process. Similarly, a time-dependent concentration interval analysis method was proposed by Liu *et al*. (2007) to solve the problems associated with the synthesis of discontinuous or batch water-using systems involving both non-mass-transfer-based and mass-transfer-based operations. Foo *et al*. (2012) proposed a systematic procedure to perform targeting and design of a batch resource conservation network involving material regeneration and waste treatment.

A new formulation was proposed by Oliver *et al*. (2008), which combines water pinch technology with mathematical modeling to design the water network for batch processes. The formulation is capable of satisfying the minimum water target while determining the minimum number of water storage tanks. Foo (2010) proposed an automated targeting technique to determine the minimum resource and waste targets for batch process integration problems. Although the technique is formulated as a mathematical optimization model, the fact that it is built on the insight-based pinch analysis technique enables the minimum resource targets to be identified prior to detailed design. Li *et al*. (2013) developed some simple design heuristics to manually generate batch water networks in systems with multiple contaminants.

In the methods above, the design of batch water networks is divided into many intervals based on the starting and finishing times of each operation. In each interval, the designer would identify freshwater consumption and the quantity of reuse water from earlier processes. It can be formulating multistage decision processes. Dynamic programming (DP) is a powerful formal framework for dealing with a large spectrum of multistage decision-making problems (Bellman 1957). DP provides a decomposition strategy for large optimization problems. It has been applied in numerous multi-stage decision processes, for example, the allocation of feed in a multi-reactor system, equipment replacement, tray-by-tray calculations in distillation and absorption, as well as multiple flash tank separation (Roberts 1964). El-Halwagi *et al*. (2003) employed DP techniques to derive the mathematical conditions and characteristics of an optimal solution strategy for material reuse/recycle networks. In the work of Diban *et al*. (2016), DP was used to obtain an optimum replanting policy that achieves minimum carbon emissions over a finite time horizon for commercial agriculture plantations.

In this work, DP is used to design a water network for batch processes. Although the procedures are similar to the stepwise method of water network design, the difference is that in every stage, the optimal solution to the decomposed problem is chosen to form the overall solution. When transforming from a stage to the next stage, the overall solution is not optimal; it will return back to the previous stage to choose another solution to ensure finding the globally optimal solution for the original problem. Furthermore, once obtaining the water network for fixed predefined schedule, the network can be evolved by rescheduling some operations, resulting in a less capacity of the tank and a simpler water network by removing some tanks. The rest of the paper is organized as follows. Section 3.2 describes the problem statement. A description of the methodology employed in this work is explained in Section 3.3. Section 3.4 presents case studies reproduced from the literature. Finally, Section 3.5 concludes the paper and suggests prospects for further research.

3.2 Problem statement

The problem addressed in this paper is formally stated as follows.

Given:

A set of batch processes *m* with specific process data, including

(i) the start and end time of each process,

(ii) the limiting water quantity and quality of each process,

(iii) the maximum storage capacity for each material,

(iv) the time horizon of interest, and

(v) general information of regeneration units, e.g., fixed outlet concentration, or the remove ratio of the contaminant.

Determine the optimum water network that achieves minimum freshwater consumption and minimum storage capacity.

3.3 Methodology

Dynamic programming (DP) is generally used to reduce a complex problem with many variables into a series of optimization problems with one variable. Thus, the decomposed problems are comparatively easy to solve. In the analysis, DP is characterized fundamentally in terms of *stages* and *states*. A difficult problem can be divided into a series of consecutive *stages*. Each stage constitutes a new problem to be solved to find the optimal result. In each stage, the system can be described or characterized by a relatively small set of parameters called the *state* variables. The states correspond to the alternative decisions which could be made in this stage, and those will often be a range of possible values for control variables.

In this work, the states for every stage are freshwater consumption, the quantity of stored water and wastewater generated. In each stage, a decision could be made on whether to use freshwater or reuse wastewater or regenerated water. No matter what stage the system is in, one or more decisions must be made in order for the analysis to proceed to the next stage. These decisions may depend on either precious stage or state or both. When a decision is made, a return cost or reward is obtained, and the system transforms the next stage. The return cost is determined by a known single-valued function of the input state. In this work, the return cost mentioned in the following sections refers to freshwater consumption. The entire process can be divided into *N* stages (1, 2, …, *k*, …, *N*) based on the start and end time of the operations. The relationship between stages and time is displayed in Figure 3.1, where ts_m and te_m represent the starting time and end time of operation *m*. It is noted that the problem was solved using the backward procedure of DP (Roberts, 1964). The stages are thus presented in reverse order.

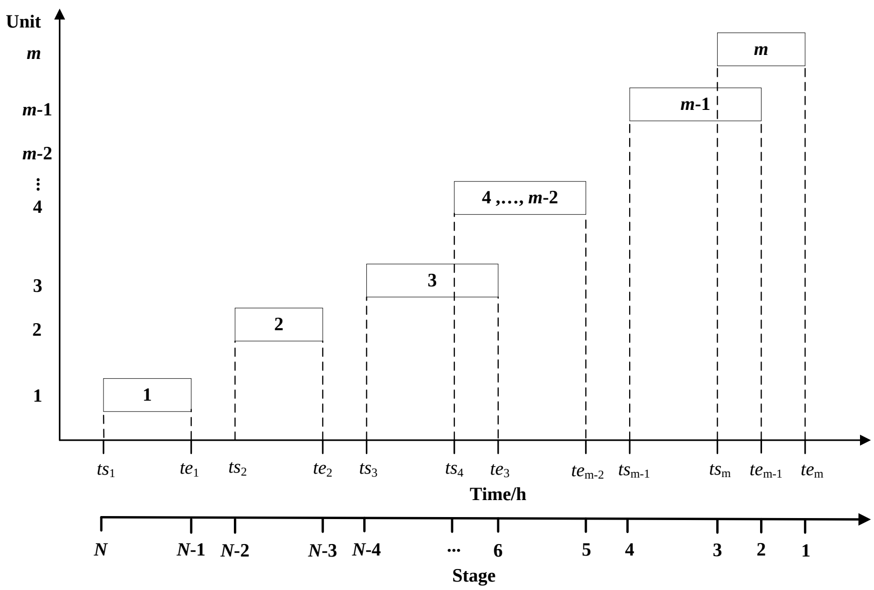

Figure 3.1 The relationship between time and stages

Suppose that in the *k*th stage there are I_k water sources and J_k water sinks, resulting in $M(k)$ possible states which are numbered 1, 2, …., $M(k)$. In other words, there are $M(k)$ possibilities about the allocation of freshwater to water sinks in the *k*th stage. The potential states in each stage are represented by the circles, as shown in Figure 3.2. Let $F_{j,k}^{Fw}$ denote the allocation state of freshwater to sink j in the *k*th stage of the process. In Figure 3.2, $F_{j,k}^{Fw}$ is represented by the arc, indicating the chosen path from the state of the previous stage to the state of the next stage. If $F_{j,k}^{Fw}$ is the state chosen in the *k*th stage, a solution to the whole problem may be denoted by the sequence $(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$. $f(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$ denotes the return cost associated with the sequence $(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$.

The objective is to minimize $f(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$ subject to any constraints which are placed on the choice of the states in each stage, and these constraints may depend on the states entered in stages 1, 2, …, *N*-1. In this work, the returned cost function is set as the total minimum freshwater consumption over the *k*th stage, which equals the minimum sum of freshwater consumption in *k*th stage ($\sum_{j=1}^{J_k} F_{j,k}^{Fw}$) in the *k*th stage and return cost results ($f_{k-1}(F_{j,k-1}^{Fw})$) from the stage (*k*-1). This work aims to find the path with the minimum result from Stage *N* to Stage 1.

The objective of the problem is defined as:

$f_k(F_{j,k}^{Fw})$ = minimum freshwater consumed over the *k* stages

Where,

$$f_k(F_{j,k}^{Fw}) = \begin{cases} \text{Freshwater:} & \sum_{j=1}^{J_k} F_{j,k}^{Fw} + f_{k-1}(F_{j,k-1}^{Fw}) \\ \text{Reuse/recycle:} & f_{k-1}(F_{j,k-1}^{Fw}) \end{cases}, \ k = 1, 2, 3, ... N \qquad (3\text{-}1)$$

$$f_0(F_{j,0}^{Fw}) = 0 \qquad (3\text{-}2)$$

Eq (3-1) represents the objection function of the problem when it is located in the *k*th stage. In every stage, the designer has two options for satisfying the water demand of operation, i.e., the freshwater scenario, reuse/recycle scenario. For the freshwater scenario, the water requirement of a sink is satisfied with freshwater in addition to any reused, recycled, and regenerated water. In this scenario, freshwater must be used to dilute wastewater to meet the water requirement. However, for the reuse/recycle scenario, no freshwater is required to satisfy the water demand. In other words, the available reusable wastewater or regenerated water is capable of achieving the target. Eq (3-2) is the objective function of the origin stage, setting as zero. It does not have a physical meaning.

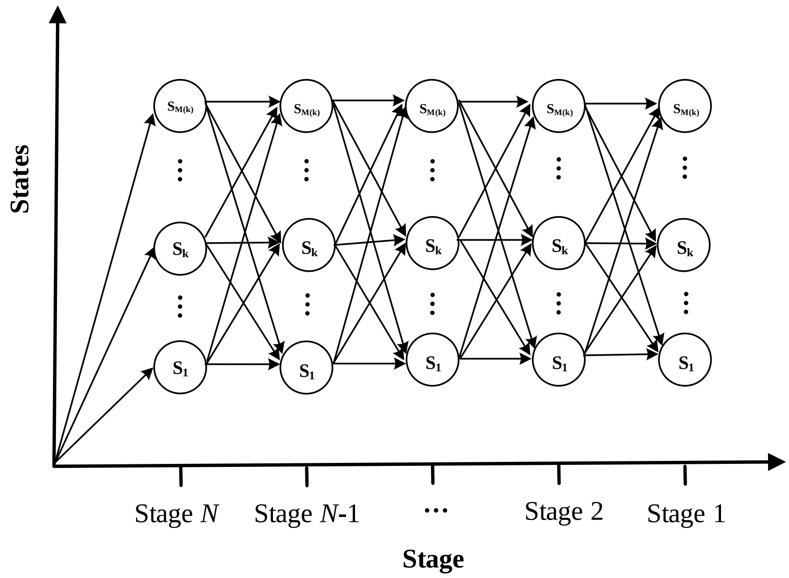

Figure 3.2 Potential states in each stage

When determining water target in each stage, two main categories of water network synthesis exist, i.e., fixed flowrate and fixed-mass load problems. For different types of problems, the resulting freshwater consumption may be different. Because the number of variables presented in the constraint equations is more than the number of equations, it is difficult to determine a sole solution of these equations for the system. Therefore, when attempting to identify the minimum freshwater consumption, a set of rules is generated to appropriately select from the available water resource and achieve the optimal design for water-using network.

1) When reuse water and regenerated water are available at the same time, reuse water should be used preferentially;
2) To reduce the cost of stored water, if a water sink has a few alternative water sources, the water source which is generated latest should be reused preferentially
3) If the process chooses a freshwater scenario which requires some reuse water, the reuse water with the highest quality, i.e., lowest concentration, should be used preferentially, in as great a quantity as possible;
4) If a process is fed solely by wastewater, i.e., no freshwater needed, wastewater with the contaminant concentration closest to the maximum inlet concentration of the process should be used preferentially, in as great a quantity as possible;
5) If the water sink has a few available water sources with the same concentration, the alternative water source with a sufficient amount of reuse water should be used preferentially.

Fixed flowrate problems

In the process industry, some units, such as boiler, cooling towers and reactors, do not involve any mass transfer. The inlet and outlet flowrates of the water-using processes may not be uniform and therefore can account for water losses or gains. The outlet streams always leave at the specified (maximum) concentrations, while the inlet streams have maximum allowable concentrations given. This model is generally known as the fixed flowrate problem (Foo, 2009; Prakash and Shenoy, 2005).

For freshwater scenario, water requirements of sinks are satisfied with freshwater, reusable wastewater, or regenerated water. The freshwater consumption in the *k*th stage can be obtained by Eqs (3-3) and (3-4). The priority of water utilization is based on the rules above. The procedure is explained as follows: Firstly, the process is to use a mixture of reuse water and freshwater to meet the water requirement. If the quantity of reuse water in the same stage is insufficient, the deficit water is supplied by regenerated water. After all the states of freshwater consumption are determined, the minimum freshwater consumption is chosen as the optimal state in this stage.

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}} + F_{j,k}^{Fw} = F_{j,k} \tag{3-3}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Reg}}^{l} + F_{j,k}^{Fw} c_{Fw}^{l} = F_{j,k} c_{j,k}^{\max,in,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,\ldots,N \tag{3-4}$$

For the reuse/recycle scenario, the specific water requirement for water sink j in the stage k can be obtained by Eqs (3-5) and (3-6). In the equations, $F_{i,j,k}^{d}$ and $F_{i,j,k}^{ind}$ represent the direct reuse of water and indirect reuse of water, respectively. Based on the rule above (2), direct reuse of water should be selected preferentially. If the quantity of direct reuse water is not enough to meet the water demand, the deficit water is supplemented by indirect reuse water. Furthermore, if the quantity of indirect reuse water is still deficient or not available, the remaining water is supplied by regenerated water.

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}} = F_{j,k} \tag{3-5}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Reg}}^{l} = F_{j,k} c_{j,k}^{\max,in,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N \tag{3-6}$$

Fixed-mass load problems:

Apart from the fixed flowrate operations, a different category termed as fixed-mass load operations is commonly used in the process industry. The operations in this category can be modelled as mass transfer mass transfer units with water being used as the only mass separating agent. It includes washing, scrubbing, and extraction operations. In the fixed-mass load problem, each operation has a fixed contaminant load and the maximum allowable inlet and outlet concentrations are specified. The flowrate of water entering and leaving the unit is the same (Foo, 2009; Prakash and Shenoy, 2005).

For fixed-mass load problems, the supplied water quantity can be less than the limiting water requirement, and the inlet concentration can also be less than the maximum allowable inlet concentration. To obtain an optimal result of freshwater consumption, it is prudent to use nonlinear programming (NLP) to determine the results of freshwater consumption and reuse water from previous processes. The NLP model is explained as follows: The objective function is to minimize freshwater consumption, as shown in Eq (3-7). Eq (3-8) states that the removal of the mass load must be greater than or equal to the limiting mass load if the outlet concentration reaches its limiting data. Eq (3-9) represents the calculation of inlet concentration. Eq (3-10) ensures that the actual removal of mass load is equal to limiting mass load. The quantity constraint is expressed in Eq (3-11). Eq (3-12) indicates that the actual inlet and outlet concentration should be limited by the limiting data.

$$\min F_{j,k}^{Fw} \tag{3-7}$$

$$\left(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Reg}}\right)\left(c_{j,k}^{\max,out,l} - c_{j,k}^{in,l}\right) \geq M_{j,k}^{l} \tag{3-8}$$

$$c_{j,k}^{in,l} = \frac{\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Reg}}^{l} + F_{j,k}^{Fw} c_{Fw}^{l}}{\sum_{i=1}^{I} F_{i,j,k}^{d} + \sum_{i=1}^{I} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}} + F_{j,k}^{Fw}} \tag{3-9}$$

$$\left(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Reg}}\right)\left(c_{j,k}^{out,l} - c_{j,k}^{in,l}\right) = M_{j,k}^{l} \tag{3-10}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Re}g} \le F_{j,k} \tag{3-11}$$

$$c_{j,k}^{in,l} \le c_{j,k}^{\max,in,l}, c_{j,k}^{out,l} \le c_{j,k}^{\max,out,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N \tag{3-12}$$

For the reuse/recycle scenario, water sinks are only fed by the available wastewater from storage tanks, or wastewater which is produced in the same stage, or regenerated water. The NLP model is expressed by Eqs (3-13)-(3-18). The difference between this scenario and the freshwater scenario is that the freshwater term is removed in all of the constraints. The objective function expresses the minimization of the sum of reuse water and the regenerated water. It applies individually to each stage.

$$\min \sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} \tag{3-13}$$

$$(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}})(c_{j,k}^{\max,out,l} - c_{j,k}^{in,l}) \ge M_{j,k}^{l} \tag{3-14}$$

$$c_{j,k}^{in,l} = \frac{\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Re}g}^{l}}{\sum_{i=1}^{I} F_{i,j,k}^{d} + \sum_{i=1}^{I} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}}} \tag{3-15}$$

$$(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Re}g})(c_{j,k}^{out,l} - c_{j,k}^{in,l}) = M_{j,k}^{l} \tag{3-16}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Re}g} \le F_{j,k} \tag{3-17}$$

$$c_{j,k}^{in,l} \le c_{j,k}^{\max,in,l}, c_{j,k}^{out,l} \le c_{j,k}^{\max,out,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N \tag{3-18}$$

For simplicity, in this work, only the states of freshwater and stored water are displayed in each stage. Once the freshwater consumption of each process is determined, the quantities of reused water and wastewater, as well as the maximum capacities of storage tanks can be identified. The problem was solved using the backward procedure of DP (Roberts 1964). In the following section, four examples, adapted from the literature, are explored in detail using the above methodology.

3.4 Illustrative examples

To illustrate the application of the proposed approach to network design in batch processes, four examples extracted from literature are investigated. Example 1 is composed of fixed quantity operations, while Example 2 is a hybrid system that includes different types of water-using operations. Example 3 and 4 are fixed-mass load operations. Example 3 considers water network design with a regeneration scheme, and Example 4 focuses on water network design with multiple contaminants.

3.4.1 Example 1

This example is taken from Majozi *et al*. (2006). In their work, all operations consume water only at the beginning of the operation and generate water only at the end of the operation, i.e., truly batch processes are considered. Additionally, water intake and discharge are assumed to take place instantly. The operations are based on a fixed water requirement. The start and end times of each operation are known *a priori*. To explain the method clearly, if an operation requires water in a certain stage, it is termed a water sink (SK). If an operation generates water which becomes available for later reuse, it is termed a water source (SR). The limiting data are summarized in Table 3.1.

Table 3.1 Limiting data for Example 1

Process	**Process number**	**Sinks**	**Time (h)**	$c^{\max,in}$ **(kg salt/kg water)**	**Water (kg)**	**Stage**
A wash	1	SK_1	0	0	1000	7
B reaction	2	SK_2	0	0.25	280	7
B wash	3	SK_3	4	0.1	400	4
C reaction	4	SK_4	2	0.25	280	6
C wash	5	SK_5	6	0.1	400	2
Process	**Process number**	**Sources**	**Time (h)**	$c^{\max,out}$ **(kg salt/kg water)**	**Water (kg)**	**Stage**
A wash	1	SR_1	3	0.1	1000	5
B reaction	2	SR_2	4	0.51	280	4
B wash	3	SR_3	5.5	0.1	400	3
C reaction	4	SR_4	6	0.51	280	2
C wash	5	SR_5	7.5	0.1	400	1

The whole process is divided into seven stages, based on the start and end times of each batch operation. The start and end times of each operation and the corresponding stages are shown in Figure 3.3. The time points 0 h, and 2 h are set as Stages 7 and 6, respectively. The end time point of the last operation, i.e., 7.5 h, is Stage 1. During each stage, the designer would decide to choose the freshwater scenario or reuse/recycle scenario to meet the water requirements. It is worth noting that in this example, water could not be reused in adjacent stages directly due to the discrete time of each stage. For example, Stage 3 is at 5.5 h, and Stage 2 is at 6 h. It is impossible to reuse the water which is available in Stage 3 to Stage 2 directly without the presence of a storage tank.

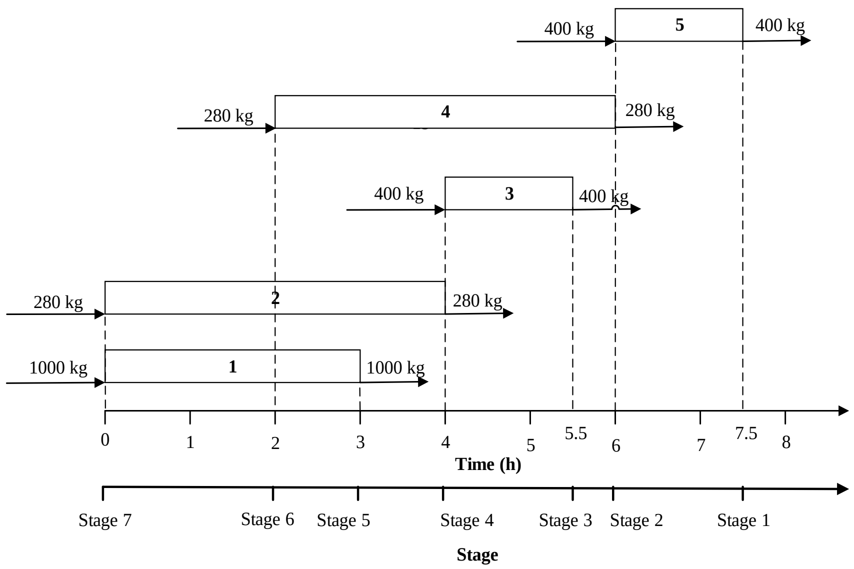

Figure 3.3 The relationship between stages and time of Example 1

In the synthesis of batch water networks for completely batch operations, first sequence and cyclic-state targeting are essential. The first sequence targeting focuses on a single batch over a relatively short time horizon of interest. The cyclic-state targeting occurs over an extended time horizon when more than one batch has to be produced in multi-stage operations. In the following subsection, the first sequence and cyclic-state scenarios are considered.

First sequence scenario

When the freshwater consumption of all the stages has been determined, the final quantities of stored water and generated wastewater can be calculated from the water balances of each operation. Furthermore, the maximum capacity of the storage vessel can also be determined. Hence, for simplicity, only the states where freshwater is consumed, and the initial quantity of stored water are displayed in this work. In every stage, the freshwater and reused water, for the freshwater scenario can be determined from Eqs (3-3) and (3-4). For the reuse/recycle scenario, the quantity of reused water is determined by Eqs (3-5) and (3-6). The detailed processes are described as follows.

Stage 7

In this stage, water sinks SK_1 and SK_2 can only be fed with freshwater because there is no available water source for reuse. Hence, there is only a state of freshwater consumption in Stage 7, with a quantity of 1,280 kg of freshwater consumed in this stage, i.e., $F_{SK_1,7}^{Fw}$ = 1,000 kg and $F_{SK_2,7}^{Fw}$ = 280 kg. As there are no alternative water sources, the quantity of stored water is zero. The selected state and return cost for Stage 7 is shown below. This work does not consider the cost of consumed freshwater consumption. Therefore, the return cost for the problem is the extent of freshwater consumption.

$$S_{Stage7} = \left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} = 1,280kg, F_{\text{Tank1}}^{St} = 0kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min \left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} + f_6(F_{j,6}^{Fw}) \right\} = \min \left\{ 1,280kg + f_6(F_{j,6}^{Fw}) \right\}$$

Stage 6

In Stage 6, there is no water available for reuse, and so the water sink SK_4 is also fed by freshwater, i.e., 280 kg. Therefore, the chosen state of Stage 6 is shown below. The recursive function of the problem could be updated by the state of freshwater consumption in Stage 6. The return cost is the sum of the minimum freshwater consumption in Stages 6 and 7 and the freshwater consumption over the remaining stages (Stages 1-5).

$$S_{Stage6} = \left\{ \sum_{j}^{J_6} F_{j,6}^{Fw} = 280kg, F_{\text{Tank1}}^{St} = 0kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min \left\{ 1,280kg + \sum_{j}^{J_6} F_{j,6}^{Fw} + f_5(F_{j,5}^{Fw}) \right\} = \min \left\{ 1,560kg + f_5(F_{j,5}^{Fw}) \right\}$$

Stage 5

In Stage 5, a water source SR_1 exists. This means the state of freshwater consumption is zero, i.e., $\sum_{j}^{J_5} F_{j,5}^{Fw}$ = 0 kg. Water source SR_1 is of a high enough quality, i.e., 0.1 kg salt per kg water that it could be sent to the storage facilities for indirect reuse in later stages. In theory, there are a great number of states of stored water in this stage, i.e., the quantity of wastewater sent to the storage tank ranges from 0 kg to 1000 kg. The available wastewater is 1000 kg. The quantity of stored water mainly depends on the water requirements of water sinks in later stages. Once the states of freshwater consumption in Stages 2 and 4 are determined, the maximum required capacity of the storage tank can be identified. At this phase of the procedure, it is assumed that all the water from the source SR_1 is sent to the stored tank, i.e., Tank 1. Note that the quantity of stored water in Stage 5 is not the final result. It will be updated if the later stage does not require the current quantity of stored water. Therefore, the selected state of stored water in Stage 5 is determined, i.e., F_{Tank1}^{St} = 1,000 kg. The state of freshwater and stored water, the return cost of the problem are expressed as follows.

$$S_{Stage5} = \left\{ \sum_{j}^{J_5} F_{j,5}^{Fw} = 0kg, F_{\text{Tank1}}^{St} = 1,000kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min \left\{ 1,560kg + \sum_{j}^{J_5} F_{j,5}^{Fw} + f_4(F_{j,4}^{Fw}) \right\} = \min \left\{ 1,560kg + f_4(F_{j,4}^{Fw}) \right\}$$

Stage 4

A water sink SK_3 and a water source SR_2 exist in this stage. To meet the water requirement of SK_3, there are two possible states of freshwater consumption. As restored water from Stage 5 has a concentration of 0.1 kg salt per kg water, which is equal to the inlet concentration of water sink SK_3, the stored water can be reused by the water sink SK_3. Hence, the first possible state is that the indirect reuse water $F_{Tank1,SK_3,4}^{ind}$ from Tank 1 is 400 kg, and the freshwater consumption is zero. The second possible state is that water sink SK_3 is fed with freshwater, i.e., $F_{SK_3,4}^{Fw}$ =400 kg. Because the stored water from Stage 5 is enough to supply the water sink in this stage, and the quality of water from the source SR_2 is inferior, i.e., 0.5 kg salt per kg water, to that of the stored water, the water from SR_2 is discharged as wastewater. The state of stored water in the Tank 1 is thus 600 kg, i.e., 1,000 kg (from Stage 5) − 400 kg (to Stage 4). The states of freshwater consumption for Stage 4 are shown as follows.

$$S_{Stage4}^{1} = \left\{ \sum_{j}^{J_4} F_{j,4}^{Fw} = 0kg, F_{Tank1,SK_3,4}^{ind} = 400kg, F_{\text{Tank1}}^{St} = 600kg \right\}$$

$$S_{Stage4}^{2} = \left\{ \sum_{j}^{J_4} F_{j,4}^{Fw} = 400kg, F_{Tank1,SK_3,4}^{ind} = 0kg, F_{\text{Tank1}}^{St} = 1,000kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{1,560kg + \sum_{j}^{J_4} F_{j,4}^{Fw} + f_3(F_{j,3}^{Fw})\right\} = \min\left\{1,560kg + f_3(F_{j,3}^{Fw})\right\}$$

Stage 3

In Stage 3, only a water source SR_3 exists. Because SR_3 has a lower concentration, i.e. 0.1 kg salt per kg water, which matches the maximum inlet concentration of sink SK_5 in Stage 2, all of the available water from SR_3 can be stored in Tank 2 for indirect reuse. The state of freshwater consumption $\sum_{j}^{J_3} F_{j,3}^{Fw}$ is zero for Stage 3. Since in the later stages, Stages 1 and 2, contain a single water sink with a demand of 400 kg, the water from water source SR_3 can be stored in a separate tank (Tank 2) for reuse. Therefore, the state of stored water in Stage 3 is 400 kg, with a concentration of 0.1 kg salt per kg water.

$$S_{Stage3} = \left\{\sum_{j}^{J_3} F_{j,3}^{Fw} = 0kg, F_{\text{Tank1}}^{St} = 600kg, F_{\text{Tank2}}^{St} = 400kg\right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{1560kg + \sum_{j}^{J_3} F_{j,3}^{Fw} + f_2(F_{j,2}^{Fw})\right\} = \min\left\{1,560kg + f_2(F_{j,2}^{Fw})\right\}$$

Stage 2

Water sink SK_5 and water source SR_4 exist in Stage 2. There are two possible states of freshwater consumption. In other words, water sink SK_5 can be fed with the stored water from Stage 3 instead of freshwater, $F_{SK_5,2}^{Fw}$ = 0 kg, or it can be fed with only freshwater, $F_{SK_5,2}^{Fw}$ = 400 kg. For the state of reuse water, the sink can use the water stored in Tank 1 from Stage 5 ($F_{Tank1,SK_5,2}^{ind}$ = 400 kg) or the water stored in Tank 2 from Stage 3 ($F_{Tank1,SK_5,2}^{ind}$ = 400 kg).

To reduce the cost of storage, it is better to select the water which was stored at the time closest to Stage 2, i.e., the water stored in Tank 2. This is the implementation of rule 2 as mentioned in Section 3. Due to the higher concentration (0.51 kg salt per kg water), all the water from water source (SR_4) should be discharged as wastewater. The states of freshwater are presented as follows.

$$S_{Stage2}^{1} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 0kg, F_{Tank2,SK_5,2}^{ind} = 400kg, F_{\text{Tank1}}^{St} = 600kg, F_{\text{Tank2}}^{St} = 0kg \right\}$$

$$S_{Stage2}^{2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 400kg, F_{\text{Tank1}}^{St} = 1000kg, F_{\text{Tank2}}^{St} = 0kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{1,560kg + \sum_{j}^{J_2} F_{j,2}^{Fw} + f_1(F_{j,1}^{Fw})\right\} = \min\left\{1,560kg + f_1(F_{j,1}^{Fw})\right\}$$

Stage 1

Stage 1 is the last stage of the problem and consists of a single water source SR_5. Therefore, the state of freshwater consumption is zero. Water from SR_5 is discharged as wastewater.

$$S_{Stage1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0kg, F_{Tank1}^{St} = 600kg, F_{Tank2}^{St} = 0kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{1,560kg + \sum_{j}^{J_1} F_{j,1}^{Fw}\right\} = \left\{1,560kg + 0kg\right\} = 1,560kg$$

At this point, it can be concluded that the total freshwater consumption is 1,560 kg. Two tanks with a capacity of 1,000 kg and 400 kg, respectively, are required to store wastewater for reuse. However, in Stage 1, Tank 1 is not empty but contains 600 kg of reuse water. This implies that only 400 kg of water from SR_1 in Stage 5 should be sent to Tank 1 and the remaining 600 kg should be discharged as wastewater. As a result, the stored water from Stage 5 is completely consumed in Stage 4; Tank 1 is empty again in Stage 3. Hence, only one tank is required for this problem. In other words, water from SR_3 in Stage 3 can be sent to Tank 1. The maximum required capacity of the tank is 400 kg.

The chosen states for the problem are represented in a solid circle, as shown in Figure 3.4. The arc represents the chosen path from the state of the previous stage to the state of the next stage. The solid arcs indicate the path from the optimal state in the previous stage to the optimal state in the adjacent stage, while the dashed arc is the alternative state. The value along each arc is the state of freshwater consumption from the present stage to the adjacent stage. Therefore, the sum of all the values along with the solid arc, is the target of freshwater consumption, i.e., 1,560 kg.

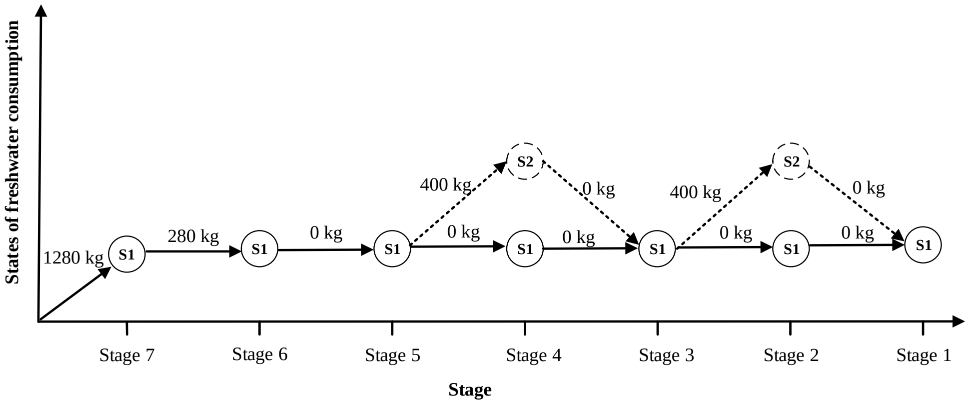

Figure 3.4 The optimal state of Example 1 (first sequence)

The final network of water flows of operations is shown in Figure 3.5. The freshwater consumption and wastewater generation of Example 1 (first sequence) are both 1,560 kg. The targets identified in this work match with those reported by Majozi et al. (2006).

As shown in Figure 3.5, the wastewater generated by operation 1 (A wash) is stored in the tank and then is reused by operation 3 (B wash). Thus, if operation 1 finishes at 4h, the tank can be removed. The other choice is to move operation 3 to 3h. However, operation 3 should start after operation 2 (B reaction) finishes. Thus, the only choice is to extend operation to 4h. Similarly, the tank for operation 5 (C wash) can be removed by starting operation 4 (C reaction). Therefore, it is not necessary to use the tank by rescheduling the operations. The final network after rescheduling operation is shown in Figure 3.6.

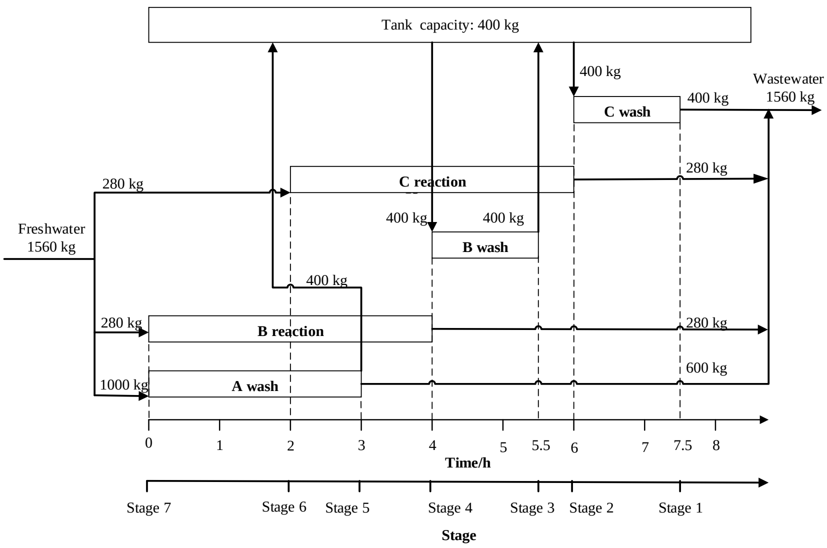

Figure 3.5 The resultant network for Example 1 (first sequence)

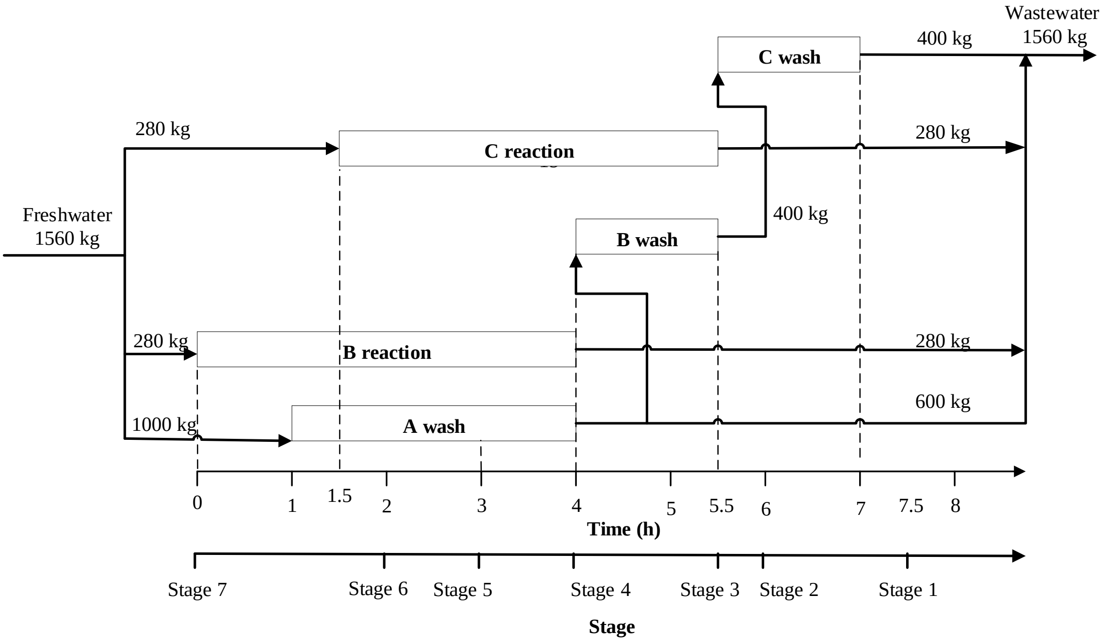

Figure 3.6 The resultant network for Example 1 after rescheduling (first sequence)

Cyclic operation scenario

In the industry, more than one batch is operated for a certain operation to achieve the required capacity or meet required product demand. Therefore, consecutive batches are repeated with the same schedule in an extended time horizon. This kind of operating mode is termed cyclic, which is the equivalent of steady state in continuous operations. In cyclic batch operations, processes can use surplus water from previous batches through the use of storage tanks. This means that later water sources in previous batches can be used to supply the earlier water sinks in later batches.

Based on the preceding analysis of the single batch case, insight on the potential reuse of water between water sinks and sources can be obtained. For example, 600 kg of high-quality water from SR_1 at 0.1 kg salt/kg water in Stage 5 and 400 kg of the same quality water from SR_5 in Stage 1 are discharged as wastewater in the first sequence scenario. These two water sources could instead be stored in a tank for reuse in the next batch case. To reduce the freshwater consumption as much as possible, water from these two water sources should be sent to a storage tank for future reuse in possible sinks. Hence, the maximum amount of stored water in Tank 1 (F_{Tank1}^{St}) is 1,000 kg, i.e., 600 kg from SR_1 and 400 kg from SR_5. It should be noted that only the stages which are different from the first sequence are presented in detail and the repeated stages are omitted.

Stage 7

Since water sink SK_1 has a maximum inlet concentration of 0 kg salt per kg water, it should be fed with freshwater. The inlet concentration of SK_2 is 0.25 kg salt per kg water, which implies that it can be supplied with stored water from previous batch cycles, which is of a concentration of 0.1 kg salt per kg water. Hence, the state of freshwater consumption in Stage 7 is determined as $F_{SK_1,7}^{Fw}$ =1,000 kg. It should be noted that the state of stored water at this point is an initial result and that will be updated based on the specific consumption of stored water.

$$S_{Stage7} = \left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} = 1,000kg, F_{\text{Tank1}}^{St} = 720kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} + f_6(F_{j,6}^{Fw}) \right\} = \min\left\{1,000kg + f_6(F_{j,6}^{Fw})\right\}$$

Stage 6

In the first sequence scenario, there is no available water for reuse in this stage, and the water sink SK_4 was still fed by freshwater, i.e., 280 kg. However, for the cyclic-state scenario, the water stored in the tank is of sufficient quantity and quality to supply SK_4. Hence, the state of freshwater consumption is zero.

$$S_{Stage6} = \left\{ \sum_{j}^{J_6} F_{j,6}^{Fw} = 0kg, F_{\text{Tank1}}^{St} = 440kg \right\}$$

$$f_7(F_{j,7}^{Fw}) = \min\left\{1,000kg + \sum_{j}^{J_6} F_{j,6}^{Fw} + f_5(F_{j,5}^{Fw}) \right\} = \min\left\{1,000kg + f_5(F_{j,5}^{Fw})\right\}$$

As the remaining stages are the same as the first sequence scenario as described in the previous section, it is not necessary to repeat this information here. The chosen states for this scenario are shown in Figure 3.7. The value along each arc is the state of freshwater consumption from the present stage to the adjacent stage. Therefore, the sum of all the values along with the solid arc is determined as the target of freshwater consumption, i.e., 1000 kg. The same method can be used to identify the target of wastewater generation.

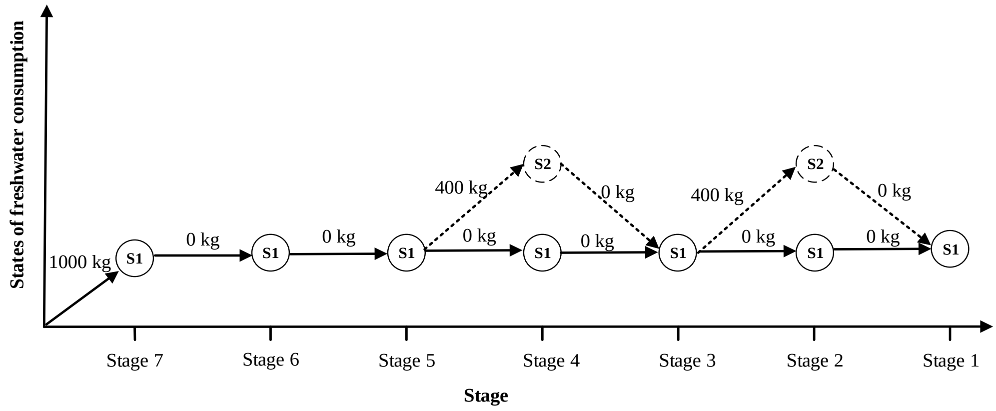

Figure 3.7 The optimal state of Example 1 (cyclic operation)

Both the freshwater demand and wastewater generation for the cyclic operation are 1,000 kg. This result is identical to the results of Majozi *et al*. (2006). Compared to the first sequence scenario, the difference here is the storage tank which provides enough water for SK_2 (Stage 7) and SK_4 (Stage 6). As a result, the maximum capacity of the storage tank is 560 kg, which equals to Majozi *et al*. (2006). The water reuse network is shown in Figure 3.8.

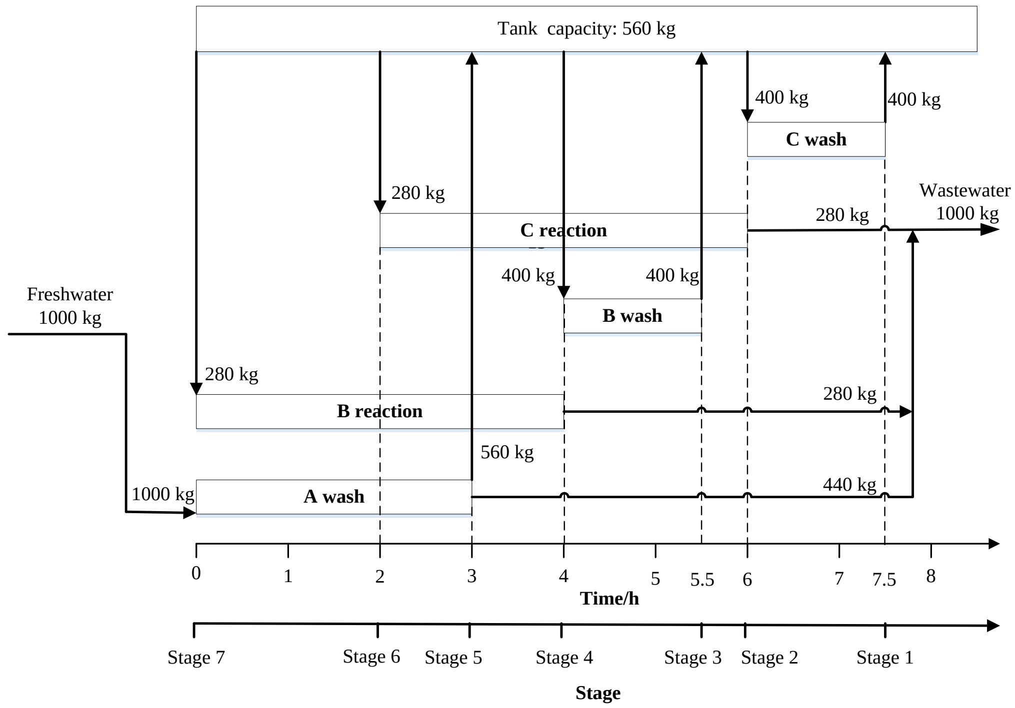

Figure 3.8 Water network for Example 1 (cyclic operation)

As shown in Figure 3.8, the stored water in the tank almost supplies all the operations, excluding operation 1 (A wash). By rescheduling the operations, it is possible to reuse the water directly, rather than storing them in the tank. This could reduce the complexity of the network and the operation time horizon. Results of rescheduling operations are presented in Figure 3.9.

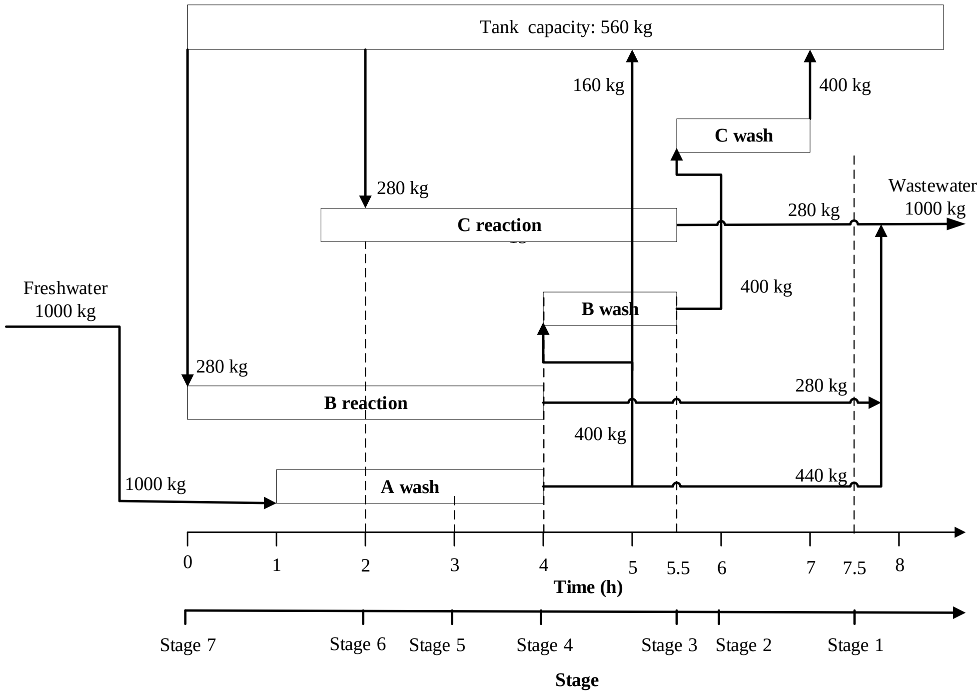

Figure 3.9 Final network for Example 1 after rescheduling (cyclic operation)

3.4.2 Example 2

In practice feeding and discharging the system is not accomplished instantly. The operations have specific processing times during input and output periods. The limiting water data for Example 2 are shown in Table 3.2, where Operations 1, 2, 4 are formulated as fixed-mass load operations and Operations 3, 5 are treated as fixed flowrate operations (Chen and Lee, 2008; Foo, 2012). Although water charging and discharging are not accomplished rapidly, the proposed method can also be applied to this example. This is because the process of decision-making is an instant action and it does not last for the whole input and output periods. It has no impact on the target of freshwater consumed in this example. Therefore, those operations can still be treated as a completely batch model.

Table 3.2 Problem specification for Example 2

Sinks	Time (h)	$C^{max,in}$ (kg salt/kg water)	Water (t)	Sources	Time (h)	$C^{max,out}$ (kg salt/kg water)	Water (t)
SK_1	0	0.0	20	SR_1	4	0.2	20
SK_2	0	0.25	16	SR_2	4	0.5	16
SK_3	5	0.1	15	SR_3	5	0.1	15
SK_4	2	0.25	24	SR_4	6	0.4	24
SK_5	7	0.1	15	SR_5	7	0.12	15

The stage is set based on the starting point of the feeding period and the discharging period, as shown in Figure 3.10.

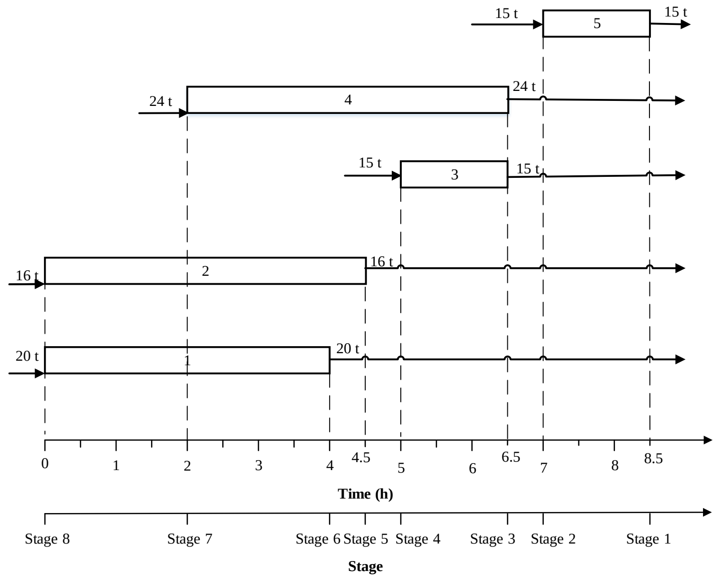

Figure 3.10 The relationship between time and stage for Example 2

For fixed flowrate operations, the freshwater and wastewater are determined by Eqs (3-3)−(3-6). For fixed-mass load operations, the freshwater and wastewater are determined by Eqs (3-7)−(3-18). In this example, the first sequence and cyclic-state batch process are also introduced.

First sequence scenario

The same procedure is repeated in this scenario. The problem can be divided into eight stages based on the charging or discharging time. The detailed calculation processes are omitted for simplicity. The chosen states for this scenario are shown in Figure 3.11. To easily understand which process has the water requirement or requires to discharge the wastewater, the limiting data of water sinks and sources are given in this example rather than the inlet and out concentration.

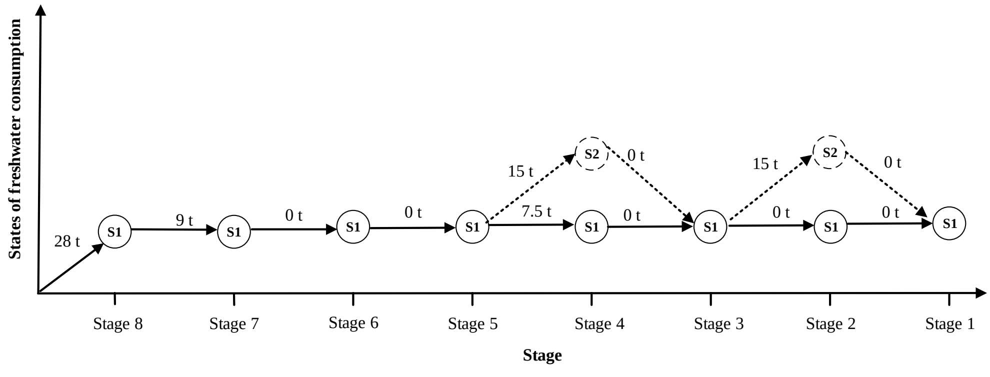

Figure 3.11 The optimal state of Example 2 (first sequence)

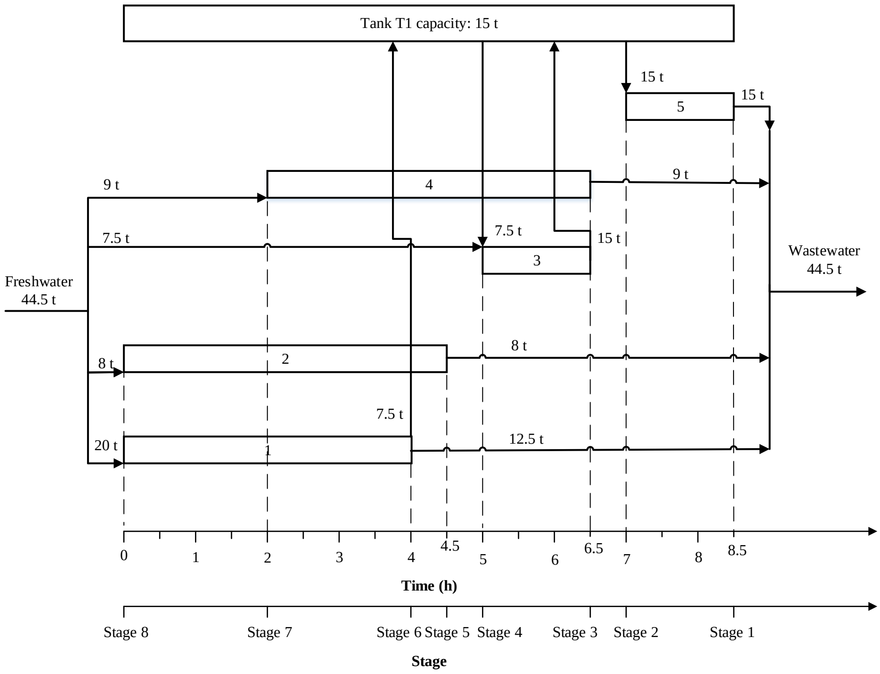

Figure 3.12 Resultant water network of Example 2 (first sequence)

During the calculation process, the water requirement at a specific stage is determined by mass load and the inlet and outlet concentration if it is formulated as a fixed-mass load process. For example, Operation 2 has a limiting quantity of 16 t. But it is formulated as a fixed-mass load process. The freshwater consumption is thus determined as 8 t, rather than the limiting water flow of 16 t. The solid arcs represent the optimal path from Stage 8 to Stage 1. Therefore, the sum of all the values along with the solid arc is determined as the target of freshwater consumption, i.e., 44.5 t. It is easily to identify the target of wastewater generation.

As a result, both the amount of freshwater and wastewater for the first sequence of Example 2 are 44.5 t. The final network is shown in Figure 3.12. The targets identified in this scenario could match with those reported by Chen and Lee (2008). It is noting that in this work, effluent of Operation 3 is not allowed to feed itself. Hence, the reference of the freshwater consumption in Chen and Lee (2008) is set as 44.5 t, not 39.5 t, which is the scenario of the effluent of Operation 3 feeding itself without any treatment.

As shown in Figure 3.12, the tank can be removed by moving operations 3 and 5 to an early time point. By rescheduling operations, the tanks can be removed, and the time horizon can be further reduced. Results after rescheduling are shown in Figure 3.13. The freshwater consumption is the same as Figure 3.12. However, the operation time for all the processes are reduced to 7 h. Furthermore, the storage tank is removed as compared to Figure 3.12.

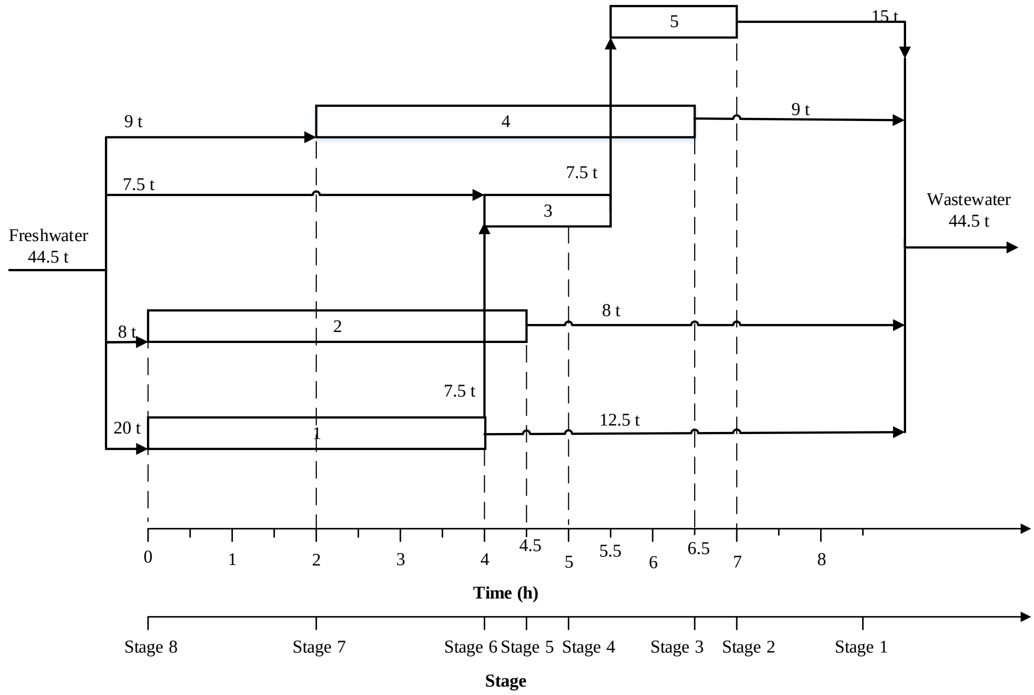

Figure 3.13 Water network of Example 2 after rescheduling (first sequence)

Cyclic-state scenario

Based on the single batch case, some insight could be obtained. For example, 12.5 t of water for Operation 1 and 15 t of water for Operation 5 are discharged as wastewater. However, Operations 1 and 5 have an outlet concentration of 0.2 kg salt per kg water and 0.12 kg salt per kg water, respectively. The water from Operations 1 and 5 could be sent to Tanks 1 and 2, respectively, and stored for future reuse. The stored water in Tanks 1 and 2 before the cyclic operation is 20 t and 15 t. The same procedure is similar to the previous section. The chosen states for this scenario are shown in Figure 3.14. Therefore, the target of freshwater consumption is determined as 26.42 t.

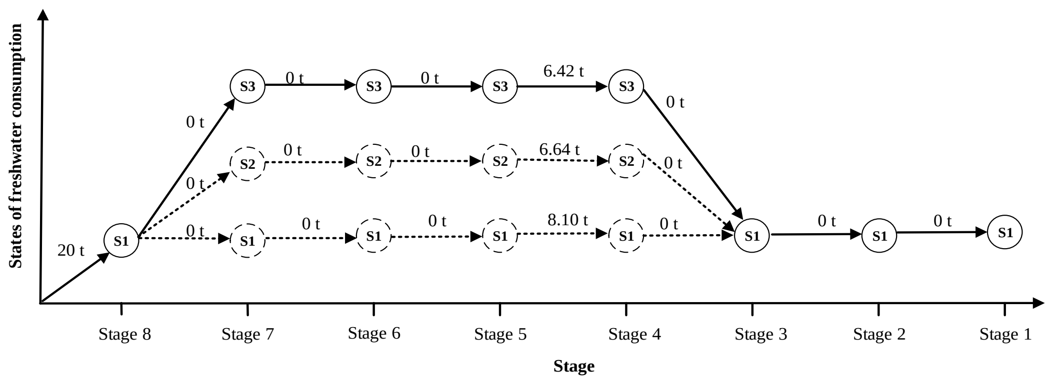

Figure 3.14 The optimal state of Example 2 (cyclic operation)

Since the quantity of freshwater consumed in this scenario is determined, the wastewater can be identified based water balance of each operation. In this scenario, both the amount of freshwater and wastewater for the cyclic operation are 26.42 t, as shown in Figure 3.15.

The targets identified in this scenario are less than those reported by Chen and Lee (2008) (27.5 t). This is because in this work all the wastewater from Operation 1 is sent to a storage tank, while in the work of Chen and Lee (2008) 1.88 t of water is discharged as wastewater. Furthermore, the freshwater consumption in this scenario is also less than that (31.021 t) of Liu et al. (2009). However, in this work, two storage tanks are used, while in Liu et al. (2009) only one tank is involved. But the results of this work have less capacity of the storage facility (20 t and 15 t) compared with those (16.22 t and 15 t) of Chen and Lee (2008). Noting that in this work, the effluent of Operation 3 is not allowed to feed itself. Hence, the result of this work can be comparable with the target of 27.5 t in Chen and Lee (2008), where the effluent of Operation 3 is not allowed to feed itself without any treatment.

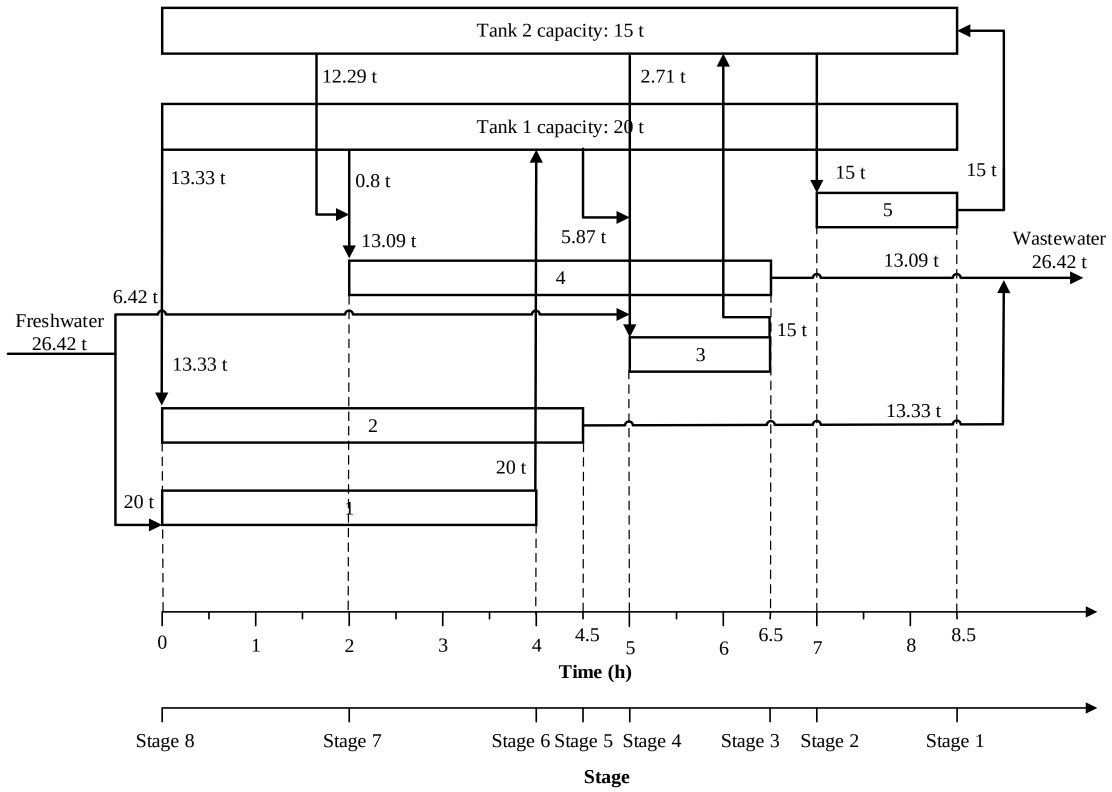

Figure 3.15 Resultant water network for Example 2 (cyclic state)

In the cyclic operation, the wastewater generated in the previous batch can be used stored in the tank and then reused by the operations of the next batch. As shown in Figure 3.15, the complexity of the network could be reduced by rescheduling some operations. For example, the wastewater generated by operation 3 can be reused by operation 5 if the operation can be moved forward. The evolved water network is shown in Figure 3.16. The capacity of tank 1 is reduced to 14.13 t, and the time horizon can be shortened from 8.5 h to 7.5 h.

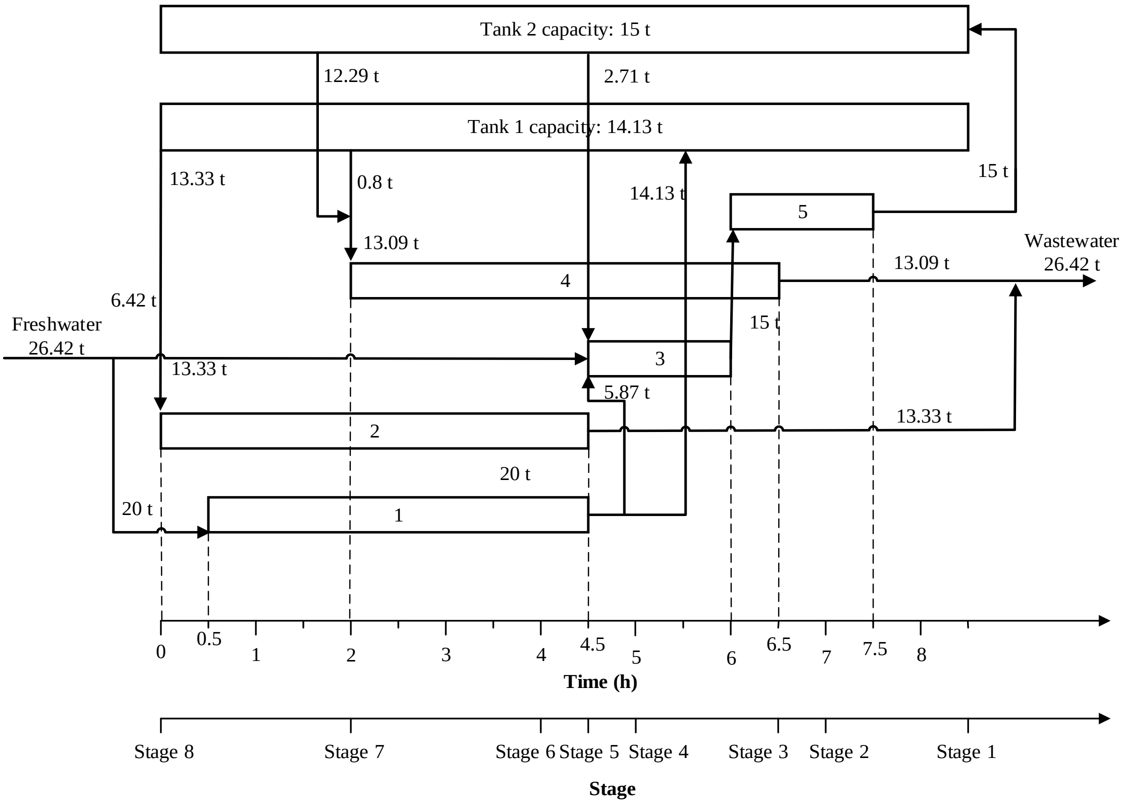

Figure 3.16 Water network for Example 2 after rescheduling operations (cyclic state)

3.4.3 Example 3

In the previous examples, the problems are mainly based on fixed flowrate assumption. Although in Example 2 some operations are fixed-mass load problems, it is not enough to prove the proposed method can be applied to fixed-mass load problems. In this section, a literature example adapted from Liu *et al*. (2009) with fixed-mass load problem is illustrated to explain the method. Two scenarios are taken into account, i.e., water reuse scenario with a central buffer tank and water reuse scenario with central buffer tank and regeneration.

Water reuse scenario with a central buffer tank

This scenario deals with the integration of a water-using system that consists of fixed-mass load operations. The limiting water data are given in Table 3.3. For fixed-mass load problems, it is improper to divide the operation into water sources and sinks. This is because the water quantity of operation is dependent on inlet and outlet concentration.

Table 3.3 Limiting water data for Example 3

Operation	Quantity/t	C^{in}/(μg/g)	C^{out}/(μg/g)	T_{in}/h	T_{out}/h	M/kg
A	50	0	400	0	2	20
B	30	100	400	3	4	9
C	10	200	500	3	6	3
D	24	350	600	3.5	7.5	6
E	40	450	700	6	8.5	10

The detail process is similar to the previous examples. For simplicity of the analysis, only the states of freshwater and stored water are shown in detail. The quantity of freshwater and wastewater is identified by the mass load and the concentration difference of each operation, i.e., Eqs (3-7)−(3-12) or Eqs (3-13)−(3-18). Based on the starting and finishing times, this batch processes comprise of 8 stages, as shown in Figure 3.17. The details of the targeting processes are described in Appendix A.

The optimal states, for example, are shown in Figure 3.18. The total freshwater consumption is identified as 80.5 t, indicating that the configuration of water reuse between different operations is also determined. Because Operations A and B have the same outlet concentration and wastewater from these two operations has a high quality, it is assumed that all the water discharged is sent to the tank during the targeting process. When the freshwater target is determined, there are surplus wastewater stored in the tank. Hence, it is necessary to check the amount of water sent to the tank to employ a minimum capacity of the tank.

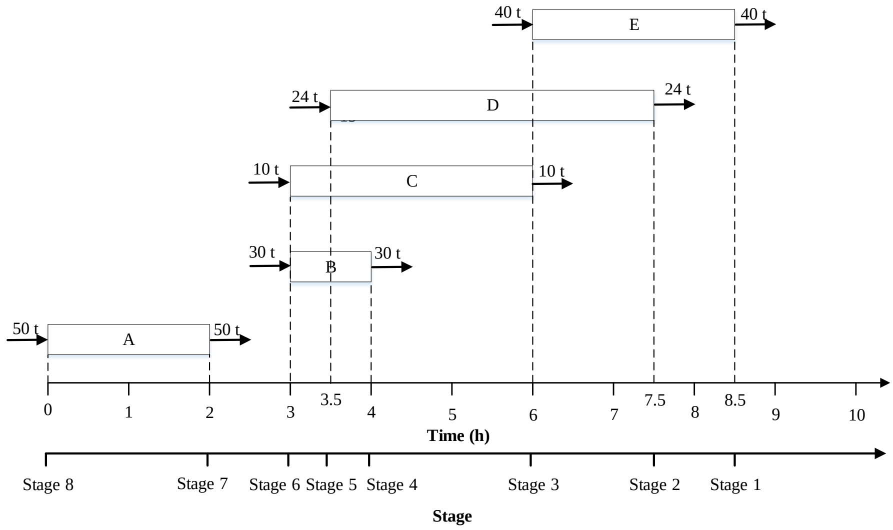

Figure 3.17 The relationship between time and stage for Example 3

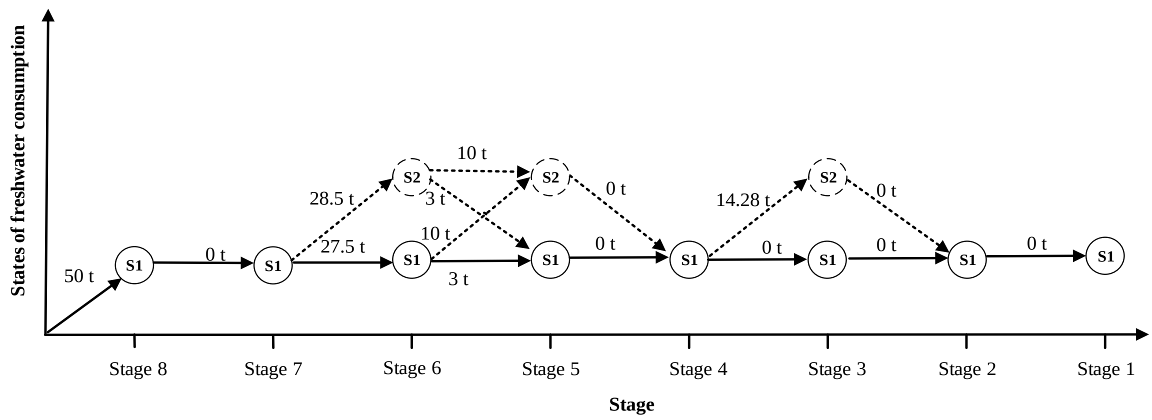

Figure 3.18 The optimal states for Example 3 (reuse scenario)

It is proper to identify the stored water in each stage using a backward approach. In other words, the stored water could be identified from Stage 1 to Stage 8. This is because Operations A and B finish early with a lower concentration and the capacity of the storage tank is mainly determined by the amount of wastewater from Operations A and B. It is easy to determine the capacity of tank based on the water requirement. For example, in Stage 3 an amount of 26.67 t water is required from Tank 1 to supply process E, that water should be stored in Tank 1 before Stage 3. In Stage 4, wastewater generated from process B is 22.5 t. The deficit quantity of 4.17 t, i.e., 26.67 t – 22.5 t, should be sourced from the previous stages. However, Operation A is the only source of stored water. The maximum capacity of Tank 1 is 30.17 t, which is the sum of indirect water at Stage 6 (5 t), Stage 5 (21 t) and the deficit water for Stage 4 (4.17 t).

The actual inlet and outlet concentrations and corresponding mass load for each operation are summarized in Table 3.4.

Table 3.4 Specification of Example 3 with central buffer tank

Operation	Quantity/t	C^{in}/(μg/g)	C^{out}/(μg/g)	M (kg)
A	50	0	400	20
B	22.5	0	400	9
C	10	200	500	3
D	24	350	600	6
E	36.67	427.27	700	10

The final results of the water network are shown in Figure 3.19. The result of freshwater consumption matches with that of literature (Liu *et al*., 2009). However, the capacity (30.17 t) of the tank in this work is less than the literature example (41.302 t). The difference is that in this work all the wastewater discharged from Operation B is sent to the tank, while in Liu *et al*. (2009) an amount of 7.37 t water is discharged as wastewater.

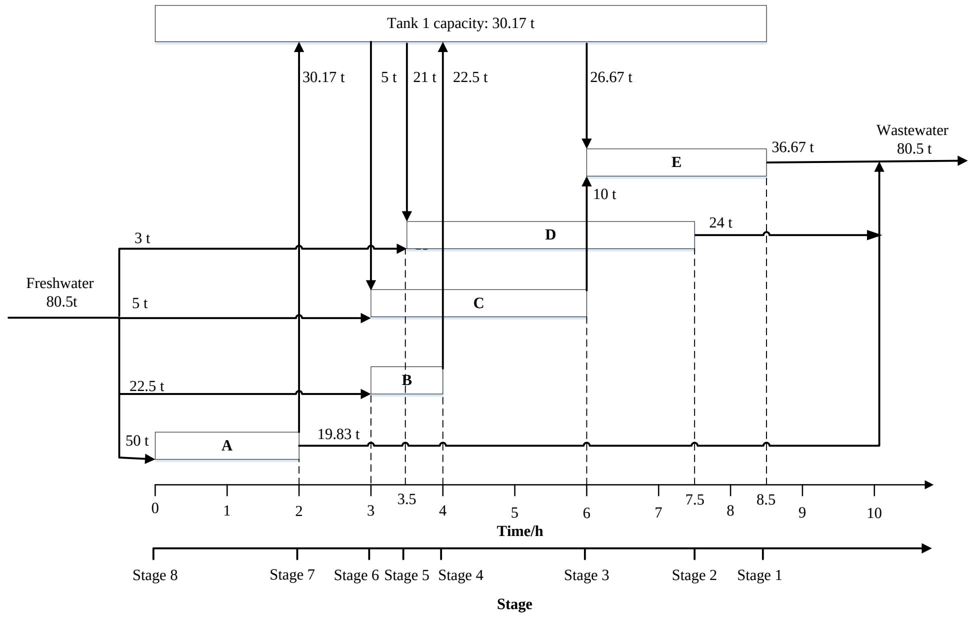

Figure 3.19 Optimal network for Example 3 (reuse scenario)

Based on the results of Figure 3.19, it is easily found that the network can be evolved to be simpler by changing the sequence of operations. The results of rescheduling operations are shown in Figure 3.20. The capacity of the tank is reduced to 4.17t.

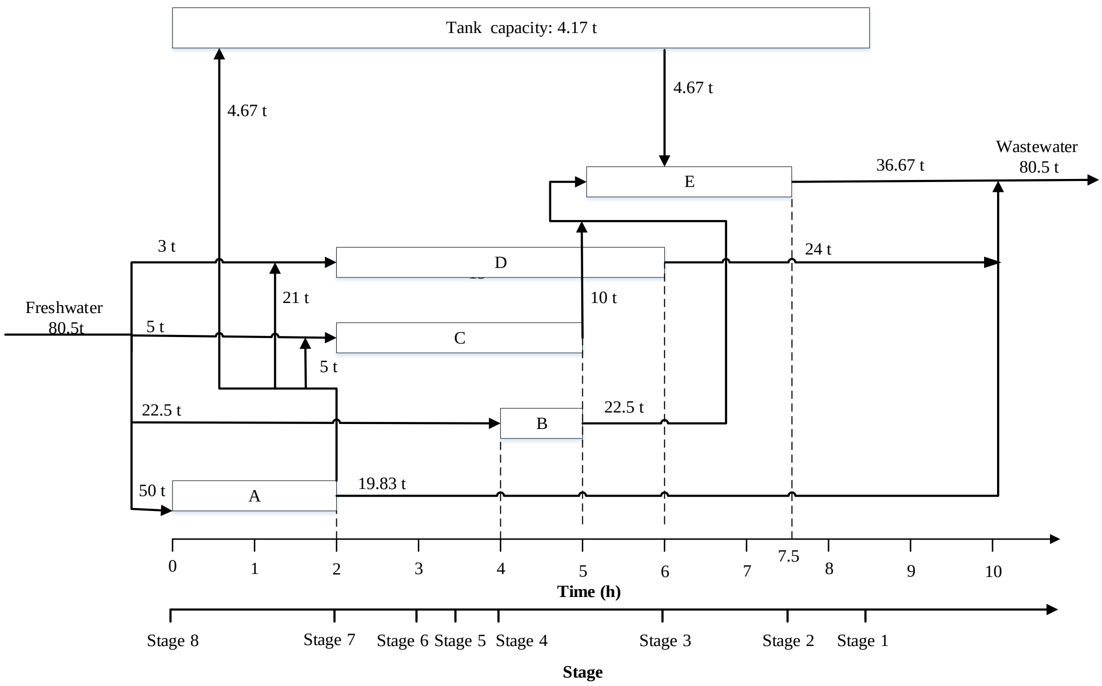

Figure 3.20 Water network for Example 3 after rescheduling operations (reuse scenario)

Water reuse scenario with a central buffer tank and regeneration

In some cases, the potential of water reuse in batch processes could be exhausted. It might, therefore, be required to employ the regeneration to purify wastewater for reuse. The outlet concentration of the central regeneration unit in this example is set to be 100 $\mu g/g$. The flowrate for regeneration is 11.875 t/h. As aforementioned, the whole batch process is divided into eight stages. The details of targeting processes are also omitted. The optimal states for the problem are shown in Figure 3.21.

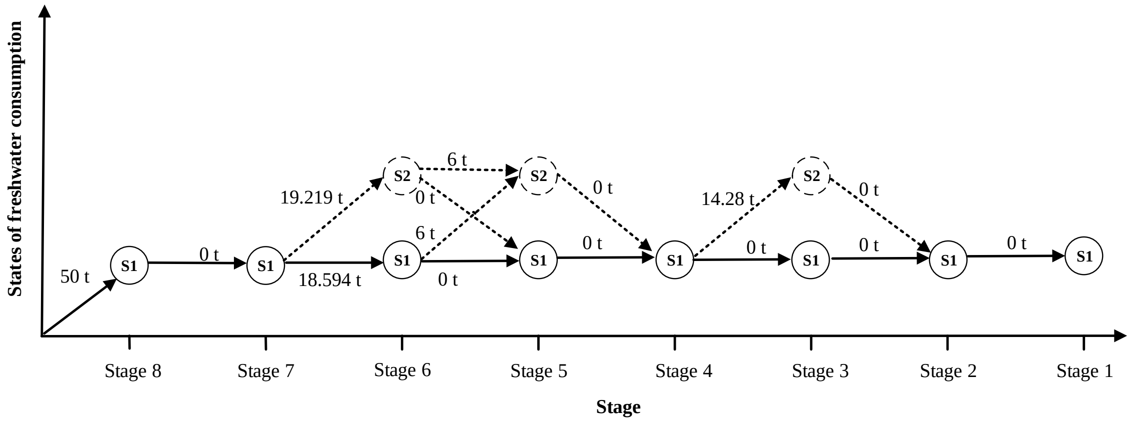

Figure 3.21 The optimal states for Example 3 (regeneration scenario)

The total freshwater of this scenario is 68.594 t. The wastewater is 25.886 t. At the end of this batch process, the remaining regenerated water in the tank is 42.708 t. The capacity of Tanks is 50 t and 42.708 t. The actual inlet and outlet concentrations are shown in Table 3.5.

Table 3.5 Specification of Example 3 with regeneration unit

Operation	Quantity/t	C^{in}/(μg/g)	C^{out}/(μg/g)	M (kg)
A	50	0	400	20
B	25.469	46.63	400	9
C	10	200	500	3
D	21.094	315.55	600	6
E	16.667	100	700	10

The final water network is shown in Figure 3.22. Compared with Liu *et al*. (2009), this work has the same target of freshwater consumption. It should be noted that this work has a higher quantity of wastewater than that of Liu *et al*. (2009), i.e., 16.316t. This is because, in Liu et al. (2009), a quantity of 9.569 t wastewater is stored in the storage tank at the end of the operation. However, the network obtained in this work has less connection. For example, in Liu et al.

(2009), water requirement of process C is satisfied by three sources, i.e., freshwater, regenerated water and indirect reuse water from process A. In this work process C is fed with freshwater and indirect reuse water from process A. Note that because this scenario considers the regeneration unit. If the timing of some operations is changed, the water network is no longer optimal. Thus, in this scenario, the rescheduling is not considered.

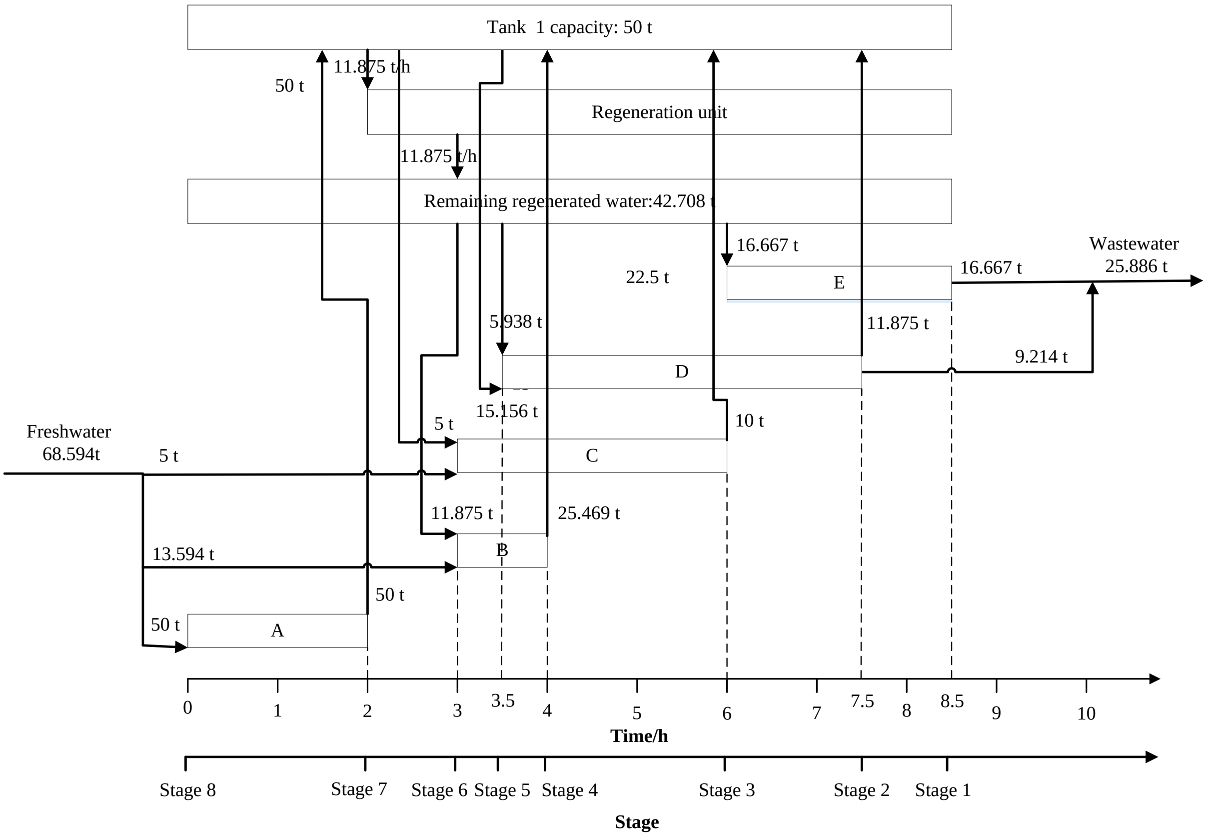

Figure 3.22 Water network for Example 3 with regeneration unit

3.4.4 Example 4

In industry, it is a common occurrence that wastewater is contaminated with multiple contaminants. Most of the wastewater minimization methodologies have been proposed to deal with single contaminant systems. This restricts the application of the methodologies to a small range of problems. Therefore, in this example, DP is used to design a batch water network with multiple contaminants. The example is extracted from the literature (Kim and Smith 2004, Majozi 2010). The example involves seven water-using operations with three contaminants presented in the system. This example is assumed to be fixed-mass load problem. The limiting data for the example are given in Table 3.6.

Table 3.6 Limiting data for Example 4

Operation	Contaminant	$C^{\max,in}$ (ppm)	$C^{\max,out}$ (ppm)	Mass load (kg)	Water (t)	Start time (h)	End time (h)
	C1	0	20	4			
1	C2	0	400	80	200	0	0.5
	C3	0	50	10			
	C1	50	100	15			
2	C2	200	1000	240	300	1	2
	C3	50	12000	3585			
	C1	10	200	28.5			
3	C2	50	100	7.5	150	2	3.5
	C3	300	1200	135			
	C1	30	75	9			
4	C2	100	200	20	200	1	2
	C3	200	1000	160			
	C1	150	300	15			
5	C2	200	1000	80	100	4	4.5
	C3	350	1200	85			
	C1	0	150	22.5			
6	C2	0	300	45	150	5.5	6.5
	C3	50	2500	367.5			
	C1	100	200	5			
7	C2	150	1500	67.5	50	8	10
	C3	220	1000	39			

The whole batch process is divided into 11 stages through starting and ending time, as demonstrated earlier in this paper. The same procedure in the previous section is applied to determine the optimal freshwater consumption in every stage. As this example considers multiple contaminants, in every stage, a nonlinear model with minimum freshwater as the objective function is constructed based on the Eqs (7)−(12) or Eqs (13)−(18). The GRG (Generalized Reduced Gradient) solver in Microsoft Excel is chosen to solve sets of nonlinear equations. The nonlinear functions are input as cells and equation residuals are minimized. The freshwater consumption and reuse water in every stage are then solved using algebraic methods. The calculation method is similar to the previous examples and is thus not explained in detail. The optimal states for the problem are shown in Figure 3.23.

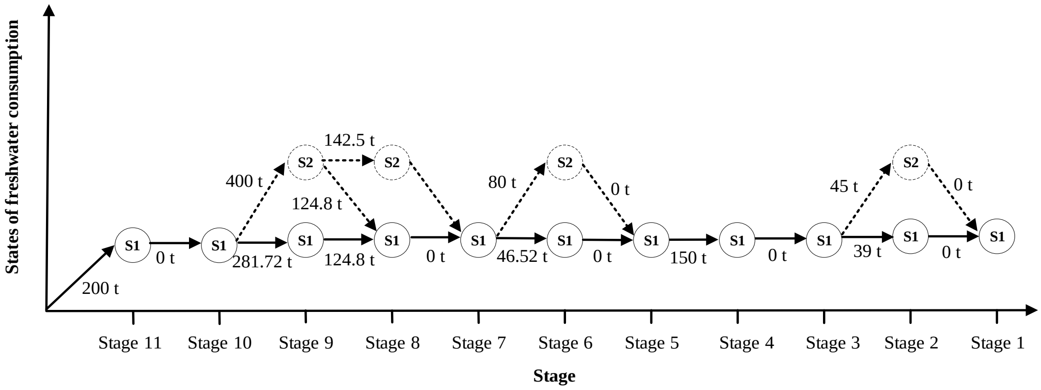

Figure 3.23 The optimal states for Example 4 with two tanks

The total freshwater consumption for the scenario with two tanks is 842.04 t. The results of Example 4 with two tanks are shown in Figure 3.24. The specific concentrations are shown in Table 3.7. It is worth noting that Kim and Smith (2004) included a second water source, other than freshwater. Consequently, the results of this work cannot be readily compared to the results of Kim and Smith (2004).

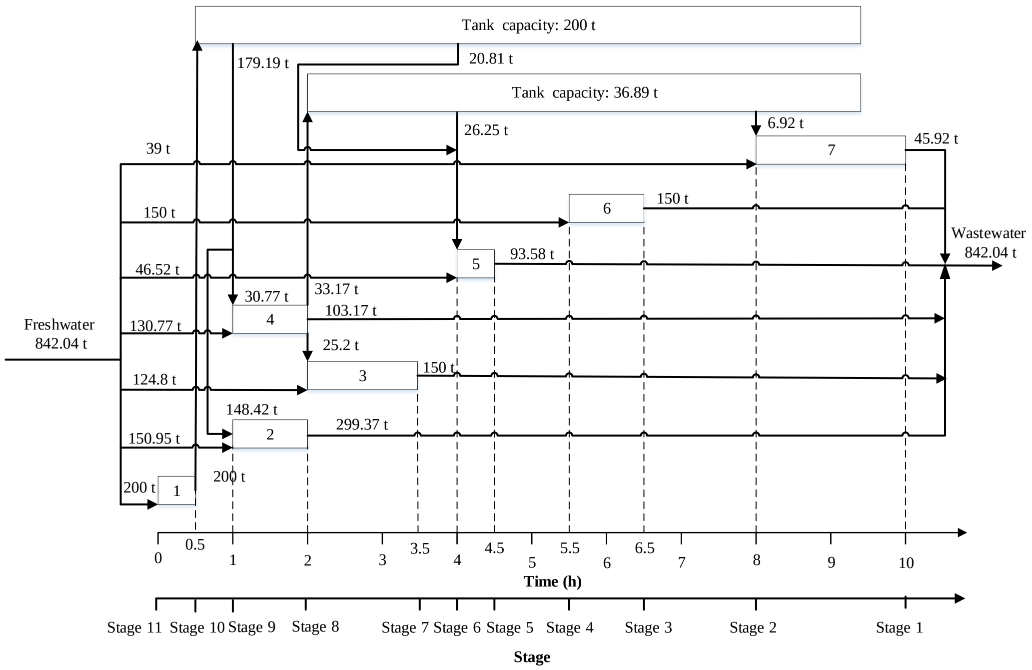

Figure 3.24 The final batch water network of Example 4 with two tanks

However, the water network obtained in the scenario with two tanks could be evolved to have one storage tank. As shown in Figure 3.25, wastewater generated from Operation 1 at 0.5 h is sent to tank for future reuse. An amount of 179.19 t wastewater is then reused by Operations 2 and 4 at 1 h and the remaining, i.e. 20.81 t, is reused at 4 h. The tank is empty from 4 h to the end time horizon of interest. It is possible to merge these two tanks into a single tank.

Table 3.7 Specification concentration of each operation

Operation	Contaminant	C^{in} /(ppm)	C^{out} /(ppm)	Mass load /(kg)	Water (t)
	C1	0	20	4	
1	C2	0	400	80	200
	C3	0	50	10	
	C1	10	60	15	
2	C2	198	1000	240	299.37
	C3	25	12000	3585	
	C1	10	200	28.5	
3	C2	33.6	83.6	7.5	150
	C3	168	1068	135	
	C1	4	59.52	9	
4	C2	76	200	20	161.54
	C3	10	1000	160	
	C1	21	181	15	
5	C2	145	1000	80	93.58
	C3	292	1200	85	
	C1	0	150	22.5	
6	C2	0	300	45	150
	C3	0	2450	367.5	
	C1	9	118	5	
7	C2	30	1500	67.5	45.92
	C3	151	1000	39	

The optimal states for Example 4 with one tank are shown in Figure 3.25. The resultant water network is shown in Figure 3.26. The freshwater consumption is further reduced, determined as 842.6 t. This is because the mixing of two different water sources results in a degradation of water quality. Compared with Figure 3.24, the difference is the quantity of freshwater consumption and reuse water of operations 5 and 7. In the scenario of one tank, the inlet and outlet concentrations of operations 5 are 19, 119, 263 ppm and 184, 1000, 1200 ppm, respectively. For operation 7, inlet and outlet concentrations are 13, 81, 180 ppm and 118, 1500, 1000 ppm, respectively. They are less than limiting concentration of operations 5 and 7.

However, the result of Example 4 with one tank is less than the result obtained by the exact model of Majozi (2010), i.e., 865.8 t and is greater than the result obtained by the relaxed model of Majozi (2010), i.e., 769.3 t. Compared with the base scenario without reuse/recycle scheme, i.e., 1076.3 t, the freshwater consumption of the scenario with one tank could be reduced by 21.7%.

The advantage of the DP method is illuminated in the calculation process. For example, when considering formulating the model of water integration of batch processes with multiple contaminants, it is difficult to determine which contaminant is reaching the maximum outlet concentration. If the designer set more than one contaminant reaching the maximum outlet concentration, it is difficult to solve the model. However, in each stage of the DP method, the complex problem is decomposed into some small problems so that it can be solved easily. If a few stages compete with the same water sources, it can also obtain the optimal results for these stages by trial and error method, such as Operation 5 in Stage 6 and operation 7 in Stage 2.

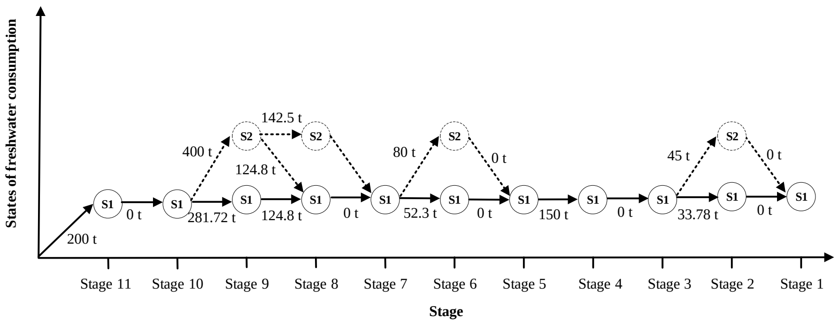

Figure 3.25 The optimal states for Example 4 with one tank

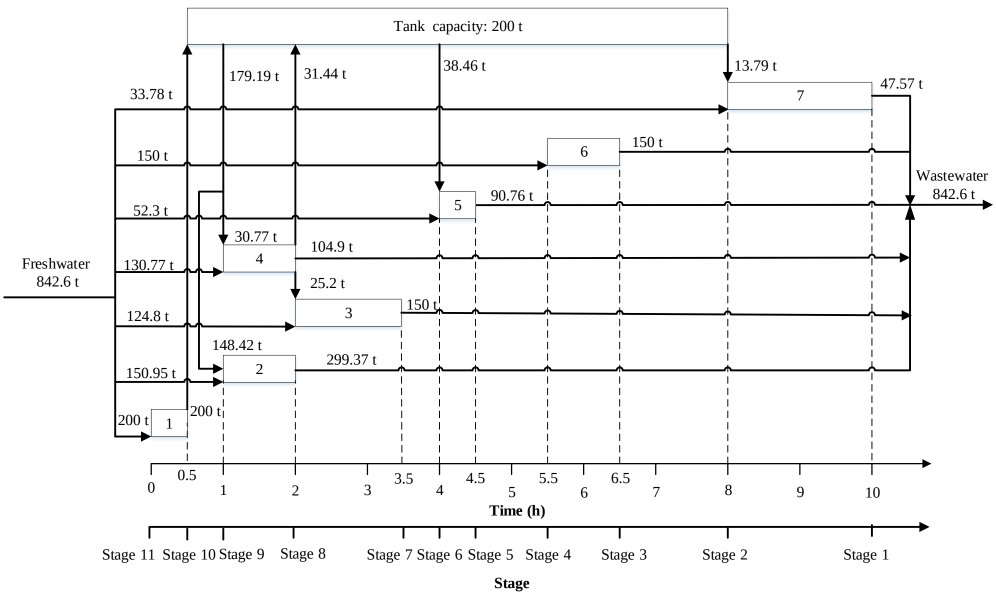

Figure 3.26 The final batch water network of Example 4 with one tank

3.5 Conclusions

A DP approach is used to identify the optimal water using policy that will achieve minimum freshwater consumption and wastewater generation, as well as the minimum capacity of the storage facility. Four examples from the literature are used to demonstrate the applicability of the proposed approach. The results obtained in this work match well with literature (Chen and Lee, 2008; Kim and Smith, 2004; Majozi, 2010; Majozi, Brouckaert, and Buckley, 2006). Furthermore, the capacity of the storage facility obtained in this work is less than that in published literature.

The advantage of the DP approach is used to decompose a complex problem with many variables into a series of problems comparatively easy to solve. For example, in Example 4, it considers water integration of batch processes with multiple contaminants. It is difficult to determine the globally optimal results using mathematical programming. This approach is simple and straightforward for the design of batch water networks. Future work should focus on exploring opportunities for water reuse/recycle and/or regeneration in batch processes with flexible product scheduling. Furthermore, it could be used to design a batch water network design with multiple contaminants in the framework of flexible scheduling. Also, other types of regeneration unit should be employed to purify the wastewater for further reuse.

Nomenclature

k the kth stage;

I_k a set of available water sources in Stage k

J_k a set of available water sources in Stage k

m the number of operations;

L a set of contaminants l

ts_m the start time of operation m;

te_m the end time of operation m;

$F_{j,k}^{Fw}$ amount of freshwater consumed by water sink j in Stage k;

F_{Tanki}^{St} amount of water stored in Tank i;

$F_{i,j,k}^{d}$ amount of directly reused water from water source i to water sink j in Stage k;

$F_{i,j,k}^{ind}$ amount of indirectly reused water from water source i to water sink j in Stage k;

$F_{i,k}^{Ww}$ amount of wastewater from water source i in Stage k;

$F_{j,k}^{\mathrm{Reg}}$ amount of regenerated water for water sink *j* in Stage *k*;

$F_{i,k}^{st}$ amount of stored water from water source *i* in Stage *k*;

$F_{j,k}$ amount of water for sink *j* in Stage *k*;

$F_{i,k}$ amount of water for source *i* in Stage *k*;

$c_{i,j,k}^{d,l}$ concentration of contaminant *l* direct reuse water from water source *i* to water sink *j* in Stage *k*;

$c_{i,j,k}^{ind,l}$ concentration of contaminant *l* of indirect reuse water from water source *i* to water sink *j* in Stage *k*;

$c_{j,\mathrm{k}}^{\mathrm{max},in,l}$ maximum inlet concentration of contaminant *l* of water sink *j* in Stage *k*;

$c_{j,\mathrm{k}}^{\mathrm{max,out},l}$ maximum inlet concentration of contaminant *l* of water sink *j* in Stage *k*;

$c_{j,\mathrm{k}}^{in,l}$ inlet concentration of contaminant *l* of water sink *j* in Stage *k*

c_{Fw}^{l} concentration of contaminant *l* of freshwater;

$c_{\mathrm{Re}g}^{l}$ concentration of contaminant *l* of regenerated water;

$M_{j,k}^{l}$ mass load of contaminant *l* of water sink in Stage *k*

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4

SYNTHESIS OF FLEXIBLE BATCH WATER NETWORKS USING DYNAMIC PROGRAMMING

4.1 Introduction

Wastewater minimization has gained significant attention from both academia and industry due to the stringent legislation on effluent and the scarcity of freshwater. Reduction of freshwater consumption not only makes the plant save operation costs but also discharges less wastewater to the environment. Batch processes have been widely used in the chemical industry because of their suitability for the production of small volume, high value-added products, and the capability of adjusting to fast market changes. Hence, it is urgent to develop a systematic approach to minimize wastewater consumption by exploiting opportunities for water reuse and removing hazardous contaminants through effective regeneration operations.

Graphical methods and mathematical programming are two different methods of effectively achieving water recovery in batch processes (Gouws *et al*., 2010). Graphical methods are mainly based on a 2-D diagram, which limits its wide application. This is because batch process considers thermodynamic constraints, as well as time feasibility, while the 2-D diagram can only consider the flowrate and quality of water streams or the flowrate and the duration of water operation simultaneously. It is impossible to consider flowrate, quality, and time constraints at the same time. Although the conventional pinch analysis is powerful for water recovery in continuous processes, it is only applicable to a single contaminant. When dealing with multiple contaminants, the targeting process is complex.

Mathematical programming is an optimization-based method which is based on the superstructure. It is capable of addressing large scale systems, as well as multiple contaminants problems. The limitation is that it only gives the results, rather than displaying the detailed targeting process. This feature could make it difficult to widely accepted by industrial practitioners. In the batch process, mathematical programming is widely used to cope with production scheduling, resources conservation problems. Especially, much effort has been placed on water integration of batch processes with the predefined schedule. However, results obtained from these studies could be suboptimal. In the work of Adekola and Majozi (2011), the optimal product schedule can result in further reduction of freshwater consumption.

Recently, more attention is paid to the simultaneous optimization of wastewater minimization and production schedule. The formulations could identify the minimum freshwater consumption together with the corresponding production schedule. Chen and Chang (2007) proposed a simultaneous optimization framework to synthesize water networks in batch processes. The interplay between these subsystems is considered, rather than individually discussed in s subsequent framework. In their work, the discrete-time model is adopted to represent the production schedule. Results show that an improvement of 5% in net profit can be obtained if production scheduling, water recovery, and wastewater treatment are optimized simultaneously. However, the limitation is that the adoption of the discrete-time model only allows the starting and ending time to locate at some fixed interval boundaries. Furthermore, the relationship between operations and equipment is not clear.

Thus, Zhou *et al*. (2009) proposed a continuous-time model to overcome the limitation. A modified state-space concept is adopted to represent the batch process. In the model, pipelines connecting splitters/mixers and equipment are actual pipelines. In contrast, in the work of Cheng and Chang (2007), some additional constraints should be incorporated into the model to translate the optimal solution into the actual pipeline network. In the solution strategy, a combination of DICOPT and GA is used to ensure global optimum. Compared with the discrete-time model, event point in the continuous-time model is obtained by a sensitivity analysis procedure. Li *et al*. (2010) extended the model of Zhou *et al*., (2009) to dealing with single- and multiple-contaminant problems in a batch process. Both discrete- and continuous-time model are introduced. Also, a modified superstructure is proposed to represent production scheduling and water recovery.

Adekola and Majozi (2011) proposed a continuous-time based formulation for wastewater minimization in a flexible product scheduling framework. A state sequence network is used to capture production scheduling schemes. Results show that a reduction of 19.2% and 26% in freshwater consumption for two case studies with flexible production scheduling can be achieved as compared to the fixed scheduling considered. In the work of Chen *et al*. (2011), an integrated model was proposed for simultaneous scheduling and water minimization in batch plants. The difference from previous work is that Resource-Task Network (RTN) is used to represent the scheduling framework. The bilinear terms in mass balance are linearized through a reformulation-linearization technique. The objective function is to maximize the profit by taking into account the net income from production and water-related costs.

In the work of Chaturvedi and Bandyopadhyay (2014), the feature is to consider the effects of multiple freshwater resources on the operating cost of batch water networks in a flexible schedule plant. In their subsequent work, Chaturvedi *et al*. (2016) compared the difference in production scheduling for single freshwater resource and multiple freshwater resources. They pointed out that the optimal schedule for a single freshwater resource is also applicable to multiple resources, resulting in the minimum operating cost. Lee and Foo (2017) incorporated the pinch-based automated targeting method into the state-task network-based scheduling model. Compared with previous work, the formulation is formulated as a MILP problem. This is because pinch-based automated targeting avoids the bilinear terms in mass balance by decomposing the mass balance into many intervals where concentrations are known, rather than variables. However, this method is restricted to a single contaminant problem. Pulluru and Akkerman (2018) employed a generic classification scheme to represent the quality of water in batch plants. This makes modeling of water recovery and regeneration in a relatively efficient manner. As for advances of simultaneous optimization of water integration and production scheduling, as well as heat integration and scheduling, one can refer to the textbook (Majozi *et al*., 2017).

These methods are all based on mathematical programming. In the process of determining freshwater consumption for batch processes, the process is divided into many stages because of the difference between starting and finishing times of each operation. At each stage, the designer can make decisions to choose the freshwater or reusable water from previous operations to meet water demand. This targeting process is similar to the dynamic programming algorithm. Dynamic programming (DP) is generally used to decompose a complex problem with many variables into a series of optimization problems with one variable in every stage (Bellman, 1957). It has been widely used for handling multistage operations. El-Halwagi *et al*. (2003) employed DP techniques to derive the mathematical conditions and characteristics of an optimal solution for material recycle/reuse networks. These conditions and characteristics are represented in a graphical form that can be readily used to determine rigorous targets for minimum usage of fresh resources.

Diban *et al*. (2016) presented a DP approach to find an optimum replanting policy for the Malaysian oil palm plantation that can achieve the minimum CO_2 emission over a finite time horizon. Peng *et al*. (2017) utilized DP to find the optimal actions at each stage for energy management in plug-in hybrid electric vehicle systems to minimize the cost of fuel consumption. Zhen *et al*. (2017) employed dynamic programming to obtain some key threshold values, which are used to determine at which ports and how much fuel the ship should be refueled. Results of experiments indicate the problem can be solved within a reasonable time and at least a reduction of 8% in fuel cost could be achieved as compared to some simple rules. Chen *et al*. (2017) proposed a dynamic programming framework for establishing a portfolio of advanced fuel technologies to achieve low-carbon development. In their work, the production quantity of each type of fuel in each year is set as a decision variable, while state variables are cumulative production quantities of each type of fuel technology by stage *n*.

The contribution of this chapter is to consider the optimization of water utilization in flexible batch processes using the DP method. It aims to investigate the opportunity to further reduce freshwater consumption and wastewater generation by optimizing operation scheduling. In the DP approach, there are three key elements, i.e., stage, state, and the return function of the decisions. In this work, each sink is seen as a stage, for which a decision is to be made. The sinks are arranged in ascending order of maximum allowable concentration. At each stage, once the designer decides to choose which water sources, the effect is represented by the return function. It is the quantity of freshwater consumption in that stage. The state not only connects the previous stage, but also relates to succeeding stages. The state for each stage is the remaining quantities of water sources up to that stage. The organization of this chapter is as follows. Section 4.2 makes a list of the given information. The methodology is introduced in Section 4.3. In section 4.4, three illustrative examples are presented. Finally, Section 4.5 concludes this chapter.

4.2 Problem statement

This chapter 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 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 optimum production schedule that achieves the minimum freshwater consumption by exploring opportunities for water recycle/reuse and regeneration.

4.3 Methodology

DP approach is usually used to address multi-stage decision-making process and try to capture the adaptive features of this decision process. It is characterized fundamentally in terms of *stage* and *state*. The original problem is decomposed into many stages. Each stage constitutes a new problem which can be modelled by a relatively small set of states. The states are the indicators of decisions that are made to move to the next stage. The recursive function is updated using the chosen state of each stage. DP approach not only assure in the present stage the optimal solution to the sub-problem is chosen, but it also guarantees the solutions for remaining stages are optimal through the minimization of the recurrence function of the problem. The principle of optimality of DP is explained in Bellman (1957). The application of the DP approach to predefined schedule is introduced in Li and Majozi (2018). In their work, the stage is defined by the starting and finishing times of each operation, while this work treats the concentration of water sink as a stage.

DP is used to determine the target of freshwater consumed in the batch process. The decision is decided whether to use freshwater and/or reuse wastewater or regenerated water. In each stage, a decision could be made on whether to use freshwater and/or reuse wastewater or regenerated water. The states are the remaining quantity of the available water source. When a decision is made, a return cost is obtained, and the system transforms the next stage. The return cost is determined by a known single-valued function of the input state. In this chapter, the return cost mentioned in the following sections refers to freshwater consumption. The entire process can be divided into *N* stages (1, 2, …, *k*, …, *N*) based on the concentrations of water sinks. The concentration of water sink is seen as a stage. The relationship between stages and the concentration of water sinks is displayed in Figure 4.1, where C_m represent the concentration of water sink *m*. It is noted that the problem was solved using the backward procedure of DP (Roberts, 1964). The stages are thus presented in reverse order.

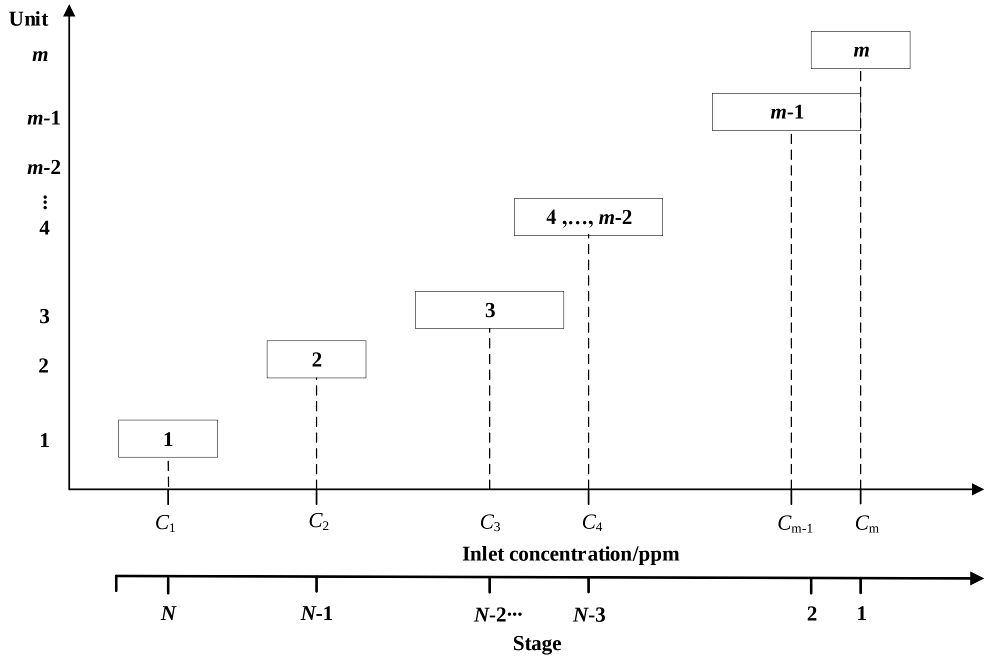


Figure 4.1 The relationship between the concentration of water sinks *and stages*

Suppose that in *k*th stage there are I_k water sources and J_k water sinks, resulting in $S(k)$ possible states which are numbered 1, 2, …., $S(k)$. In other words, there are $S(k)$ possibilities about the allocation of freshwater to water sinks in the *k*th stage. The potential states in each stage are represented by the circles, as shown in Figure 4.2. Let $F_{j,k}^{Fw}$ denote the freshwater consumption of sink j, which is used to update the return function for the *k*th stage of the process. In Figure 4.2, $F_{j,k}^{Fw}$ is represented by the arc, indicating the return cost from the state of the previous stage to the state of the next stage. If $F_{j,k}^{Fw}$ is the optimal return cost of the *k*th stage, a solution to the whole problem may be denoted by the sequence $(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$. $f(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$ denotes the total return cost associated with the sequence $(F_{j,1}^{Fw}, F_{j,2}^{Fw}, ..., F_{j,k}^{Fw}, ..., F_{j,N}^{Fw})$.

The objective is to minimize $f(F_{j,1}^{Fw}, F_{j,2}^{Fw},..., F_{j,k}^{Fw},..., F_{j,N}^{Fw})$ subject to any constraints which are placed on the choice of the states in each stage, and these constraints may depend on the states entered in stages 1, 2, …, *N*-1. In this work, the returned cost function is set as the total minimum freshwater consumption over the *k*th stage, which equals the minimum sum of freshwater consumption in *k*th stage ($\sum_{j=1}^{J_k} F_{j,k}^{Fw}$) in the *k*th stage and return cost results ($f_{k-1}(F_{j,k-1}^{Fw})$) from the stage (*k*-1). It aims to find the path with the minimum result from Stage *N* to Stage 1.

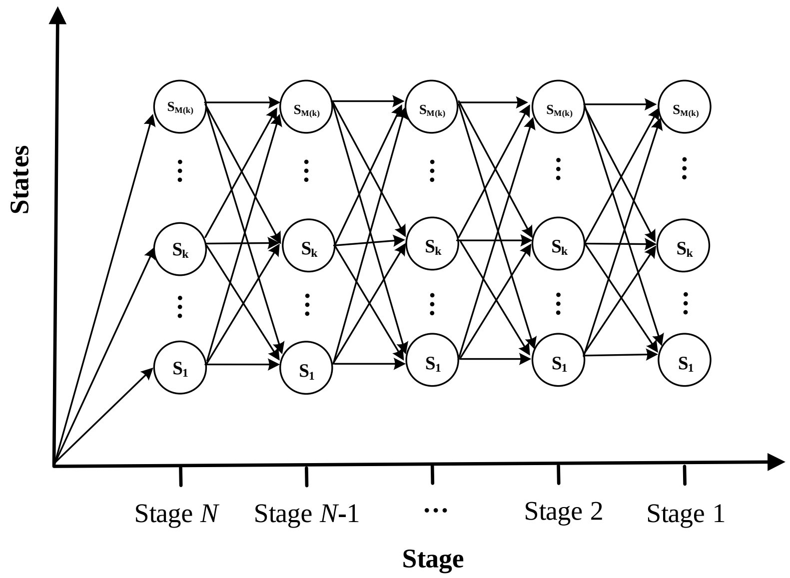


Figure 4.2 Potential state in each stage

The objective of the problem is defined as:

$f_k(F_{j,k}^{Fw})$ = minimum freshwater consumed over the *k* stages

Where,

$$f_k(F_{j,k}^{Fw}) = \begin{Bmatrix} \text{Freshwater:} & \sum_{j=1}^{J_k} F_{j,k}^{Fw} + f_{k-1}(F_{j,k-1}^{Fw}) \\ \text{Reuse/recycle:} & f_{k-1}(F_{j,k-1}^{Fw}) \end{Bmatrix}, k = 1, 2, 3, ... N \quad (4\text{-}1)$$

$$f_0(F_{j,0}^{Fw}) = 0 \quad (4\text{-}2)$$

Eq (4-1) represents the objection function of the problem when it is located in the *k*th stage. In every stage, the designer has two options for satisfying the water demand of operation, i.e., freshwater scenario, reuse/recycle scenario. For freshwater scenario, the water requirement of a sink is satisfied with by the mixture of freshwater and reused water, and regenerated water. In this scenario, freshwater must be used to dilute wastewater to meet the water requirement. However, for reuse/recycle scenario, no freshwater is required to satisfy the water demand. In other words, water demand is only met by available reusable wastewater or regenerated water. Eq (4-2) is the objective function of the origin stage, setting as zero. It does not have a physical meaning.

Because at each stage, there are too many combinations of water sources to meet water demand. Not all of them contribute to the optimal result. To reduce the search space, a set of rules is generated to select an appropriate water source.

1) When reuse water and regenerated water are available at the same time, reuse water should be used preferentially;
2) To reduce the cost of stored water, if a water sink has a few alternative water sources, the water source which is closest to the sink should be reused preferentially
3) If the process chooses a freshwater scenario which requires some reuse water, the reuse water with the highest quality, i.e., lowest concentration, should be used preferentially, in as great a quantity as possible;
4) If a process is fed solely by wastewater, i.e., no freshwater needed, wastewater with the contaminant concentration closest to the maximum inlet concentration of the process should be used preferentially, in as great a quantity as possible;
5) If the water sink has a few available water sources with the same concentration, the alternative water source with enough reuse water should be used preferentially.

When determining the amount of freshwater consumption in each stage, two main categories of water network synthesis exist, i.e., fixed flowrate and fixed-mass load problems. For different types of problems, resulting in freshwater consumption may be different.

Fixed flowrate problems

In the process industry, some units, such as boiler, cooling towers and reactors, do not involve any mass transfer. The inlet and outlet flowrates of the water-using processes may not be uniform and therefore can account for water losses or gains. The outlet streams always leave at the specified (maximum) concentrations, while the inlet streams have maximum allowable concentrations given. This model is generally known as the fixed flowrate problem (Foo, 2009; Prakash and Shenoy, 2005).

For freshwater scenario, water requirements of sinks are satisfied with freshwater, reusable wastewater and/or regenerated water. The freshwater consumption in the kth stage can be obtained by Eqs (4-3) and (4-4). The priority of water utilization is based on the defined rules. The procedure is explained as follows: Firstly, the process is to use a mixture of reuse water and freshwater to meet the water requirement. If the quantity of reuse water in the same stage is insufficient, the deficit water is supplied with regenerated water. After all the states of freshwater consumption are determined, the minimum freshwater consumption is chosen as the optimal state in this stage.

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Re}g} + F_{j,k}^{Fw} = F_{j,k} \tag{4-3}$$

$$\begin{gathered}\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Re}g}^{l} + F_{j,k}^{Fw} c_{Fw}^{l} = F_{j,k} c_{j,k}^{\max,in,l} \\ \forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N\end{gathered} \tag{4-4}$$

For reuse/recycle scenario, specific water requirement for water sink *j* in stage *k* can be obtained by Eqs (4-5) and (4-6). $F_{i,j,k}^{d}$ and $F_{i,j,k}^{ind}$ represent the direct reuse of water and indirect water, respectively. Based on the rule (2), direct reuse of water should be selected preferentially. If the quantity of direct reuse water is not enough to meet the water demand, the deficit water is supplemented by indirect reuse water. Furthermore, if the quantity of indirect reuse water is still deficient or not available, the remaining water is supplied by regenerated water.

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}} = F_{j,k} \tag{4-5}$$

$$\begin{gathered}\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Re}g}^{l} = F_{j,k} c_{j,k}^{\max,in,l} \\ \forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N\end{gathered} \tag{4-6}$$

Fixed-mass load problems

Apart from the fixed flowrate operations, a different category termed as fixed-mass load operations is commonly used in the process industry. The operations in this category can be modelled as mass transfer mass transfer units with water being used as the only mass separating agent. It includes washing, scrubbing, and extraction operations. In the fixed-mass load problem, each operation has a fixed contaminant load and the maximum allowable inlet and outlet concentrations are specified. The flowrate of water entering and leaving the unit is the same (Foo, 2009; Prakash and Shenoy, 2005).

For fixed-mass load problems, water quantity can be less than the limiting water requirement, and the inlet concentration can also be less than the maximum allowable inlet concentration. To obtain an optimal result of freshwater consumption, it is prudent to use nonlinear programming (NLP) to determine the results of freshwater consumption and reuse water from previous processes. The NLP model is explained as follows: The objective function is to minimize freshwater consumption, as shown in Eq (4-7). Eq 4-(8) states that the removal of the mass load must be greater than or equal to the limiting mass load if the outlet concentration reaches its limiting data. Eq (4-9) represents the calculation of inlet concentration. Eq (4-10) ensures that the actual removal of mass load is equal to limiting mass load. The quantity constraint is expressed in Eq (4-11). Eq (4-12) indicates that the actual inlet and outlet concentration should be limited by the limiting data.

$$\min F_{j,k}^{Fw} \tag{4-7}$$

$$\left(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Reg}}\right)\left(c_{j,k}^{\max,out,l} - c_{j,k}^{in,l}\right) \geq M_{j,k}^{l} \tag{4-8}$$

$$c_{j,k}^{in,l} = \frac{\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Reg}}^{l} + F_{j,k}^{Fw} c_{Fw}^{l}}{\sum_{i=1}^{I} F_{i,j,k}^{d} + \sum_{i=1}^{I} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}} + F_{j,k}^{Fw}} \tag{4-9}$$

$$\left(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Reg}}\right)\left(c_{j,k}^{out,l} - c_{j,k}^{in,l}\right) = M_{j,k}^{l} \tag{4-10}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{Fw} + F_{j,k}^{\mathrm{Reg}} \leq F_{j,k} \tag{4-11}$$

$$c_{j,k}^{in,l} \leq c_{j,k}^{\max,in,l}, c_{j,k}^{out,l} \leq c_{j,k}^{\max,out,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N \tag{4-12}$$

For the reuse/recycle scenario, water sinks are only fed by the available wastewater from storage tanks, or wastewater which is produced in the same stage, or regenerated water. The NLP model is expressed by Eqs (4-13)-(4-18). The difference between this scenario and the freshwater scenario is that the freshwater term is removed in all of the constraints. The objective function expresses the minimization of the sum of reuse water and the regenerated water. It applies individually to each stage.

$$\min \sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} \tag{4-13}$$

$$(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}})(c_{j,k}^{\max,out,l} - c_{j,k}^{in,l}) \geq M_{j,k}^{l} \tag{4-14}$$

$$c_{j,k}^{in,l} = \frac{\sum_{i=1}^{I_k} F_{i,j,k}^{d} c_{i,j,k}^{d,l} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} c_{i,j,k}^{ind,l} + F_{j,k}^{\mathrm{Reg}} c_{\mathrm{Re}g}^{l}}{\sum_{i=1}^{I} F_{i,j,k}^{d} + \sum_{i=1}^{I} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Reg}}} \tag{4-15}$$

$$(\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Re}g})(c_{j,k}^{out,l} - c_{j,k}^{in,l}) = M_{j,k}^{l} \tag{4-16}$$

$$\sum_{i=1}^{I_k} F_{i,j,k}^{d} + \sum_{i=1}^{I_k} F_{i,j,k}^{ind} + F_{j,k}^{\mathrm{Re}g} \leq F_{j,k} \tag{4-17}$$

$$c_{j,k}^{in,l} \leq c_{j,k}^{\max,in,l}, c_{j,k}^{out,l} \leq c_{j,k}^{\max,out,l}$$
$$\forall i \in I_k, \forall j \in J_k, \forall l \in L, k = 1,2,...,N \tag{4-18}$$

For simplicity, only the states of freshwater and stored water are displayed in each stage. Once the freshwater consumption of each process is determined, the quantities of reused water and wastewater, as well as the maximum capacities of storage tanks can be identified. The problem was solved using the backward procedure of DP (Roberts, 1964). In the following section, four examples, adopted from the literature, are explored in detail using the above methodology.

The detailed procedure for the design of flexible batch water network with or without regeneration units is shown in Figure 4.3. As shown in Figure 4.3, the first step is to divide the process into many stages. The stages can be determined based on the inlet concentrations of water sinks. Next, the target of freshwater consumption for the whole process, as well as the specific freshwater consumption for each stage can be identified using the DP method. Since the information of freshwater consumption, reused water in each stage is determined, the sequence of operation can be subsequently identified. In other words, the receiving unit should start immediately after the wastewater generating unit finishes. It can thus design the initial water network of batch processes with the constraint of time. If the initial water network is feasible, it will obtain the final batch water network.

If the process requires considering water regeneration scenario, the timing of operation for water reuse/recycle scheme can be used as the basis for further investigation. In every stage, regenerated water as a water resource is incorporated into the analysis, and the match with minimum freshwater and/or a minimum quantity of regenerated water is selected as the optimal strategy. The same procedure of water reuse/recycle is repeated to get the final batch water network.

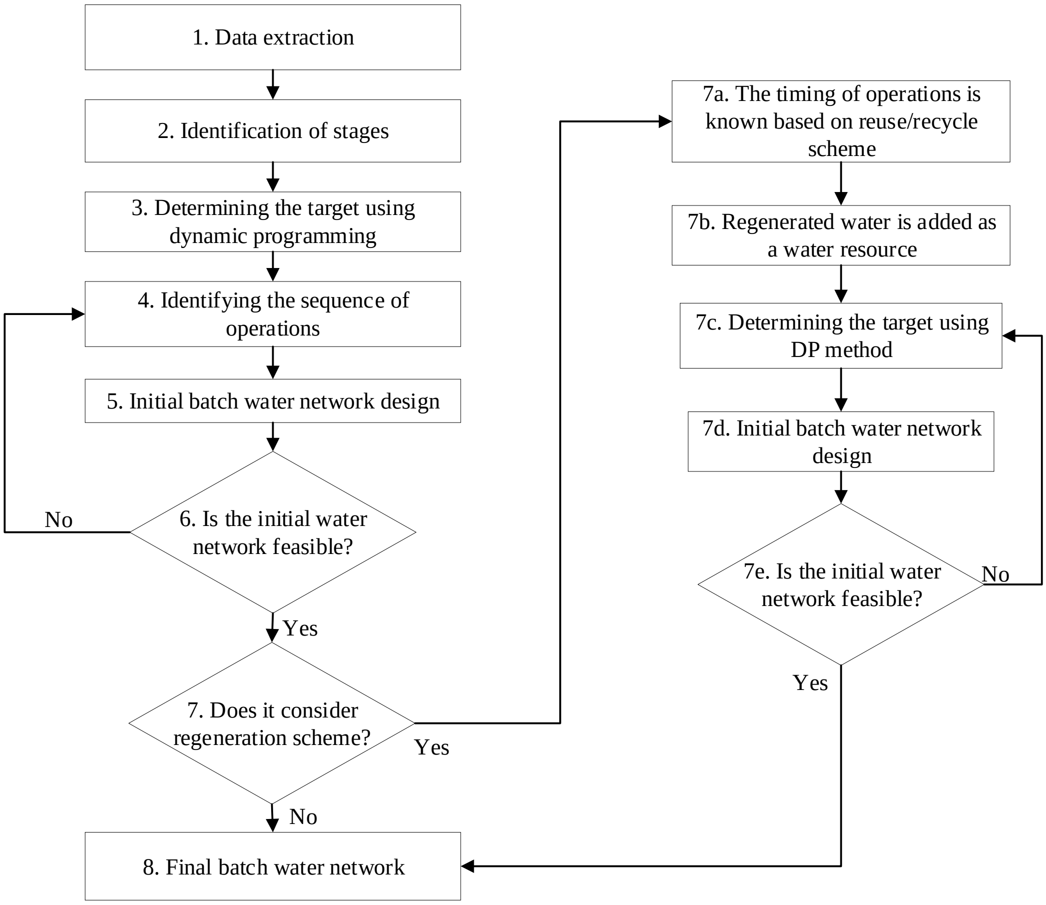


Figure 4.3 The design procedure for batch water network

4.4 Illustrative examples

To illustrate the application of the proposed approach to network design in flexible batch processes, two examples extracted from literature are investigated.

4.4.1 Example 1

A literature example adapted from Liu *et al*. (2009) is introduced to demonstrate the application of the proposed method for the optimal design of a flexible batch water network. It has five operations with a single contaminant. The limiting data for the example is shown in Table 4.1. To investigate the effect of production scheduling on water consumption, the duration of each operation is given, rather than the start and end time. Furthermore, the overall process is assumed to operate in repeated batch cycles with the cycle time being 8.5 h.

Table 4.1 Limiting water data for the Example 1

Operation	Quantity/t	C^{in}/(ppm)	C^{out}/(ppm)	M/kg	Duration/h
A	50	0	400	20	2
B	30	100	400	9	1
C	10	200	500	3	3
D	24	350	600	6	4
E	40	450	700	10	2.5

Reuse scenario

Based on the inlet concentration of operations, the whole process can be divided into five stages, as shown in Figure 4.4. In this example, all the operations have different inlet concentrations. Each stage has only one operation. Note that the cyclic batch operation is considered in this example because of the unknown timing of each operation. Cyclic batch operation is common in the industry to achieve the required capacity of the product, enabling the same schedule in an extended time horizon.

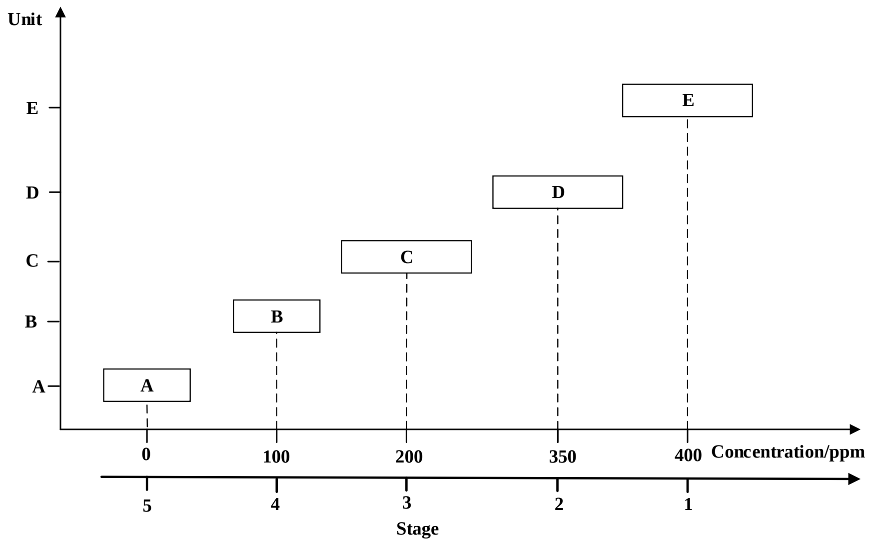


Figure 4.4 The identification of stages for Example 1

In every stage, the freshwater and reused water, for the freshwater scenario can be determined from Eqs (4-3) and (4-4). For the reuse/recycle scenario, the quantity of reused water is determined by Eqs (4-5) and (4-6). When a new stage starts, it is assumed that the operation in the previous stage is finished. For example, operation A located in Stage 5 is assumed to finish before starting operation B in Stage 4. Thus, the wastewater generated by operation A can be reused by operation B. The detailed processes are described as follows.

Stage 5

In this stage, water sinks SK_A can only be fed with freshwater because inlet concentration is zero. Hence, there is only a state of freshwater consumption in Stage 5, with a quantity of 50 t of freshwater consumed in this stage, i.e., $F^{Fw}_{SK_A,7}$ = 50 t. As there are no alternative water sources, the quantity of stored water is zero. The selected state and return cost for Stage 5 is shown below. This work only considers the freshwater consumption. Therefore, the return cost for the problem is the extent of freshwater consumption.

$$S_{Stage5} = \left\{ \sum_{j}^{J_5} F^{Fw}_{j,5} = 50\text{t}, F^{St}_{\text{TankA}} = 0t \right\}$$

$$f_5(F^{Fw}_{j,5}) = \min \left\{ \sum_{j}^{J_5} F^{Fw}_{j,5} + f_4(F^{Fw}_{j,4}) \right\} = \min \left\{ 50t + f_4(F^{Fw}_{j,4}) \right\}$$

Stage 4

In Stage 4, there is operation B, which can be fed by the mixture of reusable water from operation A and freshwater or only fed by freshwater. However, reusable water from operation A has the same concentration as operation B, i.e., 400 ppm. This reusable water cannot be used by Operation B. Otherwise it violates the necessary conditions for the optimal design of water network (Savelski and Bagajewicz, 2000). Therefore, the state of freshwater consumption is 22.5 t. The recursive function of the problem could be updated by the state of freshwater consumption in Stage 4. The return cost is the sum of the minimum freshwater consumption in Stages 5 and 4 and the freshwater consumption over the remaining stages (Stages 1-3). On the other hand, as the reusable water from operation A is not reused by operation B, the makespan is the maximum duration of these two operations, i.e., 2 h. It is noted that in the following targeting processes, the indirect reuse and direct is not distinguished. This is because the timings of each operation are not known.

$$S_{Stage4} = \left\{ \sum_{j}^{J_4} F^{Fw}_{j,4} = 22.5t, F^{St}_{\text{TankA}} = 50t \right\}$$

$$f_5(F^{Fw}_{j,5}) = \min \left\{ 50t + \sum_{j}^{J_4} F^{Fw}_{j,4} + f_3(F^{Fw}_{j,3}) \right\} = \min \left\{ 72.5t + f_3(F^{Fw}_{j,3}) \right\}$$

Stage 3

In Stage 3, there exists operation C with an inlet concentration of 200 ppm. There are two reusable water sources, operations A and B. Both of them have the same concentration.

Therefore, there are three states of freshwater consumption for this stage, i.e., freshwater, the mixture of freshwater and reusable water from operation A, and the mixture of freshwater and reusable water from operation B. For the first state, operation C is fed by freshwater, as shown in S_{Stage3}^{1}. The second state is that operation C is fed with the mixture of the reusable water from operation A and freshwater, while in the third state reusable water from operation B is sent to operation C. Therefore, the state with minimum freshwater consumption is chosen to update the recursive function of the problem. On the other hand, since the reusable water from operations A and B is possible to be reused by operation C, the minimum makespan for these operations is 3 h, the sum of the duration of operations B and C.

$$S_{Stage3}^{1} = \left\{ \sum_{j}^{J_3} F_{j,3}^{Fw} = 6t, F_{\mathrm{Tank1}}^{St} = 50t, F_{\mathrm{Tank2}}^{St} = 22.5t \right\}$$

$$S_{Stage3}^{2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 5t, F_{\mathrm{TankA},SK_C,2} = 21t \right\}$$

$$S_{Stage3}^{3} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 5t, F_{\mathrm{TankB},SK_C,2} = 21t \right\}$$

$$f_5(F_{j,5}^{Fw}) = \min\left\{ 72.5t + \sum_{j}^{J_3} F_{j,3}^{Fw} + f_2(F_{j,2}^{Fw}) \right\} = \min\left\{ 77.5t + f_2(F_{j,2}^{Fw}) \right\}$$

Stage 2

In Stage 2, operation D has an outlet concentration of 600 ppm. The reusable water from operations A, B, and C can be used as water sources of operation D. It, therefore, has seven states, i.e., freshwater, A, B, C, A-B, A-C, and B-C. For the first state, operation D is fed with freshwater, i.e., 10 t. If operation D is fed by the reusable water from operation A, the freshwater is determined as 3 t. The similar procedure is performed for operation B. These two states are shown in the second and third state. For the fourth state, operation D is fed by the reusable water from operation C, consuming a quantity of 8.33 t freshwater. Because the single source can feed the operation D, the combinations of A-B, A-C, and B-C are not considered to reduce the complexity of connections. Therefore, the state with minimum freshwater consumption, i.e. 3 t, is chosen to update the recursive function of the problem.

$$S_{Stage2}^{1} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 10t \right\}$$

$$S_{Stage2}^{2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 3t, F_{\text{TankA},SK_C,2} = 21t \right\}$$

$$S_{Stage2}^{3} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 3t, F_{\text{TankB},SK_C,2} = 21t \right\}$$

$$S_{Stage2}^{4} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 10t, F_{\text{TankC},SK_C,2} = 8.33t \right\}$$

$$f_5(F_{j,5}^{Fw}) = \min\left\{ 77.5t + \sum_{j}^{J_2} F_{j,2}^{Fw} + f_1(F_{j,1}^{Fw}) \right\} = \min\left\{ 80.5t + f_1(F_{j,1}^{Fw}) \right\}$$

Stage 1

Stage 1 is the last stage. Operation E has an inlet concentration of 450 ppm, which is higher than the outlet concentration of operations A and B. On the other hand, the outlet concentration of operation E is higher than the outlet concentration of remaining operation in the system. If the combinations of different sources are considered, there are 15 states in this stage. However, some combinations of these sources may consume freshwater. For example, the outlet concentration of wastewater from operations C and D is more than the inlet concentration of operation E, the mixture of these two sources will not comply with the minimum mass transfer without freshwater. Thus, the combination of C-D is not taken into account. For simplicity, in the analysis the single source is considered first, i.e., A, B. If the single source cannot meet the water requirement, a combination of two sources is considered, i.e., A-B. Furthermore, if the combinations of two different sources are still infeasible. One more water source is added to the combination, for example, A-B-C.

$$S_{Stage1}^{1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 14.29t \right\}$$

$$S_{Stage1}^{2} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0t, F_{\text{TankA},SK_E,1} = 33.33t \right\}$$

$$S_{Stage1}^{3} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0t, F_{\text{TankB},SK_E,1} = 33.33t \right\}$$

$$S_{Stage1}^{4} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0t, F_{\text{TankA-B},SK_E,1} = 33.33t \right\}$$

$$f_5(F_{j,5}^{Fw}) = \min\left\{ 80.5t + \sum_{j}^{J_1} F_{j,1}^{Fw} \right\} = 80.5t$$

In this stage, four states are presented here. This is because other states consume more freshwater; these states are not explained in detail. For the first state, operation E is fed by freshwater, i.e., 14.29 t. For the second state, the water requirement of operation E is met by the wastewater from operation A. A quantity of 33.33 t reusable water from operation A will be needed. In the third state, a quantity of 33.33 t reusable water from operation B is required to satisfy with the water requirement of operation E. In the fourth state, the mixture of wastewater from operations A and B is used to feed operation E. Because the residue water from operations A and B are unknown, the specific quantity of freshwater is dependent on the states in previous stages. The relationship between the states in Stage 1 and the states in Stage 2 is presented in Figure 4.5.

In Figure 4.5, the states represented by the solid circle is chosen to achieve the target of freshwater consumption. The target of freshwater consumption for the whole process can be determined as 80.5 t, which is identical to a scenario with predefined production scheduling (Liu *et al.*, 2009). It is easily found that there are three paths that can achieve this target. Furthermore, the time horizon of the processes is fixed as 8.5 h. The corresponding water network is shown in Figure 4.6(a)-(c). Although these three networks have the same target, Figure 4.6(c) has the least capacity of the storage tank. Therefore, Figure 4.6(c) is chosen as the optimal water network for this example with water reuse.

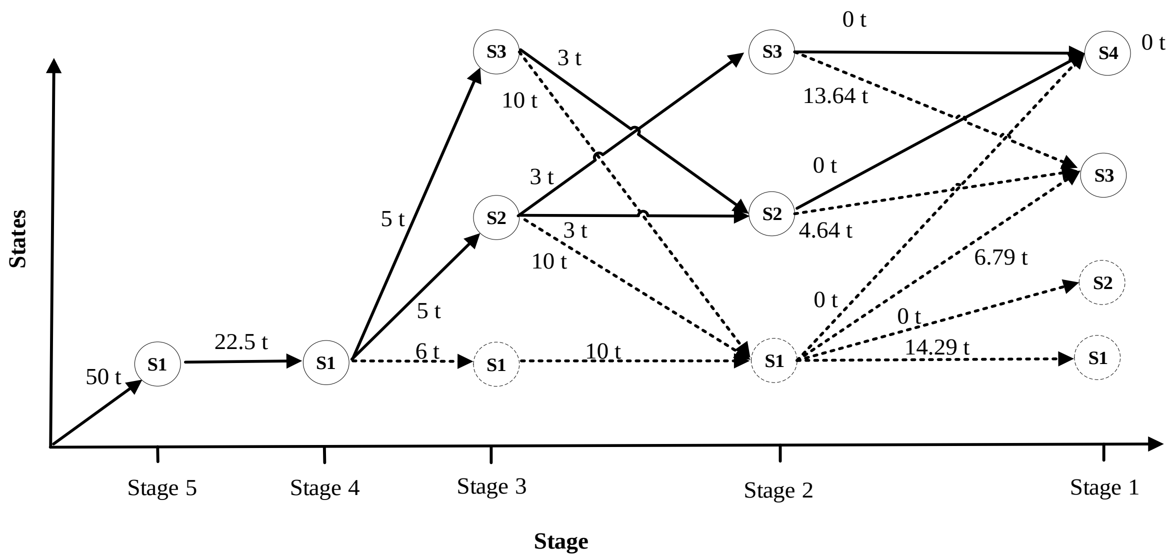


Figure 4.5 The schematic diagram of states in each stage for Example 1

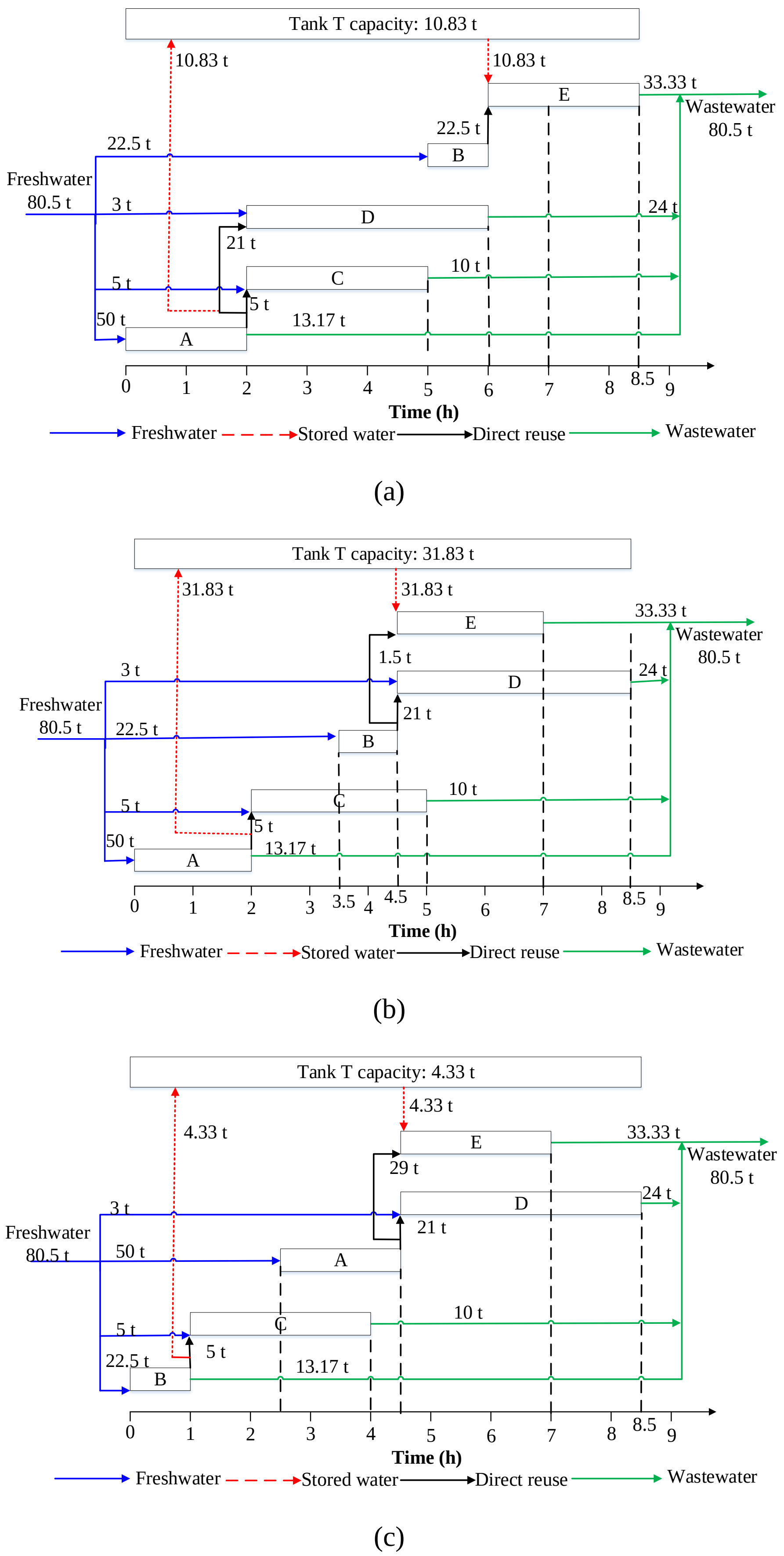
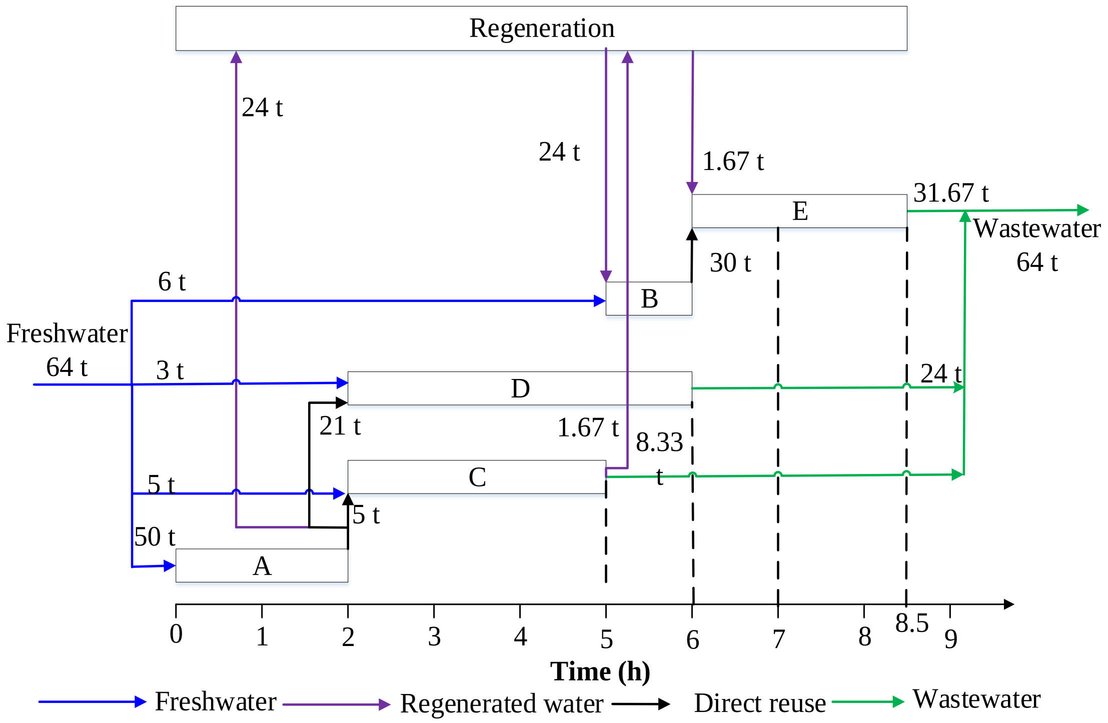


Figure 4.6 Water network of Example 1 with reuse scenario

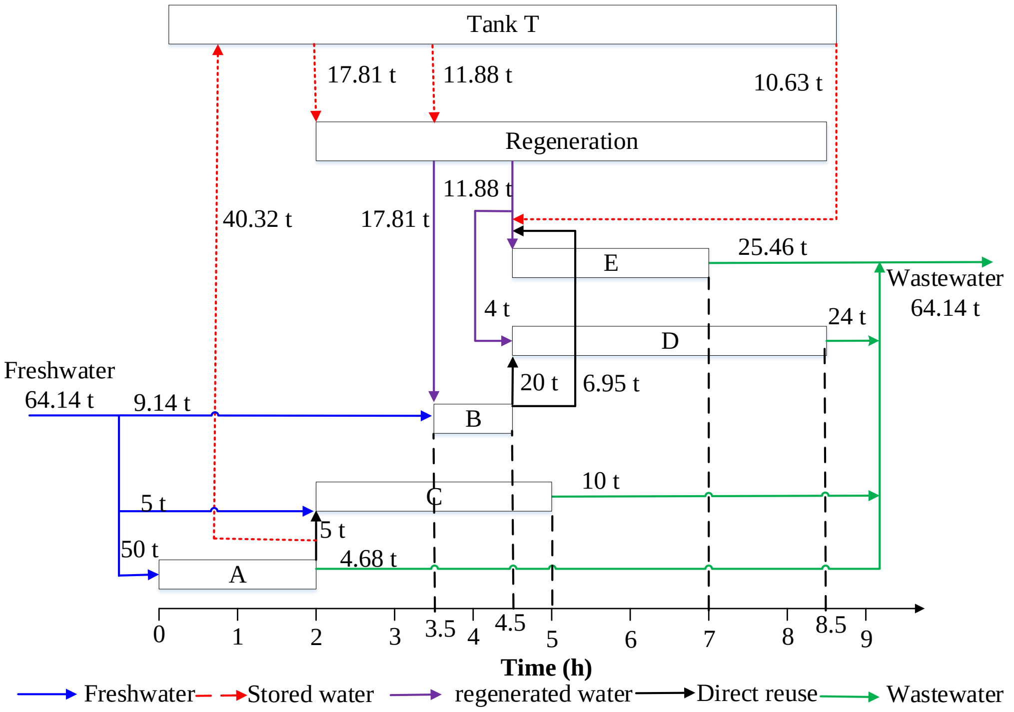
Regeneration scenario

In the reuse scenario, Figures 4.6(a)-(c) present the optimal water network that can achieve the minimum target of freshwater. The timing of each operation in the reuse scenario can be used to design the regeneration network. Thus, it is assumed that the timing of each operation in the reuse scenario is the same as the regeneration scenario. Compared with the original example with predefined scheduling in Liu *et al*. (2009), the scheduling of water operations in this work is different. Therefore, this rescheduling of water operation can be seen as flexible scheduling.

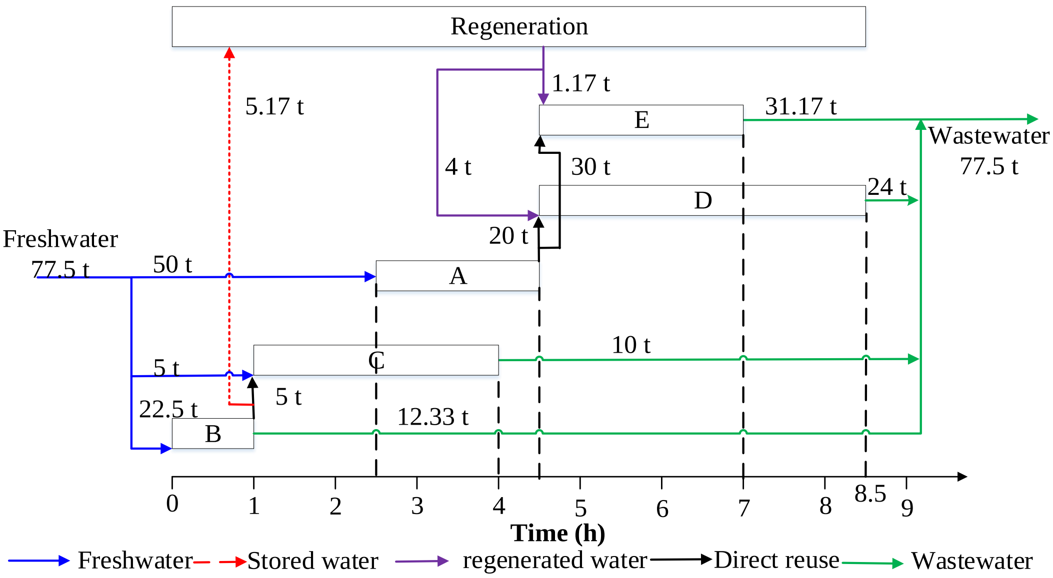
In this scenario, a regeneration unit is deployed to purify the wastewater to reduce freshwater consumption. The outlet concentration of regeneration unit is 100 ppm, and the maximum regenerated flowrate is 11.875 t/h. Since the timing of the operation is known, the targeting can be carried out by the DP method (Li and Majozi, 2018). For simplicity, the detailed procedure is not presented in this work. The corresponding regeneration networks for Figure 4.6(a)-(c) are shown in Figure 4.7(a)-(c). Note that Figure 4.7 presents the water network with regeneration for the first sequence. As shown in Figure 4.7 (a) and (b), the freshwater consumption is almost the same, which is less than that in Liu *et al*. (2009) with predefined scheduling, i.e., 68.594, but equal to the result of Adekola and Majozi (2011), i.e., 64.07 t. However, the results in Figure 4.7(c) is greater than those of Liu *et al*. (2009) and Adekola and Majozi (2011).



(a)



(b)



(c)

Figure 4.7 Water network of Example 1 with a regeneration unit

4.4.2 Example 2

To illustrate the above design procedures in detail, a literature example adopted from Li *et al.* (2013) is presented here. The limiting data of the operations are shown in Table 4.2. In this example, operations 1, 2, and 4 are regarded as fixed-load processes, while operations 3 and 5 are the fixed-flowrate processes. Note that in Table 4.2, the duration of each operation is given, rather than the starting and ending time. The charging and discharging times for water operation are included in the duration time. For operations 1, the charging and discharging of water is 1 h, while for operations 2, and 4, the intake and discharge of water operation at the start and end will take 0.5 h. In this example, the time horizon is set 8.5 h.

Table 4.2 The limiting data of Example 2

Operation	Contaminants	$C_{in,k}^{max}$ (ppm)	$C_{out,k}^{max}$ (ppm)	△m (kg)	Quantity (t)	Duration (h)
	A	0	100	3.0		
1	B	0	90	2.7	30	5
	C	0	50	1.5		
	A	40	150	8.25		
2	B	60	80	1.5	75	5
	C	20	70	3.75		
	A	170	170	0		
3	B	120	120	0	40	1.5
	C	100	100	0		
	A	110	210	3.0		
4	B	135	200	1.95	30	5
	C	60	120	1.8		
	A	170	170	0		
5	B	120	120	0	40	1.5
	C	100	100	0		

Reuse scenario

Based on the inlet concentration of operations, the whole process can be divided into four stages, as shown in Figure 4.8. In this example, all the operations have different inlet concentrations. Each stage has only one operation. Note that the cyclic batch operation is considered in this example because of the unknown timing of each operation. Cyclic batch operation is common in the industry to achieve the required capacity of the product, enabling the same schedule in an extended time horizon.

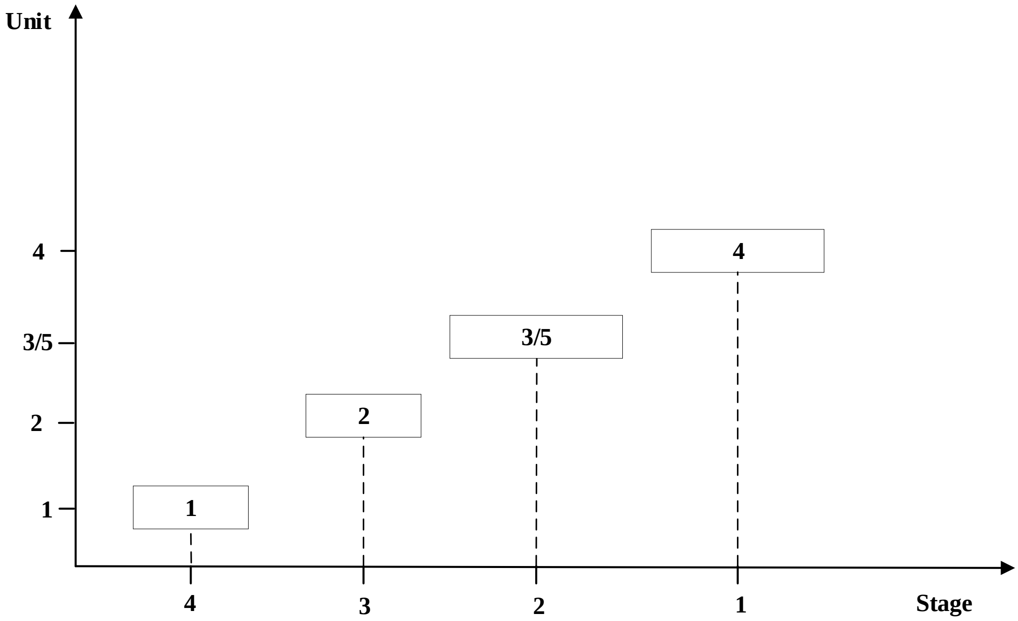


Figure 4.8 The identification of stages for Example 2

In a fixed flowrate scenario, the freshwater and reused water, for the freshwater scenario can be determined from Eqs (4-3) and (4-4). For the reuse/recycle scenario, the quantity of reused water is determined by Eqs (4-5) and (4-6). In the fixed mass load scenario, freshwater scenario refers to Eqs (4-7)−(4-12) and reuse/recycle scenario is Eqs (4-13)−(4-18). When a new stage starts, it is assumed that the operation in the previous stage is finished. For example, operation 1 located in Stage 4 is assumed to finish before starting operation 2 in Stage 3. Thus, the wastewater generated by operation 1 can be reused by operation 2. In the following analysis, the operation is divided into water sinks and sources to explain the analysis clearly. The detailed processes are described as follows.

Stage 4

In Stage 4, there is a single water operation SK_1, which can only be fed with freshwater because of the zero concentration. Hence, there is only a state of freshwater consumption in Stage 4, with a quantity of 30 t of freshwater consumed in this stage, i.e., $F_{SK_1,4}^{Fw}$ = 30 t. As there are no alternative water sources with its water quality higher than freshwater, the quantity of stored water is zero. The selected state and return cost for Stage 4 is shown below. This work aims to minimize freshwater consumption. Therefore, the return cost for the problem is the extent of freshwater consumption.

$$S_{Stage4}=\left\{\sum_{j}^{J_4}F_{j,4}^{Fw}=30\text{t},F_{\text{Tank1}}^{St}=0t\right\}$$

$$f_4(F_{j,4}^{Fw})=\min\left\{\sum_{j}^{J_4}F_{j,4}^{Fw}+f_3(F_{j,3}^{Fw})\right\}=\min\left\{30t+f_3(F_{j,3}^{Fw})\right\}$$

Stage 3

In Stage 3, there is operation 2, which can be fed by the mixture of reusable water from operation 1 and freshwater or only fed by freshwater. If operation 2 is fed with freshwater, the quantity is identified as 55 t. The corresponding state (S_{Stage3}^{1}) is that the useable water in Tank 1 is 30 t, which is from operation 1. Based on the Eqs (4-7)-(4-12), the quantity of reusable water from operation 1, and freshwater is determined as 30 t, and 45 t, respectively. In this case, all the water from operation 1 is consumed by operation 2. Therefore, the state with minimum freshwater consumption is 45 t. The recursive function of the problem could be updated by the state of freshwater consumption in Stage 3. The return cost is the sum of the minimum freshwater consumption in Stages 4 and 3 and the freshwater consumption over the remaining stages (Stages 1-2). On the other hand, as all the reusable water from operation 1 is reused by operation 2, the restored water is zero.

$$S_{Stage3}^{1}=\left\{\sum_{j}^{J_3}F_{j,3}^{Fw}=55t,F_{\text{Tank1}}^{St}=30t\right\}$$

$$S_{Stage3}^{2}=\left\{\sum_{j}^{J_3}F_{j,3}^{Fw}=45t,F_{\text{Tank1},SK_2,3}=30t\right\}$$

$$f_4(F_{j,4}^{Fw})=\min\left\{30t+\sum_{j}^{J_3}F_{j,3}^{Fw}+f_2(F_{j,2}^{Fw})\right\}=\min\left\{75t+f_2(F_{j,2}^{Fw})\right\}$$

Stage 2

In this example, the cyclic operation is considered. Thus, it is assumed the water from operation in the future stages can be used in Stage 2. There exist two water sinks (i.e., operations 3 and 5) with the same inlet concentration. The operation 2 in Stage 3 has outlet centration of 150, 80, 70 ppm, which is less than the inlet concentration of operations 3 and 5. In this stage, the alternative water sources should be operations 1, 2, and 4. Because operation 1 has a high quality, it should be preferentially reused by operation 2 in the previous stage according to rule 3 in Methodology. The option of operation 1 is removed from the alternative sources. On the other hand, the outlet concentration of operation 4 is higher than the outlet concentration of operations 3 and 5.

Operation 4 is also not suitable to supply operations 3 and 5 as a single source. Therefore, there are four possible states in this stage. For the first state, operations 3 and 5 are fed by freshwater. Operations 3 and 5 are fixed quantity operation. The freshwater consumption is 80 t, as shown in S_{Stage2}^{1}. The second state is that operations 3 and 5 are fed with the reusable water from operation 2, and the deficit is complemented by freshwater. This state consumes a quantity of 5 t freshwater. As for the third state, operations 3 and 5 are fed with a mixture of reusable water from operation 2 and operation 4. The quantity of water from operations 2 and 4 are determined as 53.34 t, and 26.66 t, respectively. To minimize the total freshwater consumption, the third state is chosen.

$$S_{Stage2}^{1} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 80t \right\}$$

$$S_{Stage2}^{2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 5t, F_{\mathrm{Tank2},SK_{3/5},2} = 75t, F_{\mathrm{Tank2}}^{St} = 0t \right\}$$

$$S_{Stage3}^{3} = \left\{ \begin{array}{l} \sum_{j}^{J_2} F_{j,2}^{Fw} = 0t, F_{\mathrm{Tank2},SK_{3/5},2} = 53.34t,\ \ F_{\mathrm{Tank4},SK_{3/5},2} = 26.66\mathrm{t}, \\ F_{\mathrm{Tank2}} = 21.66t,\ \ F_{\mathrm{Tank4}}^{St} = 3.34t \end{array} \right\}$$

$$f_4(F_{j,4}^{Fw}) = \min\left\{ 75t + \sum_{j}^{J_2} F_{j,2}^{Fw} + f_1(F_{j,1}^{Fw}) \right\} = \min\left\{ 75t + f_1(F_{j,1}^{Fw}) \right\}$$

Stage 1

In this stage, operation 4 can be feed with freshwater, and the mixture of freshwater and reusable water from previous operations, such as operations, 2, 3, and 5. Operation 1 is not considered in this stage because operation 1 should be reused by sinks with low high-quality requirement according to the defined rules; otherwise, more freshwater will be consumed. Because operation 3 has the same concentration as operation 5. In the following analysis, only operation 3 is considered. It, therefore, has four states, i.e., freshwater, a mixture of freshwater and reusable water from either operation 2, or operation 3. For the first state, operation 4 is fed with freshwater, i.e., 15 t. As for the second state, if operation 4 is fed by the reusable water from operation 2, the freshwater and reusable water from operation 2 are 8 t and 22 t, respectively. Unfortunately, the actual results for freshwater and reusable water from operation 1 are 8.34 t and 21.66 t, respectively. This is because the remaining quantity of wastewater from operation until this stage is 21.66 t. For the third state, operation 4 is fed by a mixture of freshwater and reusable water from operation 3. The freshwater and reusable water from operation 3 are determined as 18 t and 12 t, respectively. According to the results of these states, the state with freshwater consumption of 8.4 t is chosen to update the recursive function of the problem.

$$S_{Stage1}^{1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 15t \right\}$$

$$S_{Stage1}^{2} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 8.4t, F_{\text{Tank2},SK_4,1} = 21.6t \right\}$$

$$S_{Stage1}^{3} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 12t, F_{\text{Tank3},SK_4,1} = 18t, F_{\text{Tank3}}^{St} = 22t \right\}$$

$$f_4(F_{j,4}^{Fw}) = \min\left\{ 75t + \sum_{j}^{J_1} F_{j,1}^{Fw} \right\} = 83.4t$$

However, when examining the results, it is easily found that if more quantity of wastewater from operation 2 remains, the less freshwater will be consumed. The maximum quantity of wastewater from operation 2 being reused by operation 4 is 22 t. Therefore, the process should go back to stage 2 to recalculate the results. State 3 for Stage 2 are as follows. The quantity of wastewater from operation 2 to operations 3 and 5 is 53 t and 26.8 t from operation 4. Freshwater consumption is 0.1t. Thus, the total freshwater consumption is 83.1 t. However, the water network with less freshwater consumption could result in more connections. The final water network should be balanced between freshwater consumption and connection. Water network presented in this work consumes a quantity of 83.34 t of freshwater. The corresponding states are shown in Figure 4.9.

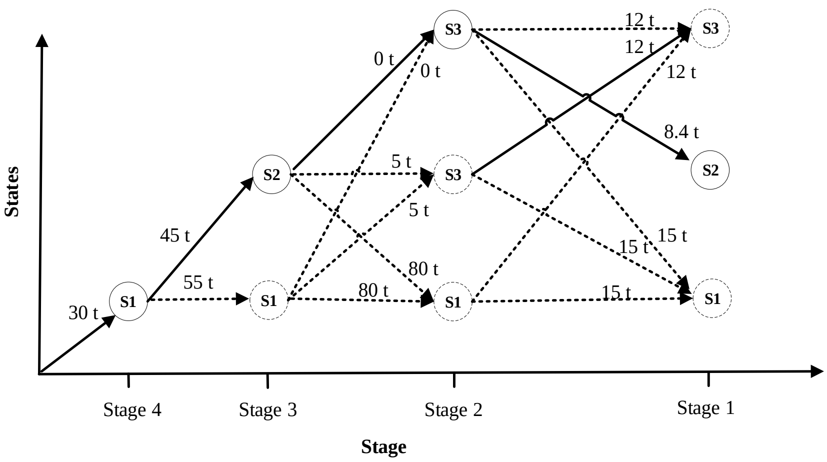


Figure 4.9 The schematic diagram of states in Example 2

Since water utilization between different operations has been identified, the water network can be configured. It is assumed that the finishing time of reusable water generating coincides with starting time of receiving operation. The water network is shown in Figure 4.10. The freshwater consumption is determined as 83.4 t. The time horizon can be shortened to 6.5 h. It is noted that in this example these operations are interdependent, otherwise the present network should be revised according to the information provided.

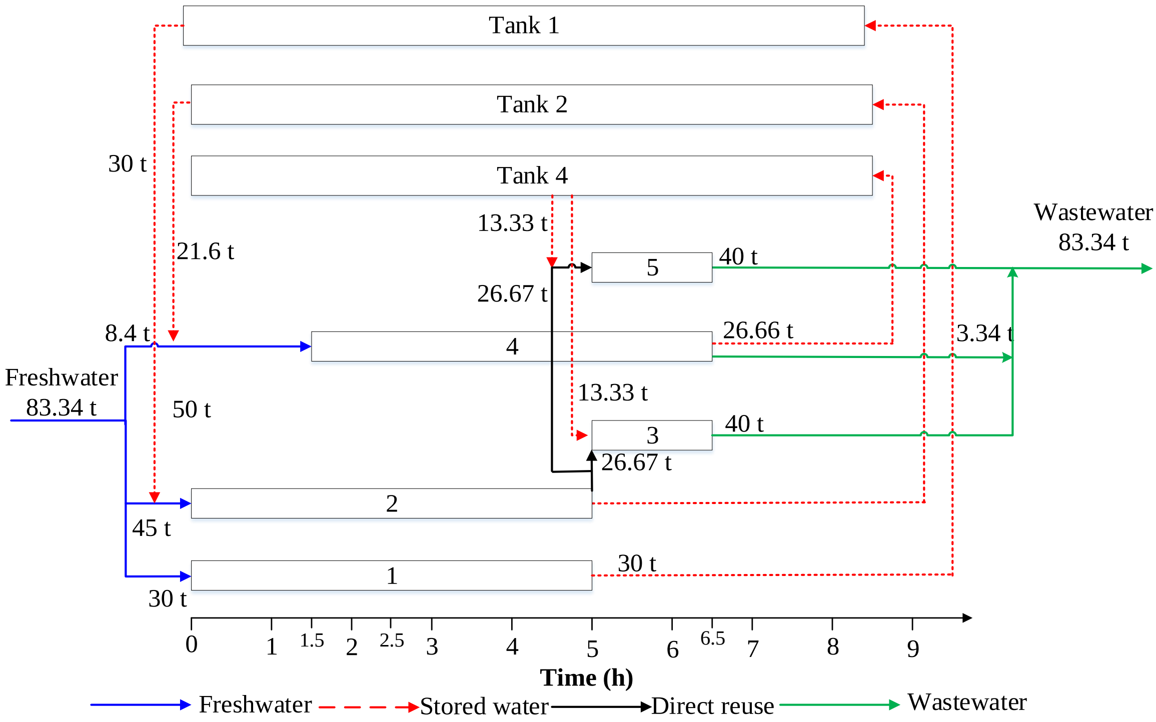


Figure 4. 10 Water network for Example 2 (reuse scenario)

Regeneration scenario

The outlet concentration of the regeneration unit for contaminants A, B, C is 40, 60, and 20 ppm, respectively. It is assumed that the timing of each operation for regeneration scenario is the same as the reuse scenario. The targeting process in Li and Majozi (2018) can be used to determine the quantity of freshwater and regenerated water. The detailed analysis is not presented in this chapter. The water network for regeneration scenario is shown in Figure 4.11. The quantities of freshwater and regenerated water are determined as 30 t, and 80 t, respectively. The flowrate of regeneration is 12.31 t/h. Compared with results of Li et al. (2018), i.e., 30 t and 75 t, this work has the same amount of freshwater and a higher quantity of regenerated water. However, this work only needs a tank.

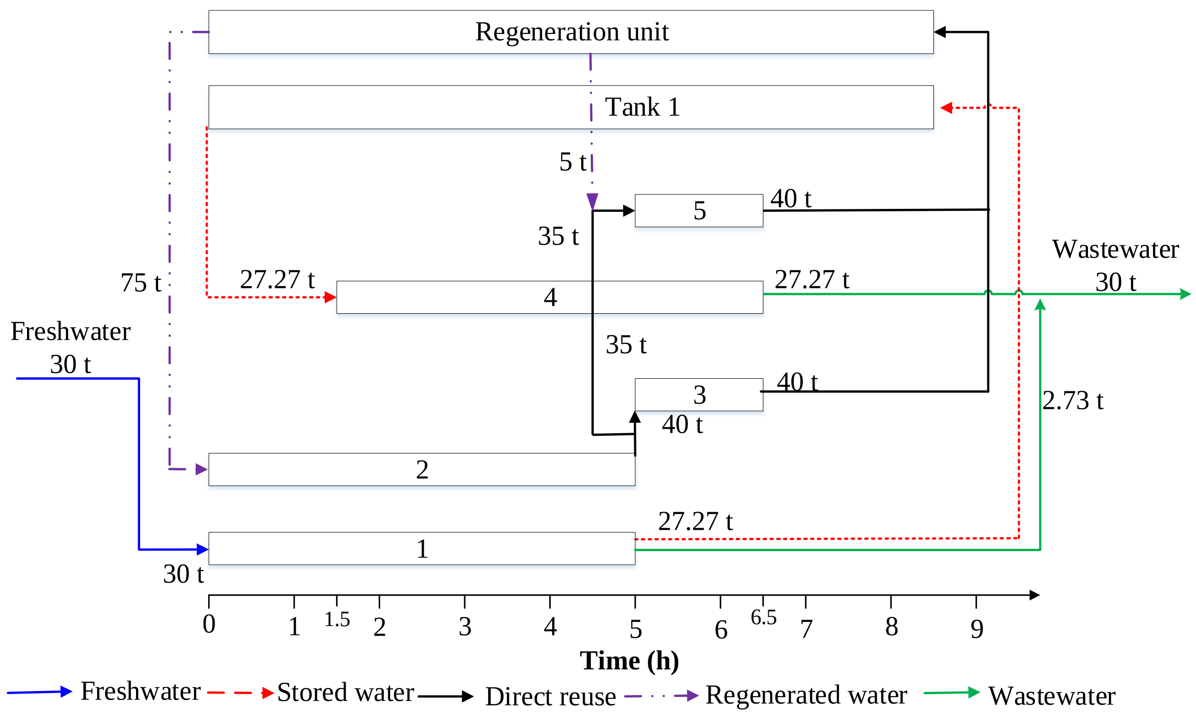


Figure 4.11 Water network for Example 2 (regeneration scenario)

4.4.3 Example 3

This example is adapted from Adekola and Majozi (2011). Four types of products are produced in the plant, i.e., shampoos, deodorants, lotions, and creams. Each product is produced by a specific mixer. The general production is described as follows. Raw material is charged to a mixer and then reacted until the required physical characteristics are obtained. After discharging the production to the delivered tank, the mixer should be washed by freshwater before next batch operation. The limiting data are listed in Table 4.3. The batches of P1, P2, P3, and P4 are 2, 3, 1, and 2.

Reuse scenario

Based on the inlet concentration of operations, the whole process can be divided into 4 stages. After a simple measure of each operation, the operation in each stage can be determined, as shown in Figure 4.12.

The operation P2 is put in the last stage because the wastewater from operation P2 cannot be reused by the remaining processes. It is noted that the sequence of each operation does not affect freshwater consumption. Because in each stage it is assumed all the wastewater generated by other processes is available.

Table 4.3 The limiting data of Example 3

Mixer	Contaminants	C_j^{in}/ppm	C_j^{out}/ppm	Limiting water/kg	△m /kg	Duration/h
P1	C1	14000	40000	576.9	15	7
	C2	0	0	0	0	
	C3	7000	7000	0	0	
	C4	3500	3500	0	0	
P2	C1	14000	14000	0	0	5.5
	C2	3500	45000	361.4	15	
	C3	7000	7000	0	0	
	C4	7000	7000	0	0	
P3	C1	14000	14000	0	0	11
	C2	0	0	0	0	
	C3	7000	50000	697.6	30	
	C4	3500	3500	0	0	
P4	C1	14000	14000	0	0	11
	C2	0	0	0	0	
	C3	7000	7000	0	0	
	C4	3500	60000	1238.9	70	

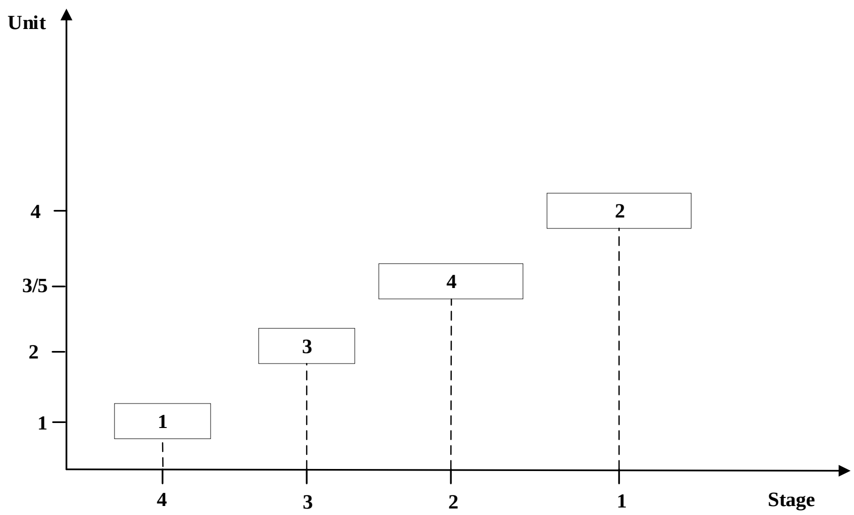


Figure 4.12 The assignment of units for each stage

The procedure of design for multiple batches is as follows. First, only a single batch operation is considered. In other words, water utilization is first considered between operations P1-P4. In the process, it could identify which process can be reused by other processes and how much water can be reused. Next, after the first single batch operation is finished, the insight obtained from the first step could be used to choose the match between the available water sources and remaining operations. The state for first single batch operation of these four mixers are shown in Figure 4.13. The detailed targeting processes for the single batch operations are described in Appendix B. In Figure 4.13; the choose states are connected by solid arcs. The insight obtained from this process could be used to choose the match between the remaining operations. For example, P2 is preferential to choose water from P3. Also, in this example, each operation can only generate a single contaminant. Thus, water from P4 could also be used by P2. For the remaining processes, such as P1, P2, and P3. The previous procedure is used to determine freshwater consumption.

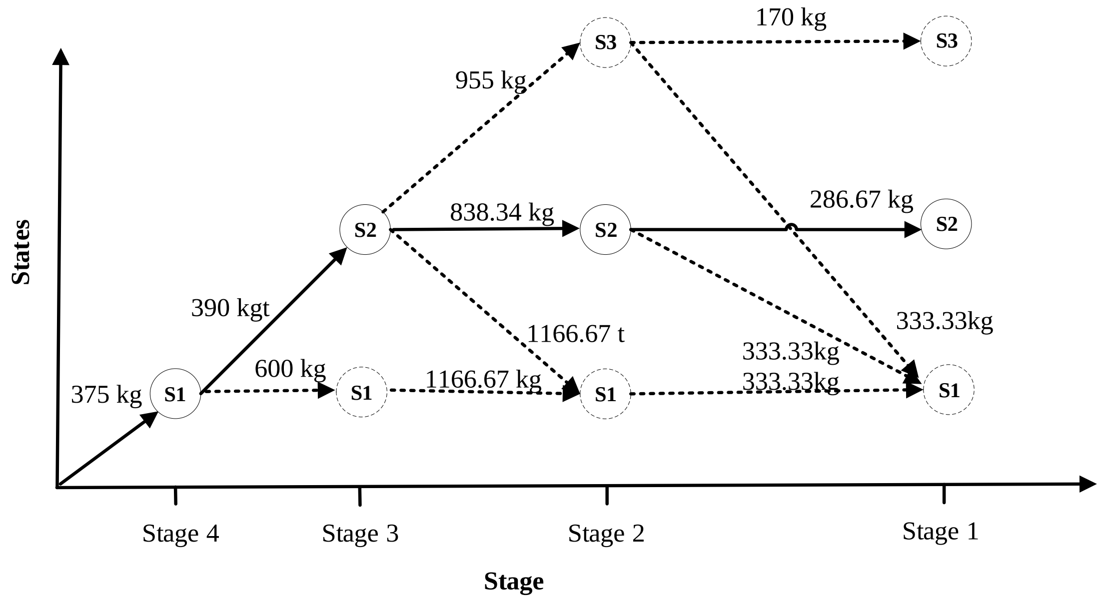


Figure 4.13 The states of each stage for a single batch operation

The resultant water network with water reuse/recycle scheme is shown in Figure 4.14. The freshwater requirement is identified as 3404.69 kg, which is less than that of Adekola and Majozi (2011), i.e., 3580 kg.

For the regeneration scenario, the timings of each operation are the same reuse scenario. The difference is to deploy a regeneration unit. Some connections are replaced by regenerated water. The final water network is presented in Figure 4.15. The result of regeneration scenario in this work is less than that of Adekola and Majozi (2011), i.e., 2653 t. The solution time of Adekola and Majozi (2011) was 464 s. However, the computational time of this work is incomparable. This is because the complex problem has been decomposed into a few small problems, which can be easily solved using a direct search algorithm.

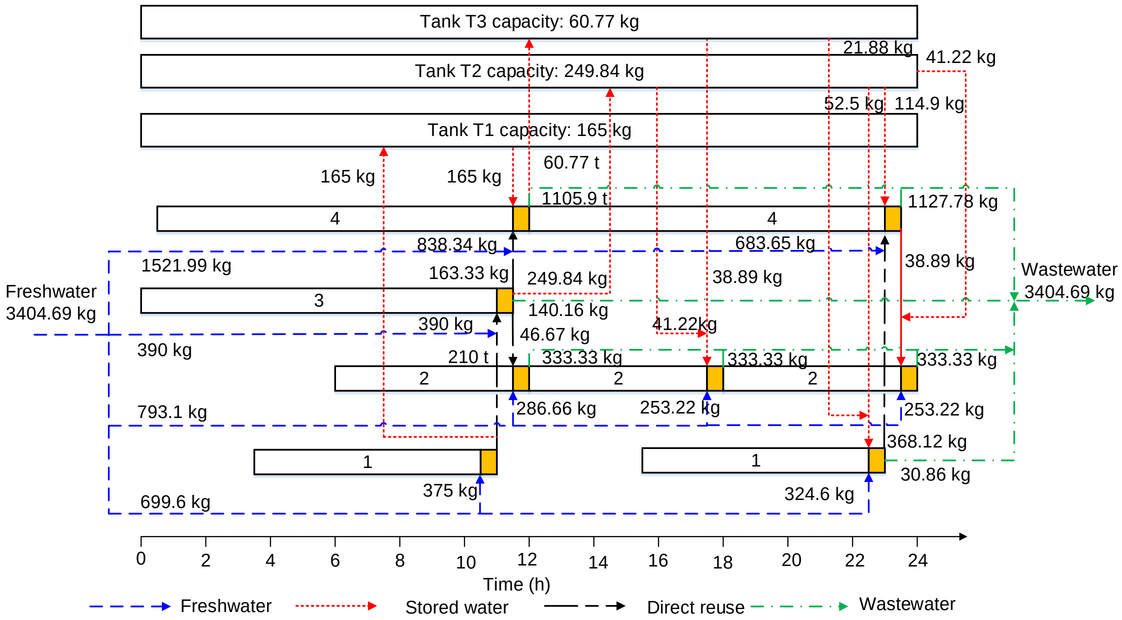


Figure 4.14 Results of Example 3 with reuse scenario

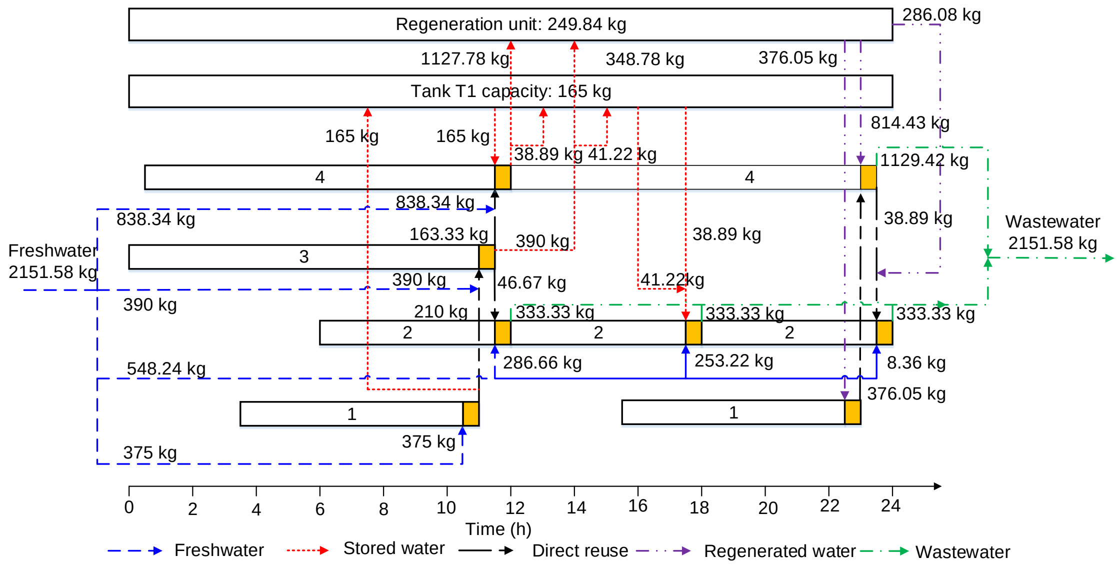


Figure 4.15 Results of Example 3 with regeneration scenario

4.5 Conclusions

A DP approach is used to identify the optimal water network for flexible batch processes. The sink with different water quality is treated as the stage. In each stage, the quantity of available water sources is seen as the state. Water utilization between different operation and target of freshwater consumption can thus be determined. Based on this target, water network could be designed. The feasibility of time constraints is then checked to determine whether the designed network is suitable or not. In the process, the water network for reuse scenario is first configured. The timings of all the operations in the regeneration scenario are assumed as the same as reuse scenario. Three different examples from the literature are used to demonstrate the applicability of the proposed approach. The obtained results match with published literature.

Compared with the predefined schedule, this work does not provide the timings of each operation before the design. Only the duration of each operation is given in the limiting data. Thus, the proposed method could be used to design a batch water network with flexible scheduling framework. The limitation of this work is that this work focuses on the scheduling of water operation. Future work should focus on the robust design of batch processes with minimum freshwater consumption and optimal product scheduling.

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5

DESIGN OF FLEXIBLE BATCH WATER NETWORK USING MATCH RANKING MATRIX METHOD

5.1. Introduction

Socioeconomic developments put increasing pressure on natural resources, especially freshwater, thereby resulting in a temporal deficit in freshwater resources. More attention is thus paid to the conservation of freshwater resources. On the other hand, more stringent regulation of environmental emissions of process industries is taken to protect the ecosystem and provide a comfortable environment for humankind. It drives the academic and industrial practitioners to find ways of reducing freshwater consumption and minimizing the environmental impact due to the wastewater discharge. Batch operations have been widely used in some chemical industries, such as pharmaceutical industry, fine and specialty chemicals because batch processing is suitable to produce specialized low volume products and are flexible to adjust to uncertainties of the market. Thus, a systematic approach is required to optimize the water utilization and maximize the output in batch plants to meet the requirements of environmental protection and cleaner production.

Water integration is a widely used method of minimizing freshwater consumption in batch chemical processes (Majozi *et al*., 2017). It not only achieves the goals of efficient utilization of water but also minimizes environmental burdens due to the discharge of wastewater. Compared with continuous processes, it is more complex to perform water reuse activities in batch processes because of the incorporation of time constraints (Majozi *et al*., 2010). Water reuse activities must obey the constraints of water quantity and quality; the feasibility of time issues should be met at the same time. Thus, the approaches developed for batch processes are more complex compared with those in continuous processes.

Among these methods, there exist two main categories in batch processes, i.e., insight-based methods and optimization-based techniques (Gouws *et al*., 2010). Optimization-based approaches are built based on the superstructure and usually formulated as a mixed integer nonlinear programming (MINLP) problem. They consist of various constraints, such as water and contaminant balances, allocation constraints, capacity constraints, storage constraints, etc. According to the difference in the treatment of time dimension, there are two main groups of addressing wastewater recovery issues in batch processes. One group is to minimize freshwater consumption in a predefined schedule scenario. In the batch plant, the timings of all the operations are known before water reuse activities. The other group is to optimize water reuse and product scheduling simultaneously, which implies that the duration of the operation is treated as a variable. Because this work considers the latter case, the approaches for the given product schedule are not discussed. One can refer to the technical books for detailed information (Majozi *et al*., 2015; Majozi *et al*., 2017).

One of the advantages of batch operation is the flexibility of adjusting its strategy to market changes. When the market demand for productions changes, batch chemical plants can adapt to these changes accordingly. Consequently, the existing water network of batch plants could not achieve the goals set for the previous production recipe. To this end, we should consider water recovery for flexible production scheduling. It has been reported that the flexibility of production schedules may lead to a further reduction of freshwater consumption compared with predefined production scheduling (Majozi *et al*., 2017; Adekola and Majozi, 2011).

Many mathematical approaches have been proposed to consider the simultaneous optimization of wastewater minimization and production schedule. The solution of these formulations can obtain the optimal production scheduling with the minimum freshwater consumption. Most of them are formulated as MINLP problems. Majozi (2005) extended the formulation of wastewater minimization in a predefined schedule environment to a flexible scheduling framework where the timings of operations are treated as optimization variables. Cheng and Chang (2007) proposed an integrated batch water model. In their formulation, the interactions between production scheduling subsystem, water-reuse subsystem, and wastewater treatment are considered, rather than considering each subsystem individually. Similarly, Zhou *et al*. (2009) used the unit-specific event point formulation to develop a comprehensive formulation representing water utilization in flexible batch plants. In this contribution, a continuous-time formulation is used to represent production scheduling. Furthermore, a hybrid strategy combining DICOPT and genetic algorithm is employed to obtain the globally optimal solution. Li *et al*. (2010) modified the state-time-space superstructure proposed by Zhou *et al*. (2009) for optimization of water allocation network in batch processes. In their modified superstructure, the employment of mixers/splitters could rule out the streams which bypass water users without any mass exchange.

In the work of Adekola and Majozi (2011), a continuous-time-based model is presented to address wastewater minimization with flexible production scheduling. A regeneration unit is deployed for further reduction of freshwater. Results showed the employment of regeneration could bring in more reduction of wastewater production compared with water reuse scenario. Chen *et al*. (2011) developed a resource-task-network based mathematical model to optimize production scheduling and wastewater recovery. In their model, both short-term and periodic scheduling are considered separately. A relaxation linearization was employed to solve the resultant formulation.

Chaturvedi and Bandyopadhyay (2014a) proposed a mathematical formulation to reduce operating cost by supplying multiple freshwater resources in flexible batch plants. The formulations in their work can be used to deal with both single and multiple-contaminant systems. In their subsequent work, Chaturvedi and Bandyopadhyay (2014b) proposed a multiple objective formulation to cope with the issues of minimizing freshwater requirement and maximizing production in a batch process at the same time. The optimal solution between the production and the freshwater consumption was obtained through the Pareto optimal front. Chaturvedi et al. (2016) optimized water utilization in the batch plant by employing multiple water resources. They pointed out that the optimal production scheduling for a single resource can also be suitable for multiple fresh resources, which also lead to a minimum operating cost. In the work of Dong *et al*. (2016), multiple wastewater regeneration modules are considered in the model to treat the wastewater for reuse. Although the superstructure-based method can find the optimal solution, the large size of the formulation usually makes the model difficult to solve. Lee and Foo (2017) proposed a mixed integer linear program (MILP) to consider simultaneous process scheduling and water minimization for a batch plant. In the model, the water reuse is modelled by pinch-based automated targeting approach. Therefore, the limitation is that the proposed model is applicable to a single contaminant problem.

Pulluru and Akkerman (2018) employed a generic classification to represent water quality to capture the characteristics of water flows in batch plants. The water-integrated scheduling approach can help understand the balance between water efficiency and production efficiency.

Unlike mathematical techniques, insight-based approaches cannot efficiently and readily handle the issues of batch water network as in continuous processes because of the incorporation of the time dimension. Although there exist numerous methods using the insight-based advantages to address water minimization of batch processes, these methods are based on the predefined schedule. Wang and Smith (1995) proposed a graphical method for water recovery in batch processes. In their approach, operations are divided into many intervals according to the given information. In the targeting process, time constraints should meet firstly, and concentration is the second constraint. In the specific concentration interval, the target of freshwater, as well as the quantity of available reuse water is determined based on the quantity vs. time diagram. The available water is cascaded into the next concentration interval until the last concentration interval. Ultimately, the final target of freshwater consumption is the summation of freshwater consumption in each concentration interval. However, in Wang and Smith (1995), water entering and discharging from the unit can occur during the course of operation, which is not true in actual batch processes.

In truly batch operations, material enters at the start and leaves at the end of the processes, respectively. In order to address this limitation, Majozi *et al*. (2006) modified the graphical method developed by Wang and Smith (1995) to cope with wastewater recovery in completely batch operations. In their targeting method, concentration is initially set as a primary constraint, while the time dimension is treated as a secondary constraint. Results indicate that the reverse of the priority of constraints can obtain the same targets. However, the limitation is that the target of freshwater consumption cannot be determined before detailed design.

In the work of Chen and Lee (2008), the target and network design can be achieved at the same time based on the graphical representation. In their approach, water demand and water source are displayed in a quantity vs. time diagram. Next, freshwater consumption is determined based on some practical constraints by using available water sources to meet water demand at a specific time point. The network can be thus designed at the same time. The water cascade analysis was extended by Foo *et al*. (2005) for the synthesis of the batch water network. The advantage of this work is capable of obtaining the results automatically using the spreadsheet. Liu *et al*. (2007) proposed a similar method to design a water network for discontinuous or batch processes. The disadvantage of their work is that the quantity of water transfer is obtained based on the results of sub-network design. It leads to the fact that the targets are not determined prior to detailed design. Foo *et al*. (2012) considered the design of a total batch water network. However, the procedure is only applicable to cyclic operations. Furthermore, the regeneration unit is operated continuously, not in a batch operation.

Kim (2011) proposed a two-stage procedure to utilize the insight of pinch analysis for synthesis of discontinuous water systems. In the first step, targets determined by conventional pinch analysis are set as the lower bound. Next, the water network is configured based on the insight from pinch analysis. Thus, the limitation of this work is that if the lower bound cannot meet the water demand, it will be difficult to identify how much additional water should be used. Li and Majozi (2018) designed the batch water network using a dynamic programming (DP) method. In their method, all the water-using operations are aggregated into N stages based on the timings of each operation. In each stage, the state with minimum freshwater consumption is selected to update the recursive objective function until the last stage is implemented. The target and network can be determined at the same time.

Although the concept of this work is similar to Kemp and Deakin (1989), this method is different from Kemp and Deakin (1989). First, they considered heat recovery in batch processes. Second, the timings of operations are given, while only the durations of operations are given in this work. Third, Kemp and Deakin (1989) utilized Cascade analysis to analyze the heat exchange in each time interval, and then it is to remove the heat storage by rescheduling processes. Therefore, the contribution of this work is to develop an insight-based method to investigate wastewater recovery as much as possible in flexible batch processes. Flexible batch process in the context of this contribution implies that the timings of each operation are treated as variables, instead of parameters. In other words, only the duration of each operation is given, and the timings of each operation are unknown. It aims to investigate opportunities for water reuse to meet the time constraints.

Although many superstructure-based methods have been developed to deal with the water integration issues in flexible batch plants, the integrated framework considers production scheduling, water utilization, as well water regeneration, which makes the model difficult to solve. Furthermore, sometimes in the industrial community, it is not necessary to get the exactly optimal results with expensive computations. These existing insight-based methods for batch processes are proposed to cope with wastewater recovery in batch processes with predefined scheduling. When the sequence of the operations is changed, the existing water network could be not optimal for the new scheduling. Thus, the method proposed in this work aims to provide a simple procedure for the designer to perform water conservation in flexible batch plants.

In the proposed method, the possibility of reuse of wastewater between water sources and sinks is first evaluated. Next, the rankings of these matches can be obtained based on these results. Thus, the optimal match for each water sink can be identified according to these rankings. The water network can then be determined based on insight obtained from the sequence of operation. For example, the link operation of wastewater should start after the wastewater source operation finishes in the case of direct reuse. The excess reusable water is stored in the tank to meet the demand of other operations or for regeneration. The structure of this chapter is introduced as follows. The following Section 5.2 is a description of the problem, where the given information about the problem is explained. A detailed description of the methodology is explained step by step in Section 5.3. Three examples reproduced from the literature are presented in Section 5.4 to explain how to use this insight-based method. Finally, Section 5.5 summarizes the conclusions and suggestions for future research.

5.2. Problem statement

This work addresses the optimization issues of minimizing freshwater in batch processes where time is an optimization variable. The given information is stated as follows:

(i) The scheduling data are given, including maximum storage capacities, duration of operations, the time horizon of interest,

(ii) limiting water data of operations are known, such as maximum inlet and outlet concentrations for each operation, the water requirement of each operation, the parameters of regeneration units,

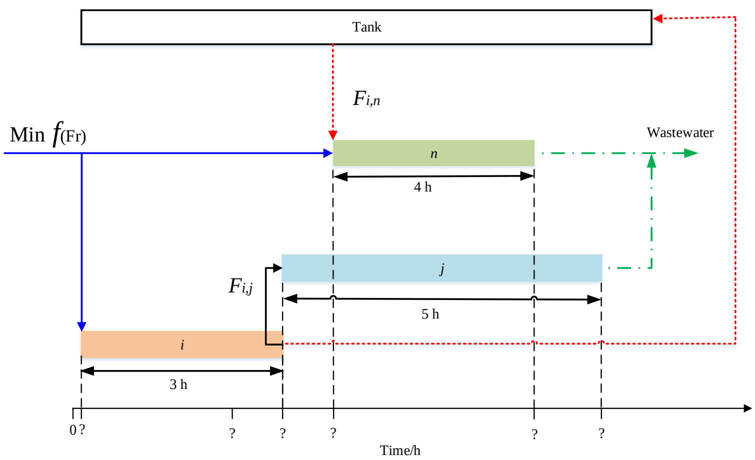

Figure 5.1 Schematic representation of the problem

The schematic of the problem is shown in Figure 5.1. It is assumed that there are *n* batch operations. The durations of these operations are known. In other words, the timings of these operations are unknown. Also, water quantity and quality of batch operations are also given. The objective is to obtain a minimum freshwater requirement for batch processes, and to determine the timings of these operations.

5.3. Methodology

In this chapter, a ranking matrix is established based on the quantity of reusable of each water source to determine the priority of the matches for each water sink. The insight obtained from the ranking of the matches can be used to identify the optimal matches and the sequence of relevant operations. Based on the chosen matches, the timing of relevant operations can be determined. Figure 5.2 presents the procedure of synthesis of the batch water network.

An example adopted from literature (Liu *et al*., 2009) is introduced to explain the procedure of the approach. Table 5.1 presents the data on water operations. Freshwater is free of contaminants. In this example, water operations are treated as fixed load problems. All the operations in this example are independent of each other. It can thus change the sequence of operation further to reduce the quantity of freshwater consumption.

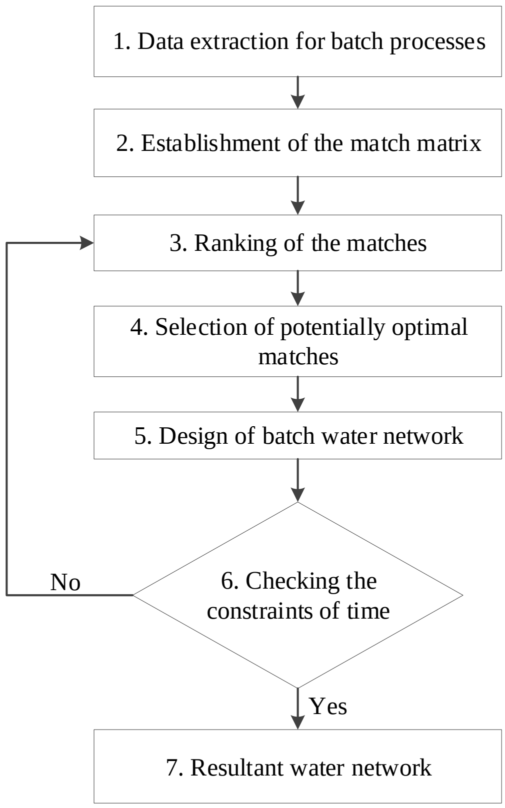

Figure 5.2 Schematic representation of the approach

Table 5.1 Limiting data for Example 1

Operation	Quantity/t	$c^{u,in}$ / *ppm*	$c^{u,out}$ / *ppm*	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

Step 1: Data extraction

The limiting data of water operation are key elements for the grassroots design of water networks and also are the basis for evaluating the potential of wastewater recovery for the retrofit. Correct identification of limiting data has a significant impact on the desired target for a given process and robustness of the network (Foo, 2012). In this work, the limiting data of examples are adapted from literature.

Step 2: Establishment of the match matrix

The matching matrix for water sources and sinks can thus be established based on the water recovery potential determined by the limiting data.

Firstly, an $m \times n$ matrix is established to characterize the potential of water reuse in the system. In the matrix, m and n represent the number of sources and sinks, respectively. Table 5.2 is a matrix of 6 × 5 representing the source-sink matches. The first value in the bracket is maximum reusable water from water sources to the sinks, and the second value in the bracket is the corresponding freshwater consumption. For example, (6, 24), in the third row, the second column of Table 5.2, indicates that a maximum amount of 6 t water from Process C can be recovered in Process B, 24 t of freshwater is required to dilute this reusable water to meet water requirement. Results of reuse water and freshwater for all the matches are determined by the specific equations in the following scenarios.

In this work, water recycling is forbidden in order to avoid the accumulation of contaminants. The values in the diagonal matches are thus zero. In some cases, the regenerator is employed to treat wastewater for further reuse. The regenerator can thus be treated as a water demand and a water source at the same time. It is noted that in this case regeneration unit is not taken into account.

Table 5.2 The matching matrix for reuse scenario (unit: t)

	A	B	C	D	E
A	(0,0)	(0, 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)

According to the concentration difference between available wastewater and water sinks, the maximum recovery of wastewater from water sources and the quantity of freshwater required to dilute the wastewater are determined based on the following three scenarios.

Scenario 1

If the inlet concentration of the water sink is zero or the concentration of reusable water exceeds outlet concentration of sinks, freshwater is the only source to meet the water requirements. This reusable water cannot be reused by the sink directly due to the high concentration, otherwise, it will cause a penalty of freshwater. Because it violates necessary optimality conditions of water utilization in process plants (Savelski and Bagajewicz, 2000). For a fixed load problem, freshwater can be identified by Eq (5-1). For a fixed flowrate problem, freshwater consumption is determined by Eq (5-2). For multiple contaminants scenario, the maximum freshwater consumption over all contaminants is selected as the freshwater requirement of this water sink.

$$F_{j,l}^{Fr}(c_{j,l}^{u,out} - c_{Fr,l}) = \Delta m_{j,l}, \forall j \in J, \forall l \in L \quad (5\text{-}1)$$

$$F_{j,l}^{Fr} = F_{j,l}, \forall j \in J, \forall l \in L \quad (5\text{-}2)$$

Where $F_{j,l}^{Fr}$ is freshwater consumption of process *j* for contaminant *l*. $\Delta m_{j,l}$ is a mass load of contaminant *l* in process *j*. $c_{j,l}^{u,out}$ is the maximum outlet concentration of contaminant *l* in process *j*. $c_{Fr,l}$ is a concentration of contaminant *l* in freshwater. $F_{j,l}$ is fixed limiting water requirement of process *j*.

Scenario 2

If the concentration of water sources, i.e. reused wastewater and regenerated water, is less than the maximum inlet concentration of water sinks, only wastewater or regenerated water is required to satisfy the water requirement of water sink. For the fixed mass load problem, the quantity of wastewater required can be identified by Eq (5-3). For the fixed flowrate problem, the wastewater required is determined by Eq (5-4). It is noted that in this stage only water reuse between one water source and one water sink is considered to rank the matches for a specific source and sink. There is only one water source in the set of *I*. Once the ranking of matches is determined, the first-place ranking is used to meet the water requirement of the specific sink. If insufficient, the deficient is compensated by the second-place ranking or freshwater.

$$\sum_{i \in I} F_{i,j,l}(c_{j,l}^{u,out} - c_{i,l}^{u,out}) = \Delta m_{j,l}, \forall j \in J, \forall l \in L \tag{5-3}$$

$$\sum_{i \in I} F_{i,j,l} = F_{j,l}, \forall j \in J, \forall l \in L \tag{5-4}$$

Where $F_{i,j,l}$ is the maximum amount of reusable water from process *i* to process *j* for contaminant *l*. $c_{i,l}^{u,out}$ is the limiting outlet concentration of contaminant *l* in the process *i*. $F_{j,l}$ is the limiting water requirement of process *j*.

Scenario 3

If the concentration of reusable water exceeds the maximum inlet concentration of water sink but is less than the maximum outlet concentration of sinks, the mixture of freshwater and wastewater should be used to satisfy the water requirement of water sinks. For the fixed mass load problem, the quantity of wastewater and freshwater consumption can be identified by Eqs (5-5) and (5-6). For a fixed flowrate problem, the wastewater and freshwater consumption is identified by Eqs (5-7) and (5-8). It is noted that in this stage it is to evaluate the reuse potential of reusable water. Thus, only one water source is included in the set of *I*.

$$\sum_{i \in I} F_{i,j,l}(c_{j,l}^{u,out} - c_{i,l}^{u,out}) + F_{j,l}^{Fr}(c_{j,l}^{u,out} - c_{Fr,l}) = \Delta m_{j,l}, \forall j \in J, \forall l \in L \tag{5-5}$$

$$\sum_{i \in I} F_{i,j,l} c_{i,l}^{u,out} + F_{j,l}^{Fr} c_{Fr,l} = (F_{i,j,l} + F_{j,l}^{Fr}) c_{j,l}^{u,in}, \forall j \in J, \forall l \in L \tag{5-6}$$

$$\sum_{i \in I} F_{i,j,l} + F_{j,l}^{Fr} = F_{j,l}, \forall j \in J, \forall l \in L \tag{5-7}$$

$$\sum_{i \in I} F_{i,j,l} c_{i,l}^{u,out} + F_{j,l}^{Fr} c_{Fr,l} = \sum_{i \in I} (F_{i,j,l} + F_{j,l}^{Fr}) c_{j,l}^{u,in}, \forall j \in J, \forall l \in L \tag{5-8}$$

Where $c_{j,l}^{u,in}$ is the maximum inlet concentration of contaminant *l* in process *j*. The remaining variables are the same as in previous scenarios.

Note that the equations above are general expressions of the problem, including single- and multiple-contaminant situations. For the single contaminant problem, it is easy to determine the quantity of freshwater and reuse water is determined directly. For multiple contaminant problems, as shown in the second illustrative example in Section 5.4.2 implemented for this application, the first step is to calculate the freshwater requirement for the specific contaminant. Next, the maximum value of the quantity of freshwater across all contaminants is chosen as the demand for freshwater requirement.

Step 3: Obtaining the match ranking matrix

Once the match matrix is constructed, the ranking for these matches can be determined on the ascending order of freshwater consumption. The match ranking matrix is then obtained, as shown in Table 5.3.

In this process, the ranking rules for these matches require to be further refined to eliminate some infeasible matches. Because in some cases there are some matches which consumed the same amount of freshwater. As shown in column 1 of Table 5.2, the freshwater consumed in all of the matches related to Operation A is the same. Operation A has, however, a zero inlet concentration, indicating that the reusable water from other operations cannot be reused by Operation A. Therefore, when performing the ranking for the matches, only the match between freshwater and Operation A is feasible.

It should be noted that this does not violate the rule of ranking based on freshwater consumption. The additional rule is to eliminate the match whose reuse water is zero, as shown in Column 1 of Table 5.2. The results of the ranking are used to select the optimal matches. It provides insight for the designer to choose which source should supply the sink preferentially. The match finally selected could be different due to other constraints, i.e. complexity of connection, availability of reuse water.

Table 5.3 The ranking matrix for water sources and sinks

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

Note: notation "–" indicating there is no water reuse between the water source and sink

Step 4: Identification of potentially optimal match

After the match ranking matrix is established, the potentially optimal matches can be determined based on these rankings. The initial matches for all water sinks are presented in Table 5.4. Insight of the rankings is then used to select the water sources to satisfy water requirements of water sinks.

Table 5.4 The potentially optimal matches

	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

Based on the information of Table 5.4, the potentially optimal matches can be determined for all the water sources and sinks. The first ranking match is preferentially chosen to meet the water demand of specific sink. If the quantity of available water from the water sources is insufficient, the water source at the second place will be used to complement the deficit. The same procedure is repeated until the water demand of water sink is satisfied. It is noted that this is an initial ranking to choose which source should be sent to the sink preferentially. The final matches between sources and sinks should consider many factors, for example, the position in the ranking list, number of tanks, and the availability of reusable water. The potentially optimal match is usually the first or second place in the ranking list, which is established based on freshwater consumption. For a specific water sink, if the quantity of water source in the first match is deficient, the second match can be selected as the potentially optimal match. This can ensure that matches with the least freshwater consumption is chosen for every sink. If no additional constraints are not considered, the selected matches can be seen as the best solutions in terms of freshwater consumption. The initial matches of sources and sinks are shown in Table 5.5.

Table 5.5 The initial potential optimal match between sources and sinks

	A	B	C	D	E
A			(5, 5)	(21, 3)	(33.33, 0)
B			(5, 5)	(21, 3)	(33.33, 0)
C					
D					
E					
Fr	(0, 50)	(0, 22.5)			

Although insight from freshwater consumption can be used to determine the potential match between water source and sink, it is not always true for all situations. As shown in Table 5.5, it is rather straightforward to determine the water utilization of Operations A and B. However; it is not obvious whether Operation A or Operation B should feed the remaining operations. Consequently, other factors, such as the time horizon, network complexity, and availability of reuse water, have to be considered.

Step 5: Design of initial batch water network

Before designing the initial network, a set of rules are set arbitrarily so as to meet the constraint of time horizon of interest and reduce the solution search space: a) The operation with zero inlet concentration is set as the first operation; b) the operation with the maximum inlet concentration is set as the final operation of this batch operation. It is noteworthy that these rules are set arbitrarily to reduce the alternative solutions so as to design the initial batch water network. The optimal network may be different from the initial water network.

Finally, the sequence of operation could be obtained based on the connection of water flows. For example, if wastewater generated by Operation A is reused by Operation B, Operation A should finish before Operation B starts. In other words, to reduce the capacity of the storage facility, the mass exchange should be achieved through the direct exchange as possible. Thus, the starting time of Operation B should coincide with the finishing time of Operation A. Therefore, the time of these operations can be determined once water utilization has been identified.

According to the rules above, the timing of Operations A and E can be determined depending on the time horizon under consideration, e.g., 8.5 h could be done in this case. Based on the insight from Table 5.5, the timing of other operations can also be determined. To reduce the network connections, Operations C and D are fed by wastewater from Operation A. This is because the quantity of available water from Operation B, i.e., 22.5 t, is insufficient to feed Operations C and D, whose total water requirement is 26 t. If all the water from Operation B is recovered by Operation E, the deficit is complemented by wastewater from Operation A, i.e., 10.83 t. The remaining water of Operation A is then emitted as wastewater. After water demand of all the sink is met, the remaining water from sources is discharged as wastewater. The initial water network is shown in Figure 5.3.

Once the initial network is configured, it is necessary to check time constraints and mass balance for each operation. If all the constraints are met, the design can be finished, and the water network is obtained. Otherwise, the network should be redesigned by removing some infeasible matches. It should be always be borne in mind that for any given target, there exist several options for the design.

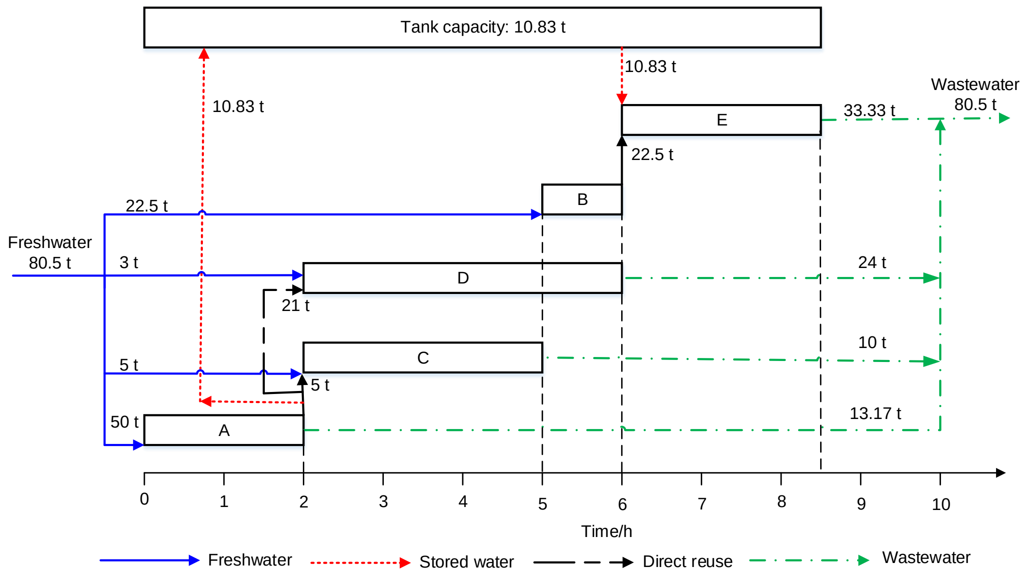

Figure 5.3 Initial water network of Example 1 with reuse scenario

5.4. Illustrative examples

Three examples adopted from literature are used to illustrate the above methodology. Example 1 considers the design of batch water network with a single contaminant, while Example 2 takes into account multiple contaminants problems. Two scenarios are considered in both examples, i.e., water reuse/recycle and regeneration scheme. In Example 1, a regeneration unit is deployed to purify wastewater. It is assumed there is no water loss during regeneration processes and outlet concentration of the regenerator is fixed. In Example 2, a regeneration unit with fixed removal ratios of contaminants is employed to further minimize freshwater consumption. Although these two examples are fixed mass load problems, the proposed method is also suitable for fixed flowrate problems. In Example 3, a batch plant with five operations is considered in which the water operations are treated as fixed flowrate problems.

5.4.1 Example 1

The example illustrated in Section 5.3 is revisited here. In water reuse/recycle scenario, a buffer tank is used to store reusable water for reuse. In regeneration scenario, the regenerator with fixed outlet concentration is considered. During the processes, the capacity of tanks deployed in the water network is restricted to 70 t.

5.4.1.1 Reuse/recycle scenario

It is assumed that all the operations are independent. Thus, these operations can be arranged at any time point only if the ending time is not extended the time horizon of interest. The time horizon of this example is set 8.5 h. When examining the results of Figure 5.3, it is easily found that the storage capacity can be further reduced by moving forward Operations B and E. It thus not only eliminates the storage facility, but it also reduces the operation time. The results are shown in Figure 5.4. Compared with Liu *et al*. (2009) with a storage capacity of 56.432 t, in this scenario the storage tank is removed. Furthermore, the time horizon is further reduced to 6 h.

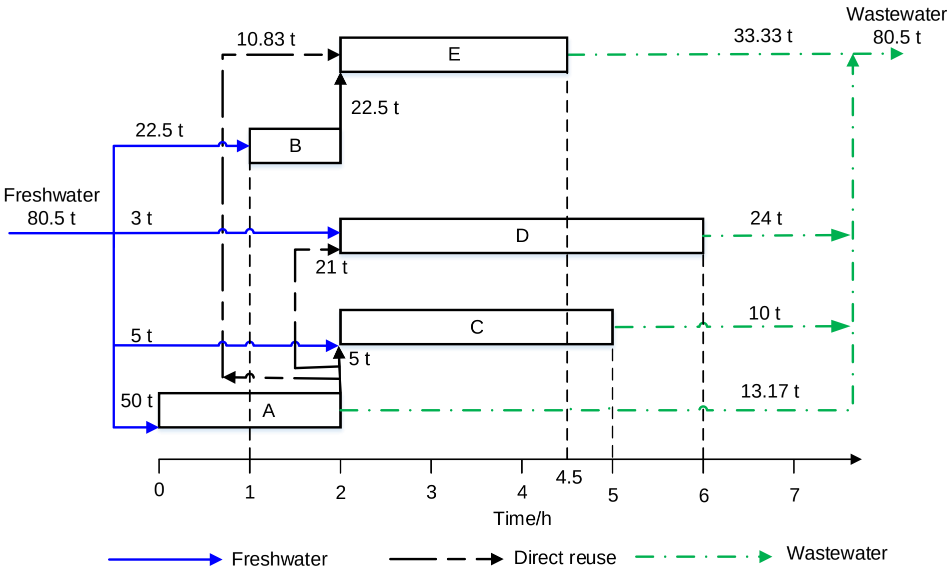

Figure 5.4 Resultant network of Example 1 (reuse/recycle scenario)

If Figure 5.4 is examined carefully, it can be found that the obtained batch water network could be evolved to reduce the number of connections and operation time. As shown in Figure 5.4, wastewater from Operation A has four destinations, i.e., Operations C, D, E, and wastewater discharge. If the wastewater from Operation B is sent to Operation D, rather than feeding Operation E, those reusable water from Operation A can be reused by Operation E. This would, therefore, reduce the complexity of water network. On the other hand, the cluster consisting of Operations B and D has nothing to do with the cluster of Operations A, C, E in terms of water reuse. Operations B can be moved forward to the start. The required time horizon of batch operations is further reduced to 5 h. The evolved batch network is shown in Figure 5.5.

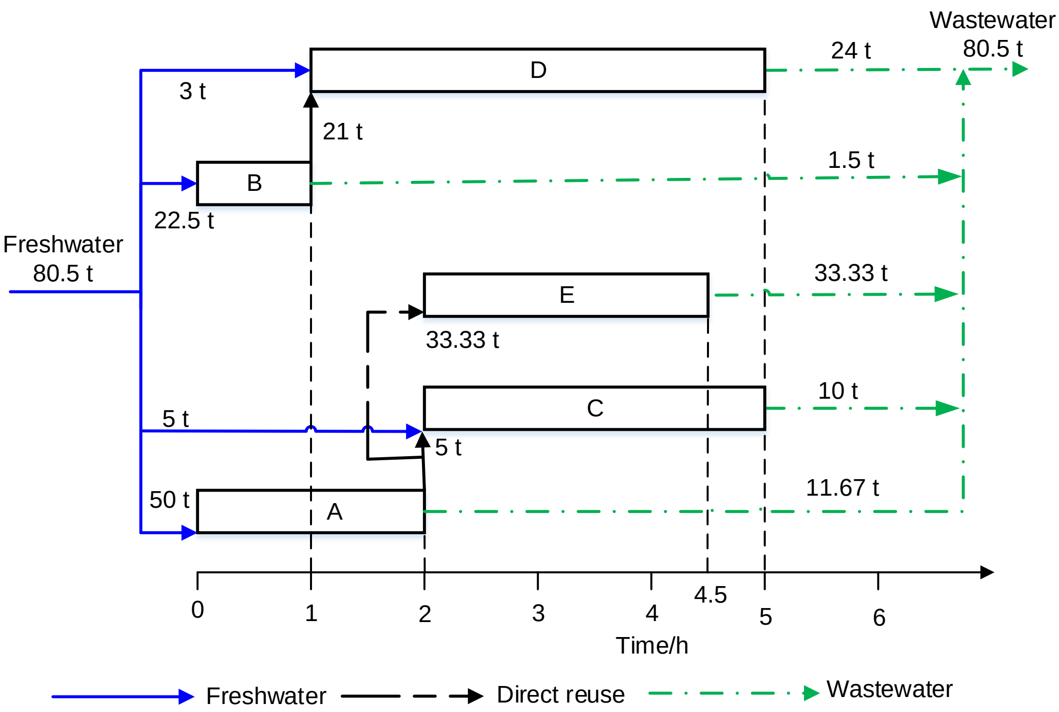

Figure 5.5 Evolved water network of Example 1 (reuse/recycle scenario)

5.4.1.2 Consideration of Regeneration

In the previous subsection, the reuse scenario has been discussed. In this scenario, a regeneration unit is employed to further reduce the quantity of freshwater requirement. The flowrate of the regenerator is 11.875 t/h, and outlet concentration is 100 ppm. The same procedure of reuse scenario is repeated for the regeneration scenario. The matching matrix for regeneration scenario is similar to the reuse/recycle scenario. The difference is that in this scenario a water source of regenerated water is added into the matrix. The value of reuse water for the regeneration unit is the limiting water quantity of each water source, as shown in Table S1 of Appendix C. The match ranking matrix and potentially optimal matches for this scenario are shown in Tables S2-S4 of Appendix C, respectively. The detailed process is explained in Appendix C.

The resultant batch water network is shown in Figure 5.6. It should be noted that two tanks must be deployed in this water network to avoid the occurrences of cross-transfer. When 10.21 t of regenerated water is leaving the regeneration unit to Tank S, 19.79 t of wastewater from Tank T is transferred to the regeneration unit at the same time. After that, the Tank T is empty until the end of all operations.

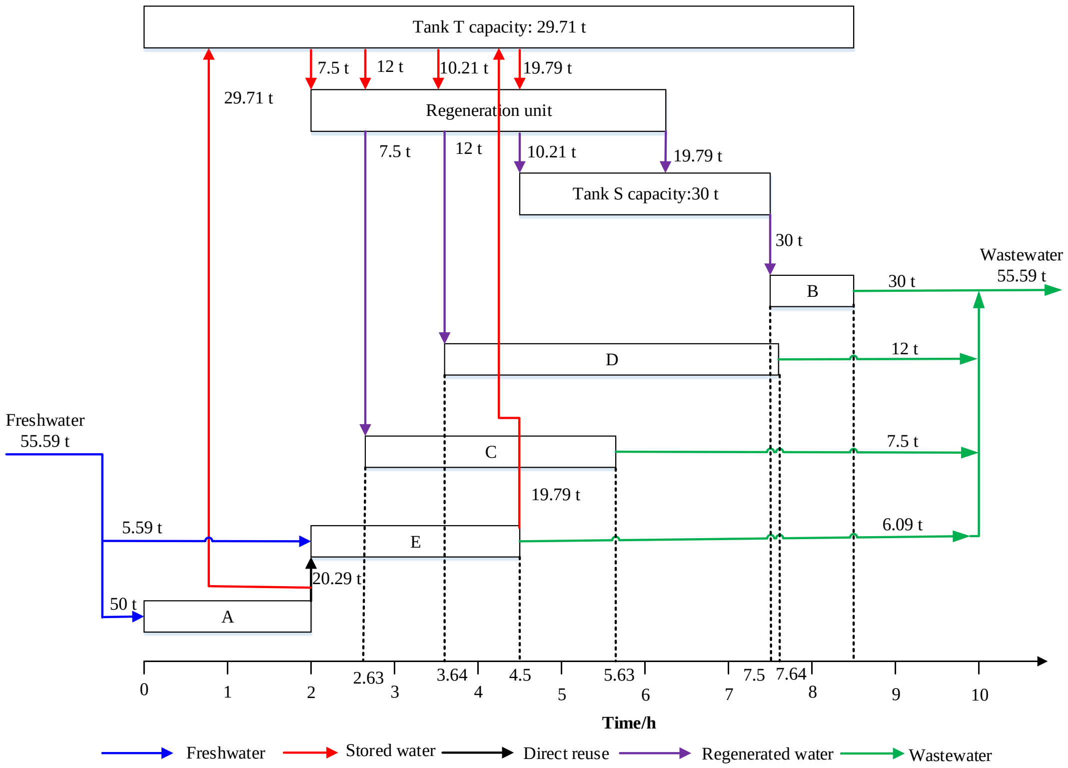

Figure 5.6 Water network for regeneration scenario of Example 1

The quantity of freshwater is determined as 55.59 t, while the result from Liu *et al*. (2009) with the predefined schedule is 68.594 t. In the work of Adekola and Majozi (2011), the freshwater is 64.07 t, where the duration of operations is treated as variables. Therefore, this work can achieve a reduction of 15.7% of freshwater for Liu *et al*. (2009) with predefined scheduling and of 9.8% of freshwater for Adekola and Majozi[5] with flexible scheduling.

If the last batch of regenerated water can be sent to Operation E directly, the storage capacity can be further reduced by moving forward Operation B. The start time of Operation B is the finishing time of the last batch of regenerated water. The total amount of regenerated water is known, the timings of the batch operation of the regeneration unit are thus determined. Furthermore, the operation time is also reduced to 7.64 h, as shown in Figure 5.7.

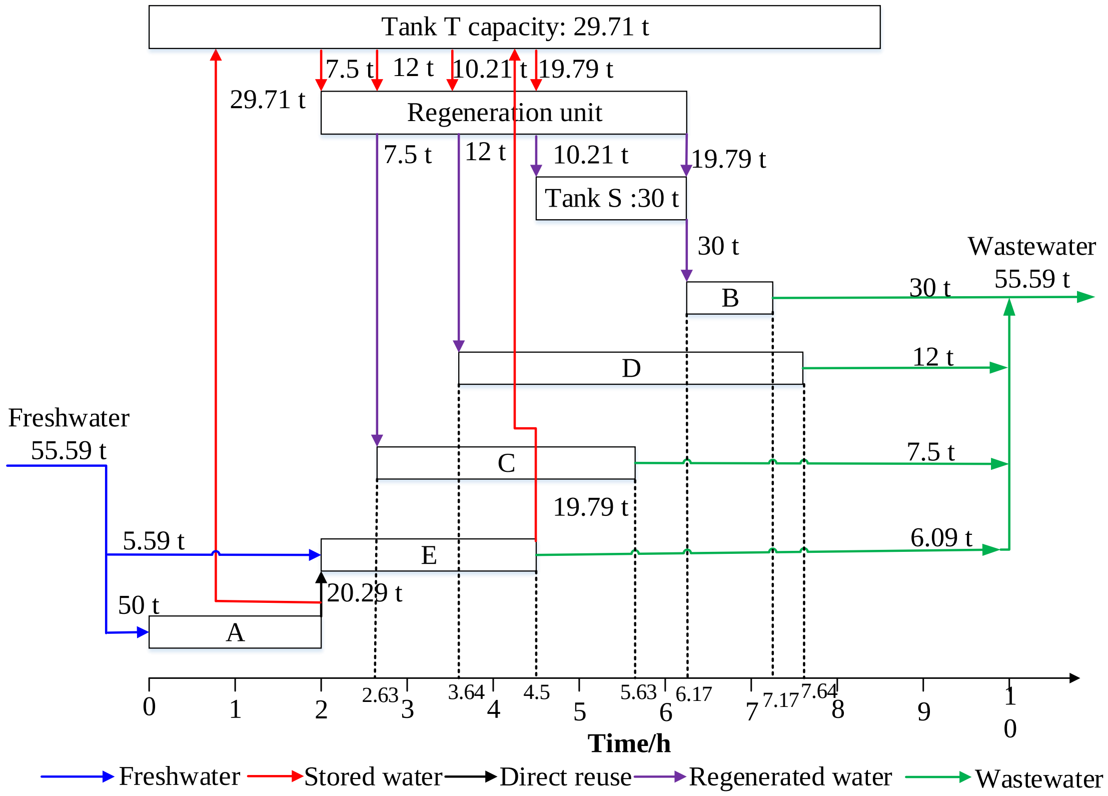

Figure 5.7 Evolved water network of Example 1 (regeneration scenario)

5.4.2 Example 2

In the previous section, a batch plant with a single contaminant is introduced to explain the application of the proposed method. In this example, multiple contaminants problems are considered. The example is reproduced from the literature (Adekola and Majozi, 2011). The limiting data are summarized in Table 5.6.

In the plant, four different products were produced by four different mixers. Each mixer is dedicated to a specific product. Raw materials are first charged to the mixer and then reacted until the required qualities are obtained. After the production are discharged from the mixer, the mixer should be washed for the next batch. The number of batches for these mixers over a 24 h time horizon is 2, 3, 1 and 2, respectively. The water washing operations is seen as fixed load problems. In this example, each mixer can produce a specific contaminant. The wastewater from different mixers can be mixed to meet the water demand of washing operation by appropriately arranging these operations.

Table 5.6 The limiting water data of Example 2

Mixer	Contaminants	$C_j^{u,in}/ppm$	$C_j^{u,out}/ppm$	Water demand/kg	△m /kg	Duration/h
P1	C1	14000	40000	576.9	15	7
	C2	0	0	0		
	C3	7000	7000	0		
	C4	3500	3500	0		
P2	C1	14000	14000	0	15	5.5
	C2	3500	45000	361.4		
	C3	7000	7000	0		
	C4	7000	7000	0		
P3	C1	14000	14000	0	30	11
	C2	0	0	0		
	C3	7000	50000	697.6		
	C4	3500	3500	0		
P4	C1	14000	14000	0	70	11
	C2	0	0	0		
	C3	7000	7000	0		
	C4	3500	60000	1238.9		

5.4.2.1 Reuse/recycle scenario

The match ranking matrix and potentially optimal matches for this scenario are shown in Tables S5-S9 of Appendix C, respectively. The detailed procedure is introduced in Appendix C. The total freshwater consumption for reuse scenario is 3404.69 kg, as shown in Figure 5.8.

As shown in Figure 5.8, 37.11% of freshwater consumption can be reduced based on the original problem without any reuse. A water saving of 5.1% is obtained, compared with results of Adekola and Majozi (2011). It should be noted that this work requires less freshwater compared to Adekola and Majozi[5]. However, more storage tanks are employed in this work. In practice, the final network should trade off the operation cost and capital cost, and other aspects that require mathematical modeling.

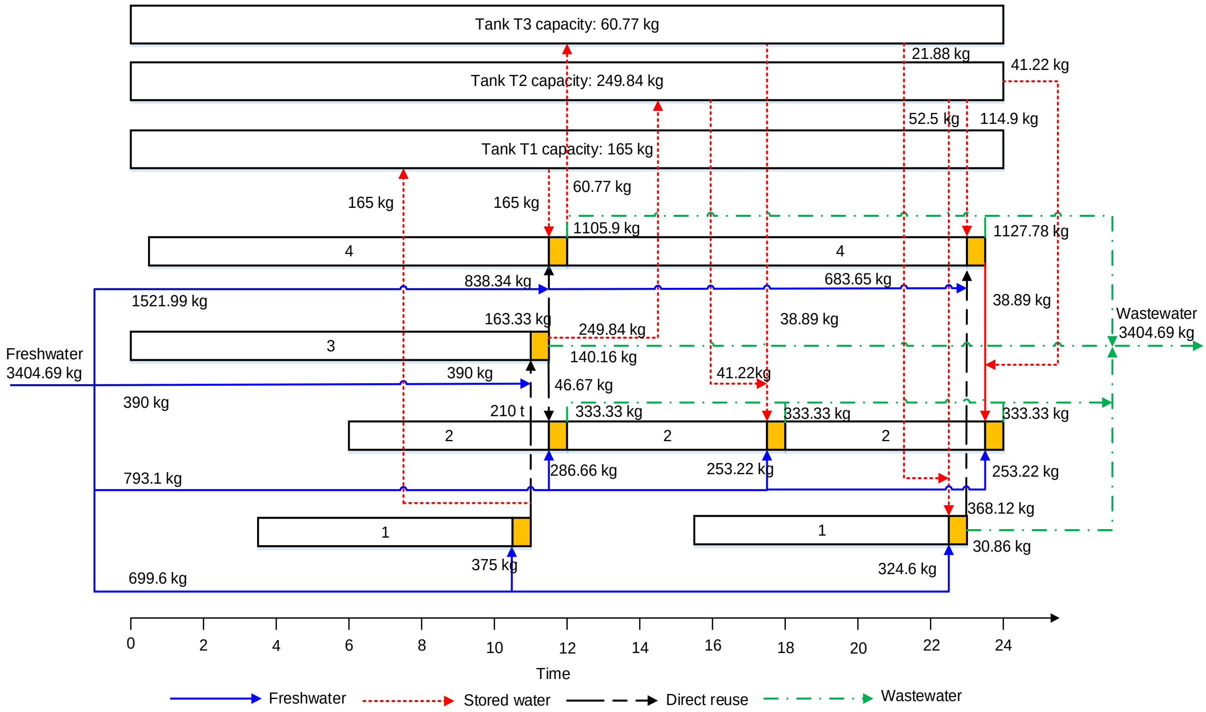

Figure 5.8 Resultant water network for the reuse scenario of Example 2

5.4.2.2 Consideration of Regeneration scenario

In the regeneration scenario, a regeneration unit with given removal ratios is considered. The removal ratio of C1, C2, C3, and C4 are 0.95, 0.99, 0.96 and 0.98, respectively. The regenerator has a flowrate of 466 kg/h. Because the regeneration unit is a type of given removal ratio, the outlet concentration is dependent on the inlet concentration if no water loss or gain occurs. It thus is not obvious to rank the matches between water sinks and regeneration unit. However, insight from the ranking matrix for reuse scenario can also be used to determine the water network through trial and error method.

In this scenario, most of the optimal matches are the same as the reuse scenario. The difference is that in some matches the wastewater is replaced by regenerated water. The total freshwater consumed in this scenario is determined as 2151.58 kg, while the results of Adekola and Majozi[5] are 2653 kg. However, more storage tanks are required in this work. The final network is shown in Figure 5.9.

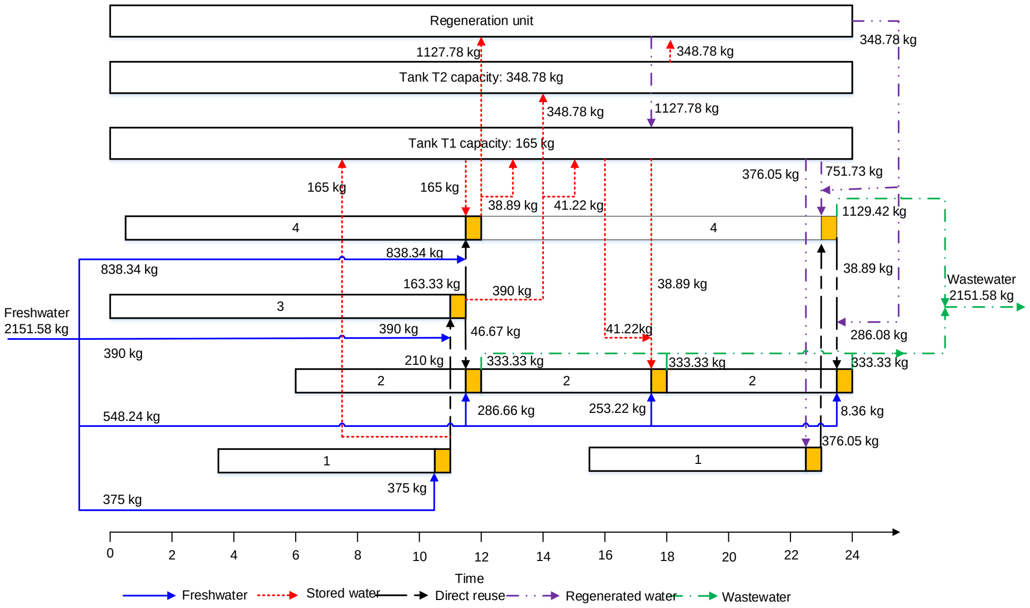

Figure 5.9 Resultant water network of Example 2 (regeneration)

5.4.3 Example 3

To extend the method to fixed flowrate problem, a case study adopted from Majozi *et al*. (2006) is introduced. The limiting water data are presented in Table 5.7.

Three products, i.e., A, B, and C, are produced in the batch plant. The procedure in the plant is as follows. The reaction took place in process 1 to produce A. Water is treated as a solvent to wash the salt. In process 2, water was used as the reaction solvent. In process 3, an additional quantity of water was required to wash the product produced in process 2 to meet the quality of production. The same procedure took place in processes 4 and 5 to produce C. Therefore, when rescheduling the processes, processes 2 and 3 should happen in sequence because of their dependence, so were processes 4 and 5. It is assumed that these operations have a fixed water requirement.

Table 5.7 The limiting data of Example 3

Operation	Quantity/kg	Concentrations /(kg of salt /kg of water) $c^{u,in}$	Concentrations /(kg of salt /kg of water) $c^{u,out}$	Duration/h
1	1000	0	0.1	3
2	280	0.25	0.51	4
3	400	0.1	0.1	1.5
4	280	0.25	0.51	4
5	400	0.1	0.1	1.5

Based on the scenarios introduced in section of Methodology, the freshwater for all the matches is determined. The matching matrix and ranking results of Example 3 are shown in Tables S10 and S11, respectively. For simplicity, the detailed process for the design is omitted. The freshwater is determined as 1560 kg. The resultant water network is displayed in Figure 5.10. Compared with the predefined scheduling (Majozi *et al*., 2006), a storage tank with a capacity of 400 kg is removed by rescheduling the operations. Furthermore, the time horizon is shortened to 5.5 h.

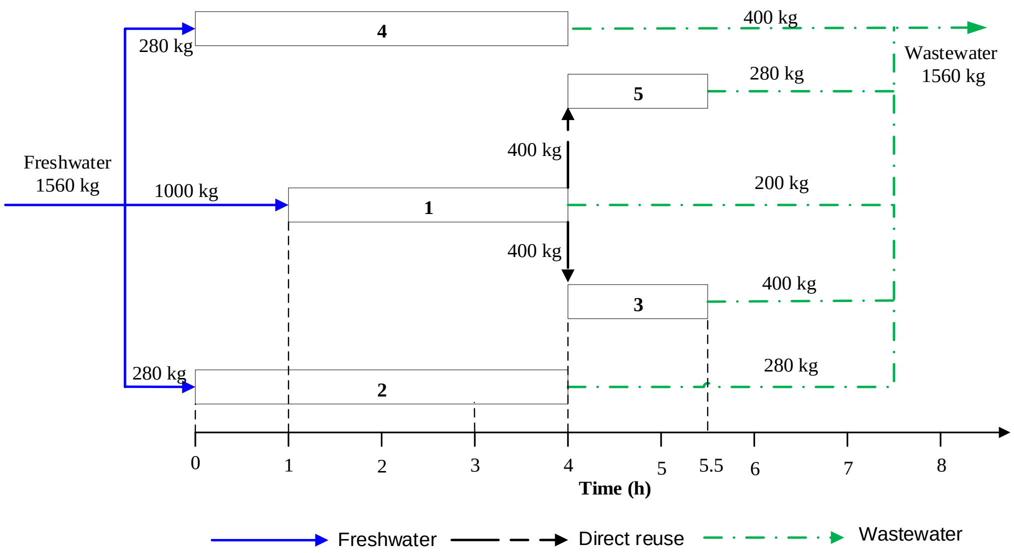

Figure 5.10 Resultant water network for Example 3 (First sequence)

5.5. Conclusions

This work has proposed an insight-based method to design a flexible batch water network. By evaluating the reuse potential of wastewater from sources, a match ranking matrix is then constructed to choose potentially optimal source-sink matches. Thus, a water network can be configurated to achieve minimum water consumption. To further reduce freshwater consumption, two types of regenerator are employed to purify wastewater in illustrative examples. The proposed approach can be used to deal with water system with single- and multiple-contaminant problems. Although the method proposed cannot be proved by rigorous mathematics, the method can assist the designer without a strong background of mathematics to design a flexible batch water network. Furthermore, the results obtained by the method are not worse than those of mathematical programming methods.

This method is simple for the synthesis of the water network in flexible batch processes. Three examples adopted from literature are considered in this work. Results in this work have better performance than those in Adekola and Majozi (2011) in terms of freshwater consumption, indicating that this approach is capable of dealing with single- or multiple-contaminant problems. The method can also be used to large scale problems. However, the design process maybe more complex compared with simple examples of this work. For example, for a specific water sink, maybe there are multiple matches with the same ranking. Furthermore, some other problems may arise. Some operations have no connection with other operations. In this case, the timing of these operations is difficult to be determined. Thus, more additional constraints about the operation should be given.

In this work, the match ranking matrix method is proposed to design batch water networks. It aims to minimize the freshwater consumption for the batch plants and design the batch water network with minimum operating time by rescheduling some processes. The proposed method is similar to a two-stage technique. The first stage is to identify the minimum freshwater consumption and the second stage is to design a batch water network to achieve the goal of freshwater consumption obtained in the first stage. These two stages are repeated until all the water sinks are satisfied. In the iterative process, the batch water network with minimum batch time is chosen by eliminating the batch water networks with longer batch time. Therefore, Hence, future work can combine the match ranking matrix approach with the superstructure-based method to simultaneously minimize the freshwater consumption and operating time for the batch plants.

Nomenclature

$F_{j,l}^{Fr}$	freshwater consumption of process *j* for contaminant *l*
$F_{j,l}$	limiting water requirement of process *j* for contaminant *l*
$F_{i,j,l}$	amount of water transferred from process *i* to process *j* for contaminant *l*
$c_{j,l}^{u,in}$	maximum inlet concentration of process *j* for contaminant *l*
$c_{j,l}^{u,out}$	maximum outlet concentration of process *j* for contaminant *l*
$c_{i,l}^{u,out}$	The maximum outlet concentration of process *i* for contaminant *l*
$c_{Fr,l}$	concentration of freshwater for contaminant *l*
$\Delta m_{j,l}$	mass load of process *j* for contaminant *l*

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6

SYNTHESIS OF FLEXIBLE BATCH WATER NETWORKS BASED ON PINCH ANALYSIS

6.1 Introduction

Although continuous processes are dominant in the production of bulk chemicals, batch processes are still used extensively in the chemical industry, especially in the manufacture of small-scale and high-value-added products. A batch process is comprised of a set of steps that can be independently operated by a predefined recipe. This advantage allows for ease of altering its production schedule to adapt to the fluctuation of the market and have good control of product quality and yield (Majozi *et al*., 2017). Once the product recipe of the batch plant is changed, it is inevitable to redesign its utility network, such as water networks. Therefore, a systematic method of designing a batch water network with flexible production scheduling is of great significance.

For continuous processes, there are many insight-based methods of determining the target of the processes. For batch processes, the insight-based methods are rarely reported. Wang and Smith (1995) introduced the graphical representation concept to target the freshwater consumption for batch processes. In the targeting processes, time feasibility is firstly checked for a specific concentration interval when considering water reuse in this concentration interval, and then the remaining water is cascaded into the next concentration interval. The detailed procedure is explained as follows. The streams are divided into a few concentration intervals and time intervals based on the given information. Next, in every concentration interval, the freshwater requirement is determined by considering water reuse in the same interval. The remaining reusable water is cascaded to the next interval. The same procedure is repeated until the water demand in the last concentration interval is satisfied. The quantity of freshwater for the whole process is the sum of freshwater consumed in each concentration interval. However, the limitation is that if an operation covers too many time intervals, wastewater from other operations can be reused in the current operation in terms of concentration. It is not feasible from the point of view of time. Because in truly batch processes, the charging and discharging of water is not allowed to happen during the operation.

To address this limitation, Majozi *et al*. (2006) reversed the priority of constraints proposed by Wang and Smith (1995) to coping with water minimization issues of completely batch operations. Results indicate the reverse priorities of constraints do not affect the target of freshwater consumption. Thus, whether choosing time as a primary constraint or not should depend on the number of intervals, which can determine the complexity of the analysis. Although these graphical methods for batch processes are similar to water pinch analysis (Wang and Smith, 1994) and could determine the target before detailed design, these methods have the assumption that operations are fixed mass load problems. Chen and Lee (2008) considered design optimal batch water network with fixed mass load and fixed quantity operations. In their method, water sources and sinks are displayed in quantity vs. time diagram. It is easily found which source is available at a specific time and how much water can be recovered from that source. Targeting and network design are performed simultaneously based on the timing of each operation. However, this method does not provide more physical insight, as shown in pinch analysis diagram (Wang and Smith, 1994).

Therefore, Kim (2011) extended pinch analysis to target freshwater requirement for discontinuous processes. Firstly, the target of minimum freshwater consumption obtained by pinch analysis is set as the lower bound. Secondly, a water network is designed based on the insights provided by pinch analysis. However, the addition constraint of time in batch processes limits the application of this method. Although the graphical method provides physical insight for the designer, the targeting is usually performed through the shift of the composite curve, which sometimes give inaccurate results. Except for these graphical methods for batch processes, other algebraic targeting methods, such as waster cascade analysis method, have also been reported to evaluate the opportunities of water recovery in batch water systems. This is because algebraic methods have higher accuracy as compared to graphical methods. For example, Foo *et al*. (2005) extended the water cascade analysis for the synthesis of the batch water network. The advantage of this work is capable of obtaining the results automatically using the spreadsheet. Liu *et al*. (2007) proposed a similar cascade analysis to design a water network for discontinuous processes. In their work, both fixed mass load problems and fixed flowrate problems are considered. The disadvantage of their work is that when considering the reusable water transferred between different time interval, the quantity of water transfer is obtained based on the existing network design. It leads to the fact that the targets are not determined before detailed design.

Foo *et al*. (2012) proposed a systematic procedure for the design of a total batch water network. However, the procedure is only applicable to cyclic operations. Furthermore, the regeneration unit is operated continuously, not in a batch operation. Taking advantage of insight provided by graphical representation, Oliver *et al*. (2008) embedded the insight from pinch analysis into the mathematical modeling to design batch water network. The solution of the formulation can determine the addition of freshwater consumption above the target obtained by pinch analysis and the number of tanks. The limitation of their work is that the multiple contaminants are not considered. Li *et al*. (2013) developed a manual design procedure for a batch water network with single- and multiple-contaminants. However, the proposed method is a manual design method, not applicable to large scale problems. Also, it cannot ensure the designed network is cost-effective. Li and Majozi (2018) designed a batch water network using the dynamic programming (DP) method. In their method, water-using operations are allocated into different stages, which is defined based on the starting and ending time. The targets can be determined by choosing the optimal states through which the analysis can transfer from the previous stage to the next stage.

In batch processes, more complexity arises in the process of wastewater recovery due to the incorporation of time constraints. These methods above are proposed for batch processes with predefined production scheduling. When the batch chemical plant changes its production strategy, the existing water network might not achieve the goal of minimum freshwater requirement. To this end, there is a need for considering the recovery of wastewater for the flexible production scheduling. It has been reported that the flexibility of production scheduling may result in more reductions of freshwater consumption compared with predefined production scheduling (Majozi *et al*., 2017).

Many mathematical approaches have been developed to simultaneously consider water recovery and production schedule. The solution of these formulations could determine the minimum freshwater requirement and corresponding scheduling. Most of these formulations are formulated as mixed integer nonlinear programming (MINLP) problems. Cheng and Chang (2007) proposed an integrated batch water model comprising of the water-reuse subsystem, production scheduling subsystem, and wastewater treatment subsystem. In the production schedule, a discrete-time representation is adopted. Although the model of Cheng and Chang (2007) could capture the characteristic of water flows in flexible batch processes, discrete time representation leads to more binary variables and the time points of operation is only allowed to locate at fixed interval boundaries. Zhou *et al*. (2009) developed a continuous time-based model to optimize batch water networks and process schedules simultaneously. A modified state-space concept is proposed to represent the batch processes. Furthermore, a hybrid method combining DICOPT and Genetic Algorithm was used to solve the problem to guarantee the global optimum. Li *et al*. (2010) modified the superstructure of Zhou *et al*. (2009) by employing splitters and mixers in the water network. This can rule out the streams bypassing water users without mass exchange. Also, deterministic and stochastic searching techniques were used to enhance the possibility of finding global solutions.

Adekola and Majozi (2011) proposed a continuous time-based model to consider the effect of employing regenerator on the flexible batch water network. The model can cope with single-and multiple-contaminant problems. However, the model is difficult to solve because of its large size. Chen *et al*. (2011) developed a resource-task-network based representation to consider simultaneous wastewater minimization and scheduling in multipurpose batch plants. Two different formulations are proposed for short-term and periodic scheduling, respectively. In some cases, there are multiple fresh resources with different quality. In the work of Chaturvedi and Bandyopadhyay (2014a), multiple freshwater resources are used to feed the water users. Because of the intake of inferior freshwater resources with lower cost, the operating cost can be further reduced.

Unlike the literature above, Chaturvedi and Bandyopadhyay (2014b) considered the production scheduling problem and water recovery as a multiple objective problems. The optimal results are obtained by the Pareto frontier. However, the epsilon-constraint method is adopted to solve the formulation, which usually obtain weakly Pareto optimal solutions. Chaturvedi *et al*. (2016) considered employing multiple water resources to feed the flexible batch water network. Results show that the optimal scheduling for the single freshwater resource is also applicable to the scenario of multiple fresh resources. To formulate a simple model, Lee and Foo (2017) combined pinch-based automated targeting model and discrete time-based scheduling. Compared with other models above, the formulation is mixed integer linear programming. The limitation is that the pinch-based automated targeting method is only applicable to single contaminant problems. Dong *et al*. (2016) presented a systematic approach for optimal batch water network synthesis based on state space superstructure. In their model, multiple wastewater regeneration methods are taken into account. Pulluru and Akkerman (2018) employed a general water classification method to capture the quality of water, rather than the concentration. The method can reduce the computational complexity caused by the modeling of contaminations.

Therefore, the objective of this chapter is to evaluate the potential of maximum water recovery in batch processes based on the graphical method. By rescheduling the operations, it is to achieve the target of minimum freshwater consumption obtained by pinch analysis through the direct and indirect water reuse schemes. The contribution of this work is described as follows: 1) it provides physical insight for the designer to design a feasible batch water network; 2) the configured water network not only achieves the goal of minimum freshwater consumption, but also meets the time constraints of operations. The paper is organized as follows. In Section 6.2, a brief introduction of the problem is stated. Section 6.3 introduces the graphical method in this work. Illustrative examples are discussed in Section 6.4. Finally, the conclusions and limitations are explained in Section 6.5.

6.2 Problem statement

This work aims to address the problem of minimizing freshwater utilization by rescheduling batch operations. It is assumed that the water operation is not bound with production scheduling. The rescheduling is only applicable to water operations. The relevant information for the problem is shown as follows.

- There are a set of operations in batch plants. The duration for each operation and the capacity of storage tanks are given. The time horizon of the processes is also known.
- For each operation, the limiting water data are given, including the mass load of contaminants, the maximum inlet and outlet concentration, as well as water quantity requirement.

The objective is to determine an optimal network which not only satisfies the time constraints but also achieves the target of maximum water recovery as possible.

6.3 Methodology

In this chapter, a three-stage procedure is presented to design optimal batch water network based on pinch analysis. The detailed explanation for the procedure is summarized in Figure 6.1.

In the first step, the operations are considered as continuous processes. The target of the minimum freshwater requirement is determined by pinch analysis. The pinch point divides the whole process into two separate regions, i.e., below the pinch (higher quality region, HQR) and above the pinch (lower quality region, LQR) (Foo, 2012). The source at pinch point is called pinch causing source. The pinch causing source can allocate its flowrate to both HQR and LQR.

A few “golden rules” can then be derived for the HQR and LQR to design the water network (Foo, 2012).

1. Water sources in the HQR (including freshwater) are not allowed to feed the sinks in the LQR and may not be mixed with sources in the latter region. If a source that belongs to the HQR is allocated to the LQR, leading to a penalty of a fresh resource in the water network.
2. The water source having the same concentration as pinch point can be allocated to both HQR and LQR. The horizontal distance of the segment for this source in the HQR and LQR represents its allocated flowrate in the respective regions.
3. Freshwater should only be used in the HQR. If an additional fresh resource is used in the LQR, the waste discharge from the water network also increases with the same magnitude.

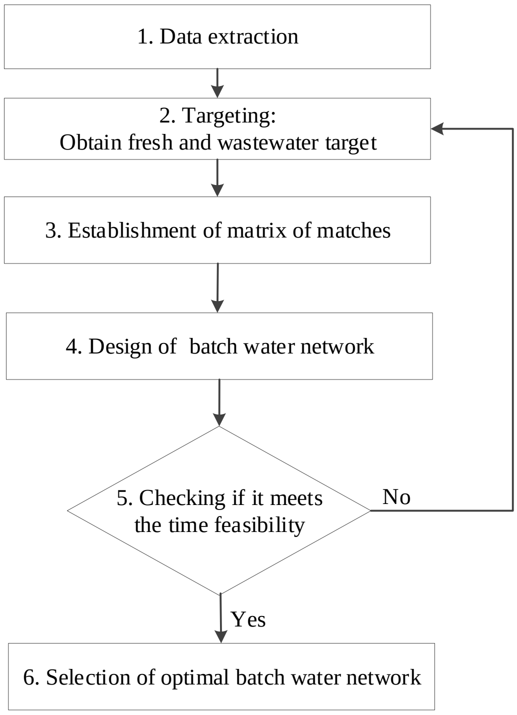


Figure 6.1 The design procedure of the proposed method

In the second stage, a matrix of the source-sink match in each region is presented to represent the water utilization. The value in the matrix is the freshwater consumption for the specific match. Once the potential matches in each region are determined, the initial batch water network can be configured based on water utilization. If the network meets the time constraints, the network can be seen as the desired results if no more constraints are required to meet. The establishment of the matrix is described as follows. First, water sinks are put in the column and water sources in the row in ascending order of concentration. Next, based on the insight from the first stage, two lines representing pinch point is drawn to separate the LQR and HQR, as shown in Figure 6.2. The whole matrix is divided into four regions. According to golden rules of pinch analysis, water sources in the HQR cannot be reused by the water sinks in the LQR, so are water sources in the

LQR not allowed to feed water sinks in the HQR. The shadowed area in Figure 6.2 represents the forbidden match. Otherwise, more freshwater consumption will be required to meet the water requirement. Note that pinch source can feed the water sinks in both HQR and LQR. Therefore, it can be split into two sub-streams, which are locating in HQR and LQR, respectively. For simplicity, it is not presented in Figure 6.2. Also, it is assumed that water recycling is not considered because of the accumulation of contaminants. In the matrix, the symbol “-" refers to that the match is forbidden. The symbol “×" represents that the match is infeasible in terms of concentration. Otherwise it will violate the golden rules of pinch analysis.

HQR

Water sinks / Water sources	SK_1	...	SK_k	...	SK_n	*WW*
FR	$F1^{R1}$	...	Fk^{R1}	×	×	—
SR_1	—	...	$F1k^{R1}$	×	×	×
...	...	...	..	×	×	×
SR_k	×	×	×	$Fkn\text{-}1^{R1}$	Fkn^{R1}	Fkw^{R1}
...	×	×	×	...	...	...
SR_n	×	×	×	$Fnk\text{-}1^{R1}$	—	Fnw^{R1}

HQR (rows FR to ...); LQR (rows SR_k to SR_n); Pinch point; Pinch point; LQR

Figure 6.2 The matrix for water sources and sinks

In the third step, the aim is to find a feasible solution while meeting the target obtained by pinch analysis and time feasibility. When choosing the matches, matches are selected in order of freshwater consumption, beginning with the least freshwater consumption.

If two matches have the same freshwater consumption, the order of preference is determined based on the following criteria. 1) The water source which can be reused by multiple water sinks without the usage of storage tank should be preferentially chosen. In other words, after feeding a water sink, the residue of the reusable water for this source can be used immediately to feed at least one other water sink. 2) The operation with less duration time should be selected to reduce the operation time for the whole processes.

If the match is selected, the end time of the supplier and the start time of the receiver should coincide. It is noted that in this work the truly batch operations are considered. In other words, the charging and discharging of water only occur at the start and end time of the operation, respectively, rather than during the course of the operation. Once the initial water network is designed, the feasibility of time constraints will be checked. If the networks meet the time constraints, the final batch water network is determined.

6.4 Case studies

Four case studies adopted from published papers are solved to demonstrate the application of the method. Although these examples are about fixed mass load problems, the method is also applicable to fixed flowrate problems.

6.4.1 Example 1

To facilitate understanding of the proposed method, an example from Wang and Smith (1995) is considered. The example comprises three processes, and its limiting data are shown in Table 6.1. It should be noted that the inlet and outlet concentrations setting to the maximum values are to ensure that there is maximum driving mass transfer force among different water operations. The duration of each operation is given, rather than its starting and ending time. The cycle time for the overall process is set to be 5 h.

Table 6.1 Limiting water data for Example 1

Operation	Concentration (ppm)		Limiting flowrate	Duration	Limiting flow
	Inlet	Outlet	(t/h)	(h)	(t)
1	100	400	100	1	100
2	0	200	80	0.5	40
3	100	200	50	0.5	25

The operations are treated as continuous processes. The material recovery pinch diagram developed by Prakash and Shenoy (2005) and El-Halwagi et al. (2003) for the continuous process is extended to batch processes. In this graphical representation, the horizontal axis represents the accumulative quantity of water, rather than accumulative flowrate of water. The graphical representation of targeting is shown in Figure 6.3.

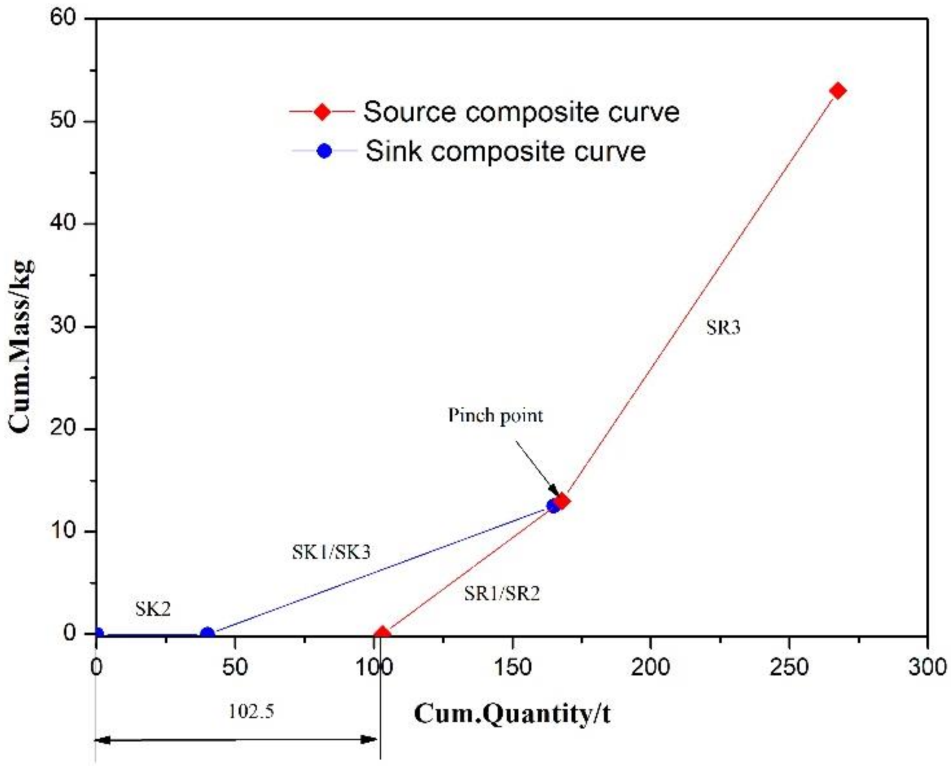


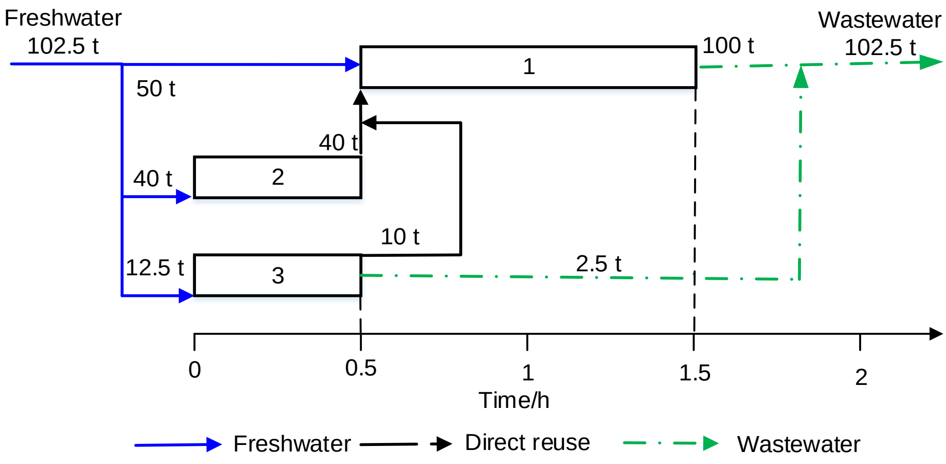
Figure 6.3 The graphical representation of targeting for Example 1

As shown in Figure 6.3, the pinch point is 200 ppm, and freshwater consumption is determined as 102.5 t. SR_1 and SR_2 are thus pinched point sources. Water sinks, i.e., SK_1, SK_2, and SK_3, are located in the HQR. For water sources, SR_1 and SR_2 are in the HQR, while the remaining source, i.e., SR_3, is completely located in the LQR. The matrix of the matches is shown in Figure 6.4. Because SR_1, SR_2 are pinch point sources, these two sources can allocate water to HQR and LQR. In the matrix, both of them are divided into two sub-streams. To display the HQR and LQR clearly in the matrix, the wastewater treatment is treated as a water source in LQR.

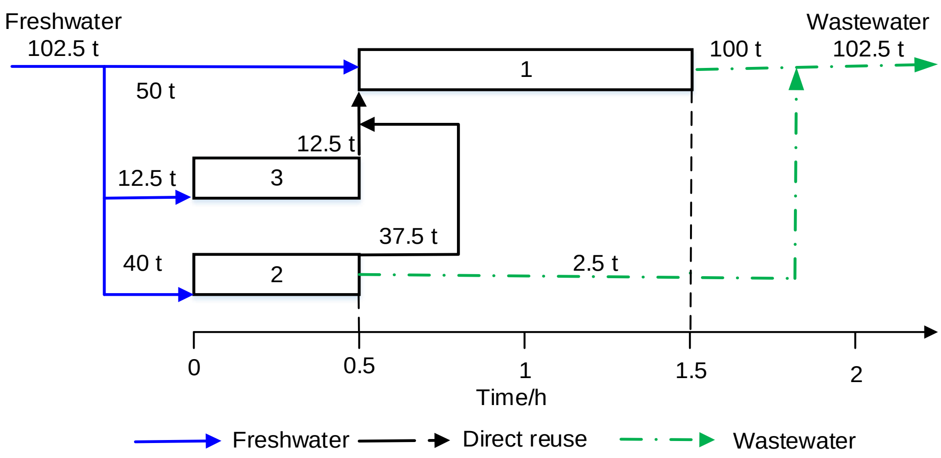
Once the matrix is constructed, the next step is to choose the appropriate matches of water sinks and sources to achieve the target obtained above. Sub-networks for HQR and LQR can be configured based on insight from the matrix. As shown in Figure 6.4, in the HQR, water sinks, both SK_2 and SK_3 have only one match. These two water sinks are supplied by freshwater, i.e., 40 t, and 12.5 t, respectively. For SK_1, the match of SR_2-SK_1 should be preferentially chosen to achieve the targets because of this match having the least freshwater consumption. However, SR_2 has a deficit in water quantity to feed SK_1. Furthermore, for SK_1, there are two alternative matches, as shown in Figure 6.4. Therefore, to achieve the target of freshwater consumption, both SR_2-SK_1 and SR_3-SK_1 should be chosen to meet the water requirement.

Water sources \ Water sinks	SK_2	SK_1	SK_3	WW
FR	40	100	25	—
$SR_{2\text{-}1}$	—	55	×	×
$SR_{3\text{-}1}$	×	62.5	—	×
$SR_{2\text{-}2}$	×	—	—	0
$SR_{3\text{-}2}$	×	×	×	0
SR_1	×	×	×	0

Figure 6.4 The matching matrix of Example 1



(a)



(b)

Figure 6.5 Water network of Example 1

However, there are two alternative water networks achieving the same target, as shown in Figure 6.5. More information, such as distance, consumer priority, should be given to assist in determining which network should be selected. The freshwater consumption is determined as 102.5 t, which is identical to the target for predefined production scheduling in Wang and Smith (1995). However, in the work of Wang and Smith (1995), water reuse can happen during the course of the operation, which is not true in truly batch processes.

6.4.2 Example 2

This example is adapted from Kim and Smith (2004). There are four operations in the processes. The limiting data for this example are shown in Table 6.2. In order to assess the effect of process scheduling on water integration, the durations of these operation are given, instead of starting and finishing times. The cycle time for the overall process is 5 h. The water operations are assumed as fixed mass load problems.

Table 6.2 Limiting water data for Example 2

Operation	Concentration (ppm)		Limiting flowrate	Duration	Limiting flow
	Inlet	Outlet	(t/h)	(h)	(t)
1	0	100	20	1	20
2	50	100	100	2.5	250
3	50	800	40	3	80
4	400	800	10	2	20

First sequence scenario

The targeting process is similar to Example 1. The targeting process is graphically shown in Figure 6.6. Note that the term of SK1/SK2 in Figure 6.6 means that the segment presents these water sinks because these sinks have the same concentration.

As shown in Figure 6.6, the pinch point is 100 ppm, and freshwater consumption is determined as 185 t. SR_1 and SR_2 are thus pinched point sources. Water sinks, i.e., SK_1, SK_2, and SK_3, are located in the HQR and SK_4 is in the LQR. For water sources, freshwater is in the HQR, while the other sources, i.e. SR_3 and SR_4, are in the LQR. From Figure 6.6, the amount of water from pinch sources to HQR and LQR can also be determined as 165 t and 105 t, respectively. The matrix of the match is shown in Figure 6.7. Because SR_1, SR_2 are pinch point sources, these two sources can allocate water to HQR and LQR. In the matrix, both are divided into two sub-streams.

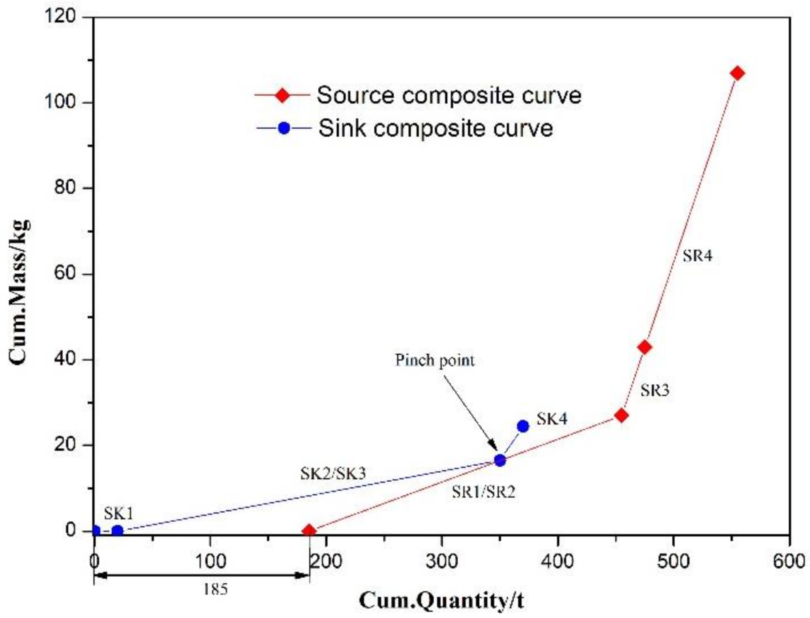


Figure 6.6 Material recovery pinch diagram of Example 2

Sub-networks for HQR and LQR can be configured based on the insight from the matrix. As shown in Figure 6.7, in the HQR, water sinks, both SK_1 and SK_2 have only one match. These two water sinks are supplied by freshwater, i.e., 20 t, and 125 t, respectively. For SK_3, the match of SR_2-SK_3 should be preferentially chosen to achieve the targets obtained, and the match of SR_1-SK_3 should be deleted in the matrix. However, the match of SR_2-SK_3 is infeasible if taking time into account. This is because the overall time for the match is 5.5 h, which exceeds the 5 h. Finally, the match SR_1-SK_3 is chosen to meet the freshwater target.

HQR (sources: FR, SR_{1-1}, SR_{2-1}; sinks: SK_1, SK_2, SK_3) — Pinch point — LQR (sources: SR_{1-2}, SR_{2-2}, SR_3, SR_4; sink: SK_4)

Water sources \ Water sinks	SK_1	SK_2	SK_3	SK_4
FR	20	125	75	10
SR_{1-1}	—	×	57.5	×
SR_{2-1}	×	—	40	×
SR_{1-2}	×	×	—	11.43
SR_{2-2}	×	×	×	11.43
SR_3	×	×	×	×
SR_4	×	×	×	×

Figure 6.7 The matching matrix of Example 2

Since there is no reusable water in the storage tank in the first sequence, the deficit of SR_1 is supplemented by freshwater, increasing freshwater consumption. In LQR, there only exists a water sink SK_4. Since SR_1 is used up in HQR, SR_2 is the sole water source that is available in LQR. Therefore, SR_2-SK_4 is chosen in LQR.

The final water network for the first sequence scenario is shown in Figure 6.8. The actual time horizon of operation is reduced to 4.5 h. The freshwater consumption for the first sequence scenario is 202.5 t, which is less than the target for the base case without water integration, i.e., 225 t.

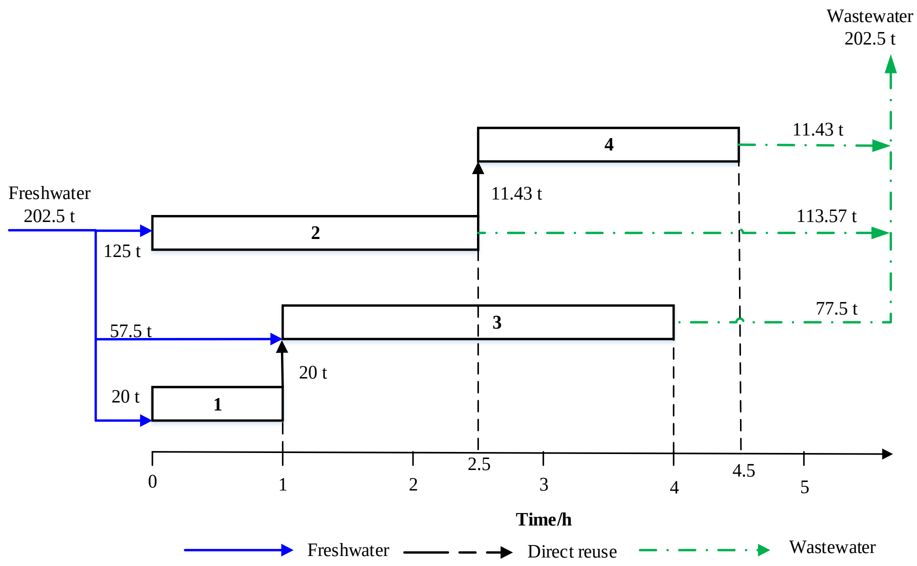


Figure 6.8 The final water network for Example 2 (first sequence)

Cyclic operation scenario

The design procedure for the first sequence scenario is repeated. In this scenario, the source-sink matches are the same as the first sequence scenario. The difference is that the quantity of reusable water for some matches are changed.

In the first sequence scenario, the deficit of SR_1 is supplied by freshwater, not by SR_2, which leads to a penalty of freshwater consumption. In cyclic operation, because the same production recipe is repeated. The wastewater generated in the previous batch can be stored and then be reused in the next batch. Therefore, the penalty of freshwater for the match of SR_1-SK_3 can be removed by the wastewater in the previous batch.

The freshwater requirement in cyclic operation is 185 t, which agrees with the results of Lee and Foo (2017). The batch water network is shown in Figure 6.9. However, the storage capacity of this work is larger than the that of Lee and Foo (2017), i.e., 2.86 t. This is because in this work, we consider these operations as truly batch processes, while Lee and Foo (2017) allows water recovery to occur during the course of operation.

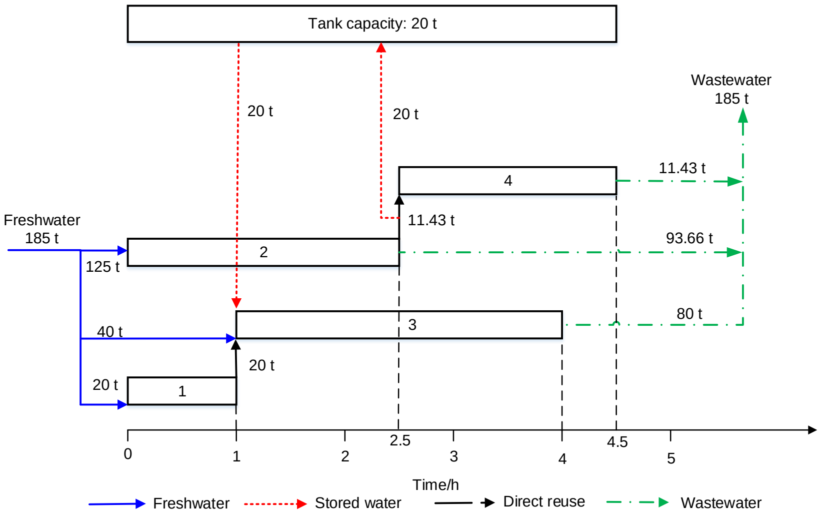


Figure 6.9 The final water network of the cyclic batch for Example 2

6.4.3 Example 3

This example is adopted from Liu et al. (2009). It includes five operations. The limiting data are shown in Table 6.3. The duration of each operation is given for these operations, as shown in Column 4 of Table 6.3. The water-using processes involve the mass transfer and are treated as fixed mass load problems. The time horizon of interest for this example is 8.5 h. Two scenarios are considered, i.e., reuse/recycle, and regeneration scenario.

Table 6.3 Limiting water data for Example 3

Operation	Limiting concentration (ppm)		Duration	Limiting flow
	Inlet	Outlet	(h)	(t)
1	0	400	2	50
2	100	400	1	30
3	200	500	3	10
4	350	600	4	24
5	450	700	2.5	40

The material recovery pinch diagram is presented in Figure 6.10. The horizontal distance from the origin indicates a quantity of 80.5 t freshwater is required. The pinch point is 400 ppm. Note that in Figure 6.10. SR1/SR2 is combined and represented in the same segment because of the same concentration. Therefore, SR1 and SR2 are pinch sources. These two sources can be divided into two sub-streams in both HQR and LQR. The quantity of water from pinch sources to HQR and LQR is 33.5 t and 46.5 t, respectively. Water sinks, i.e., SK_1, SK_2, SK_3, and SK_4, are located in the HQR and SK_5 is in the LQR. For water sources, freshwater is in the HQR, while the other sources, i.e., SR_3, SR_4, and SR_5, are in the LQR. Based on the insight of material recovery pinch diagram in Figure 6.10., the matrix of the source-sink match is shown in Figure 6.11.

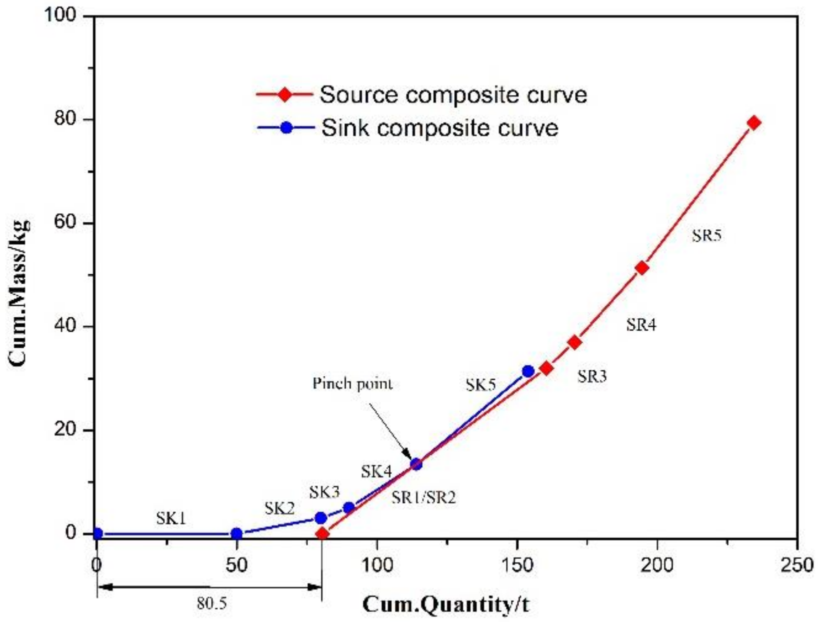


Figure 6.10 Graphical representation of the targeting process of Example 3

HQR

Water sources \ Water sinks	SK_1	SK_2	SK_3	SK_4	SK_5
FR	50	22.5	6	10	×
SR_{1-1}	—	×	5	3	×
SR_{2-1}	×	—	5	3	×
SR_{1-2}	×	×	×	×	0
SR_{2-2}	×	×	×	×	0
SR_3	×	×	—	×	4
SR_4	×	×	×	—	10
SR_5	×	×	×	×	—

HQR (rows FR, SR_{1-1}, SR_{2-1}); LQR (rows SR_{1-2} to SR_5); Pinch point

Pinch point
LQR

Figure 6.11 The matching matrix of Example 3

Based on the insight of matrix, sub-networks for HQR and LQR can be configured. As shown in Figure 6.11, in the HQR, water sinks, both SK_1 and SK_2 have only one match. These two water sinks are supplied by freshwater, i.e., 50 t, and 22.5 t, respectively. For SK_3 and SK_4, the matches between these two sinks and the existing water sources SR1 and SR_2 have the same freshwater consumption. According to the rules defined in Section 6.3, water sources can kick off a water sink completely; the reusable residue water can also be used by another water sink immediately. This type of water source should be chosen preferentially. In this example, SR_1 has a quantity of 22.5 t reusable water. It cannot meet the total water requirement of SK_3 and SK_4. Furthermore, in HQR, SR_1 is also not enough to supply SK_5, whose water demand is 33.33 t. However, if in the LQR, the matches of SR_1-SK_3 and SR_2-SK_4 are selected, the reusable residue water from SR_1 is sent to SK_5. This is in accordance with the rules in Section 3. Finally, the remaining quantity of wastewater from these water sources is sent to wastewater treatment.

The final water network is shown in Figure 6.12. It should be noted that in Figure 6.10, the amount of water from pinch sources to HQR is 33.5 t. However, the actual water transferred from pinch sources to HQR is 26 t. This is because the water operation is divided into water sinks and water sources. In this example, if the water sources and sinks are considered separately, SR_2 can be used to satisfy the water demand of SK_2. However, it is assumed water recycling for the same operation is not allowed. Therefore, the remaining water, i.e., 7.5 t, is not transferred to the HQR. The freshwater requirement is determined as 80.5 t, which is the same as the target for the predefined schedule (Liu *et al.*, 2009). However, the water storage tank can be removed in this work, as shown in Figure 6.12. Furthermore, the time horizon of operation can be reduced from 8.5 h to 5 h.

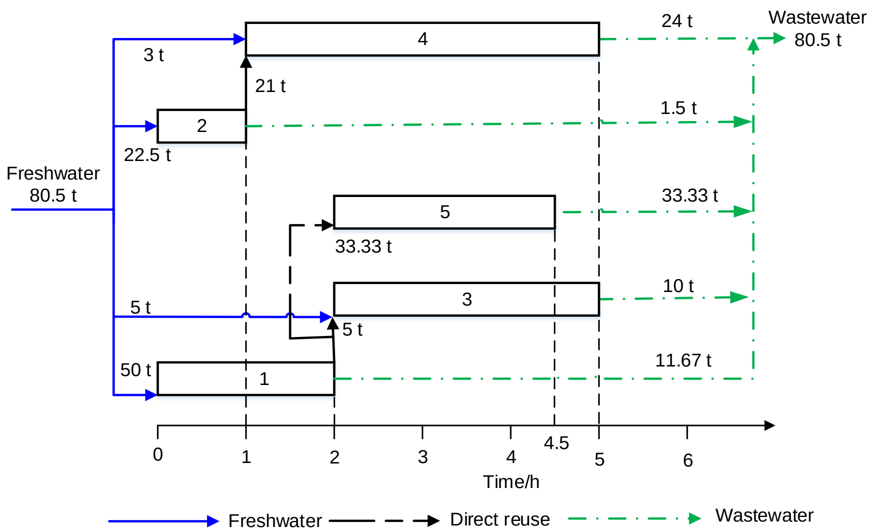


Figure 6.12 The water network of Example 3

6.4.4 Example 4

This illustrative example is adopted from Gouws et a. (2008) involving four water-using operations. Each operation is dedicated to producing a product. Water is used as a solvent to remove the inorganic salts left in batch vessels. The data for the illustrative example are shown in Table 6.4. The durations of operations are presented in Column 6 of Table 6.4. The batches of operations 1-4 over the 12 h time horizon are 4, 3, 2, and 3, respectively.

Table 6.4 Limiting water data for Example 4

Operation	Concentration (ppm)		Mass load	Limiting flow	Duration
	Inlet	Outlet	(kg)	(t)	(h)
1	100	400	30	100	3
2	0	200	8	40	5
3	100	200	2.5	25	5
4	200	300	4	40	4

The graphical representation of the targeting of a single batch for this example is shown in Figure 6.13. As shown in Figure 6.13, the pinch point is 300 ppm, and freshwater consumption is determined as 115 t. SR_4 is the pinch point source. All the water sinks, i.e., SK_1, SK_2, SK_3, and SK_4, are located in the HQR. For water sources, SR_1 and SR_2 are in the HQR, while the remaining source, i.e., SR_1, is completely located in the LQR. The matrix of the source-sink match is shown in Figure 6.14. Because SR_4 are a pinch point source, this source can allocate water to HQR and LQR. Therefore, in the matrix, this water source is divided into two sub-streams.

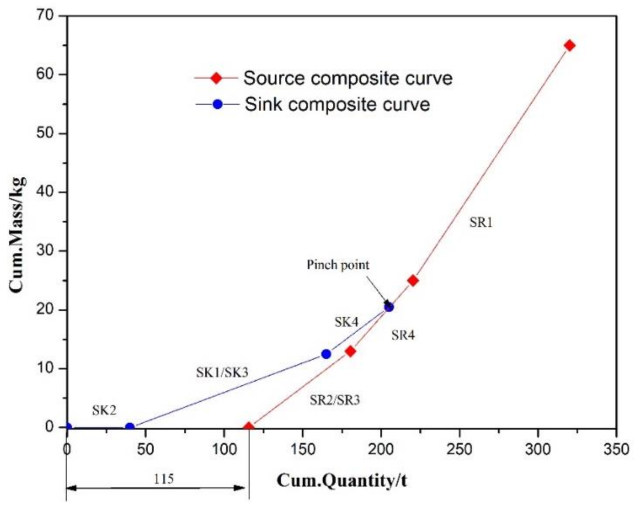


Figure 6.13 Graphical representation of targeting for Example 4

The matrix of matches between water sinks and sources are shown Figure 6.14. All the sinks having the concentration lower than pinch point are sent to the HQR. To display the HQR and LQR clearly, the wastewater treatment is treatment as a water sink in the LQR.

Water sources \ Water sinks	*SK₂*	*SK₁*	*SK₃*	*SK₄*	*WW*
FR	40	75	12.5	13.33	—
SR₂	—	55	×	0	×
SR₃	×	68.75	—	5	×
SR₄₋₁	×	66.67	×	—	0
SR₄₋₂	×	×	×	×	0
SR₁	×	×	×	×	0

HQR (sinks SK_2, SK_1, SK_3, SK_4; sources FR, SR_2, SR_3, SR_{4-1}); LQR (sink WW; sources SR_{4-2}, SR_1); Pinch point

Figure 6.14 The matching matrix of Example 4

As shown in Figure 6.14, in the HQR, water sinks, both SK_2 and SK_3 have only one match. These two water sinks are supplied by freshwater, i.e., 40 t, and 12.5 t, respectively. For SK_1, the match of SR_2-SK_1 should be preferentially chosen to achieve the targets because of this match having the least freshwater consumption. However, SR_2 has a deficit in water quantity to feed SK_1.

Therefore, to achieve the target of freshwater consumption, both SR_2-SK_1 and SR_3-SK_1 should be chosen to meet the water demand of SK_1. The quantity of reusable water from SR_2 and SR_3 are 40 t and 10 t, respectively. For SK_4, because the quantity of SR_2 has been used up, the match of SR_2-SK_4 should be deleted, and SR_3 is selected to act as the water source. The final work for the first batch water network is shown in Figure 6.15.

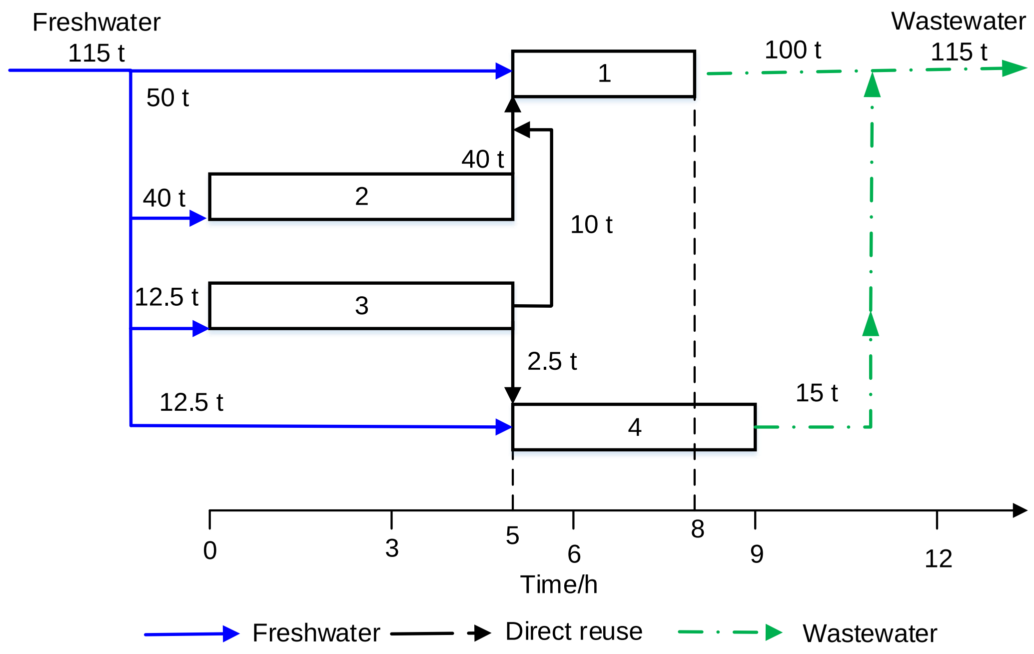


Figure 6.15 The water network for Example 4 (single batch)

In the single batch, the time constraints are removed to achieve the target of freshwater. When considering the time constraints, some connection between different operation should be removed. The insight from a single batch can be used to design the multiple batch operations. For example, the reusable water from operation 2 and 3 can be sent to operation 1. However, the connection between operations 3 and 4 should be removed unless the storage tank is used. The amount of freshwater, for example, is thus identified 420 t. The water network is shown in Figure 6.16. A reduction of 35% freshwater can be achieved compared with 650 t without reuse/recycle.

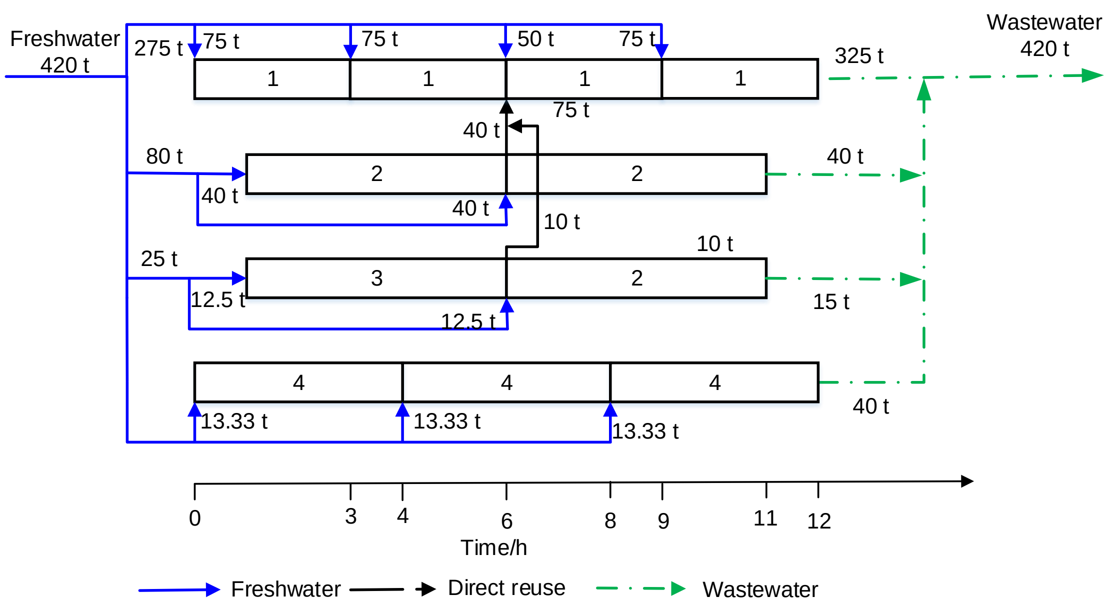


Figure 6.16 Gantt chart for Example 4

6.5 Conclusions

Batch processes have the advantage of producing low volume, high value-added products and accommodating for the changes of the market. It is of significance to consider water recovery in a flexible scheduling framework to meet the requirement of environmental regulation. In this work, a three-stage procedure is presented to synthesize the optimal batch water network that will achieve minimum freshwater consumption and meet the time requirements of production scheduling. In the method, conventional pinch analysis is used to determine the initial target of freshwater consumption. Based on the insights of pinch analysis, the water network could be configured to meet the obtained target. Next, the feasibility of timing for each operation is checked for the configured water network. If it violates the time constraints, the target of freshwater consumption is relaxed, and the same procedure is repeated until obtaining the desired water network. Four examples from the literature are illustrated to explain how to design a batch water network using the proposed method. Results show that freshwater consumption in a flexible scheduling environment could be further reduced compared to the scenario of a predefined production schedule. Furthermore, the time horizon and the capacity of the tank could also be reduced. This approach makes good use of the insight from the water pinch analysis and can assist the designer in designing a flexible batch water network.

It is worth noting that this work only considers the recovery of wastewater generated by washing operations in batch processes. In some cases, if the amount of wastewater generated is dependent on the capacity of reaction processes, mathematical methods have the advantage of determining the optimal capacity of reaction and the optimal production schedule. Future work should also focus on batch water network design with multiple contaminants. Also, it can also explore the opportunity of combining the insight-based method with mathematical programming to simultaneously optimize wastewater minimization and process scheduling.

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7

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

Batch processing is a widely accepted procedure in the chemical industry because of the flexibility in changing the production recipe and the suitability of producing small-quantity products. The environmental pressure and increasing demand for products call for an improved design of batch plants and a requirement of making better use of existing facilities. It is thus required to improve the efficiency of resource utilization. Most of the work in published literature in the area of water network optimization for multipurpose batch plants focuses on mathematical modeling, with very limited conceptual analysis. This has led to the models that are very difficult to solve at best and almost impossible to solve at worst. In this work, a conceptual analysis is performed to maximize wastewater recovery for batch processes with flexible scheduling.

In Chapter 2, a literature review is presented to introduce the techniques of production scheduling and water integration methods for continuous and batch processes. For batch processes, most of the techniques are based on mathematical programming. Few papers based on insight-based methods are published to address wastewater minimization problems because of the additional constraints of time. Among these insight-based papers, the timings of all of the batch operations are given. Also, the future development of wastewater minimization in the batch chemical industry is briefly discussed.

Chapter 3 presents a dynamic programming (DP) approach to identify the optimal water using policy, achieving the minimum freshwater consumption for predefined scheduling. Four examples from the literature are introduced to demonstrate the applicability of the proposed approach. The results obtained in this work match well with the literature. In some cases, it could obtain better results. For example, the capacities of storage facility obtained for some examples are less than those in literature. Furthermore, the DP approach can also be used to consider wastewater recovery in batch processes with multiple contaminants, which is difficult to determine the globally optimal results using mathematical programming. Based on the results obtained by DP, some indirect water reuse schemes are eliminated by rescheduling water operations.

An extension of the DP method is developed in Chapter 4 to address water integration of batch processes with flexible scheduling. The durations of all of the batch operations are given, rather than the starting and finishing times. The sinks with different water quality are treated as the stages. In each stage, the quantity of available water sources is seen as the state. Water utilization between different operation and the target of freshwater consumption can thus be determined by solving the problem using the backward procedure. Based on the water utilization, batch water networks could be designed. The feasibility of time constraints is then checked whether the designed network is suitable or not. In the proposed method, the water network for reuse scenario is first configured. The timings of all of the operations in the regeneration scenario are assumed as the same as the reuse scenario. Three different examples from the literature are used to demonstrate the applicability of the proposed approach. The obtained results match with the published literature.

In Chapter 5, an insight-based method is proposed to design a flexible batch water network. A match ranking matrix is constructed to choose potentially optimal source-sink matches based on the reuse potential of wastewater from sources. Thus, a water network can be configurated to achieve the minimum water consumption according to the insight of rankings. To further reduce freshwater consumption, two types of regenerator are employed to purify wastewater in illustrative examples. The proposed approach can be used to deal with water system with single- and multiple-contaminant problems. Although the method proposed cannot be proved by rigorous mathematics, the results obtained by the method are not worse than those of mathematical programming methods. The method can assist the designer without a strong background of mathematics in designing a flexible batch water network.

In the previous chapters, targets of freshwater consumption and wastewater generation and network design are obtained simultaneously. In Chapter 6, a three-stage procedure is presented to synthesize the optimal batch water network that achieves minimum freshwater consumption and meets the time requirements of production scheduling. First, the batch process is treated as a continuous process. Conventional water pinch analysis is extended to determining the initial target of freshwater consumption. Based on the insight of pinch analysis, a matching matrix is constructed to assist the design of batch water network in meeting the obtained target. Next, the feasibility of timing for each operation is checked for the configured water network. If it violates the time constraints, the target of freshwater consumption is relaxed, and the same procedure is repeated until obtaining the desired water network. Four examples from the literature are illustrated to explain how to design a batch water network using the proposed method. Results show that freshwater consumption in a flexible scheduling environment could be further reduced compared to the scenario of a predefined production schedule. Furthermore, the time horizon and the capacity of the tank could also be reduced.

7.2 Recommendations

As water shortage has been a global problem, it is becoming increasing important to consider wastewater minimization in the batch chemical industry. Although the method proposed in this thesis could assist the designer in designing the batch water network, it is required to develop a rigorous approach for batch water integration. It is recommended to develop a novel tool of combining the advantages of mathematical programming and graph theory. The model for water minimization in batch processes is usually formulated as a MINLP formulation, which is difficult to solve. This limitation can be overcome by the methods of the graph theory. For example, the existing P-graph can address wastewater recovery issues for continuous processes in a simple manner. The formulated model can be solved quickly, and the method can provide a few near optimal solutions. However, P-graph is difficult to be extended to addressing wastewater minimization in flexible batch processes because of the constraints of time. On the other hand, the durations of batch operations can be simulated in the Petri-net method. The limitation of the Petri-net method is that it is complicated to consider wastewater recovery issues.

Therefore, the future tool should have the advantages of mathematical programming, P-graph, and Petri-net. Furthermore, more attention should be paid to water-energy nexus. Sometimes, the minimum freshwater consumption in the plant could result in more water footprint for the whole supply chain, because the deployment of water-saving equipment can bring in more energy consumption.

Appendix A

The detailed process for Chapter 3 is as follows:

Example 3 with central buffer tank

The detail process of Example 3 with a central buffer tank is shown as follows.

Stage 8

Since this case considers the first sequence operation of batch processes, it is required to consume a quantity of freshwater to feed Operation A. On the other hand, the inlet concentration of Operation A is zero. Hence, Operation A can be only fed with freshwater with a quantity of 50 t.

$$S_{Stage8} = \left\{ \sum_{j}^{J_8} F_{j,8}^{Fw} = 50t, F_{Tank1}^{St} = 0t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ \sum_{j}^{J_8} F_{j,8}^{Fw} + f_7(F_{j,7}^{Fw}) \right\} = \min\left\{ 50t + f_7(F_{j,7}^{Fw}) \right\}$$

Stage 7

At this stage, water from Operation A has a low outlet concentration (400 $\mu g.g^{-1}$). It could be reused by the process E in Stage 6. Therefore, all the outlet quantity of Operation A is assumed to send the tank for reuse in later stages. It should be noted that the stored water at this stage is just an initial result.

$$S_{Stage7} = \left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} = 0t, F_{Tank1}^{St} = 50t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 50t + \sum_{j}^{J_7} F_{j,7}^{Fw} + f_6(F_{j,6}^{Fw}) \right\} = \min\left\{ 50t + f_6(F_{j,6}^{Fw}) \right\}$$

Stage 6

In Stage 6, both Operations B and C have a freshwater demand of 22.5 t and 6 t, respectively. If Operation B is to reuse the stored water in Tank 1, it assumes a quantity of 22.5 t freshwater. Hence, Operation B is only supplied with freshwater 22.5 t. For Operation C, if it is fed with a mixture of freshwater and stored water, the quantity of freshwater and stored water is identified as 5 t and 5 t, respectively. Therefore, Operation B is only supplied with freshwater, while Operation C is satisfied with the mixture of freshwater and stored water in Tank 1.

$$S_{Stage6} = \left\{F_{B,6}^{Fw} = 22.5t, F_{C,6}^{Fw} = 5t, F_{A,C,6}^{ind} = 5t, F_{Tank1}^{St} = 45t\right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{50t + \sum_{j}^{J_6} F_{j,6}^{Fw} + f_5(F_{j,5}^{Fw})\right\} = \min\left\{77..5t + f_5(F_{j,5}^{Fw})\right\}$$

Stage 5

At this stage, Operation D has an inlet concentration of 350 $\mu g. g^{-1}$, which is very close to the concentration of stored water 400 $\mu g. g^{-1}$. The quantity of freshwater and restored water supplied for Operation D is determined as 3t and 21 t, respectively. The remaining water in Tank 1 is 24 t.

$$S_{Stage5} = \left\{F_{D,5}^{Fw} = 3t, F_{A,C,5}^{ind} = 21t, F_{Tank1}^{St} = 24t\right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{77.5t + \sum_{j}^{J_5} F_{j,5}^{Fw} + f_4(F_{j,4}^{Fw})\right\} = \min\left\{80.5t + f_4(F_{j,4}^{Fw})\right\}$$

Stage 4

The outlet concentration of process B is the same as process A. Hence, the outlet quantity of water from process B could be mixed with the stored water in Tank 1. It should be noted that at this moment, it is impossible to decide the total quantity of reuse water used in the later stages. All the available water is set to be stored in Tank 1 for future reuse. The maximum quantity of water until this stage is 46.5 t.

$$S_{Stage5} = \left\{\sum_{j}^{J_5} F_{j,5}^{Fw} = 0t, F_{\mathrm{Tan}\,k1}^{St} = 46.5t\right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{80.5t + \sum_{j}^{J_4} F_{j,4}^{Fw} + f_3(F_{j,3}^{Fw})\right\} = \min\left\{80.5t + f_3(F_{j,3}^{Fw})\right\}$$

Stage 3

From the time dimension it is the finishing time of Operation C and starting time of Operation E. On the other hand, the outlet concentration of Operation C is close to the

Operation E. The quantity of reuse water is identified as 26.67 t from Tank 1 and 10 t from Operation C.

$$S_{Stage3} = \left\{ F_{E,3}^{Fw} = 0t, F_{C,E,3}^{d} = 10t, F_{Tank1,E,3}^{ind} = 26.67t, F_{Tank1}^{St} = 19.33t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 80.5t + \sum_{j}^{J_3} F_{j,3}^{Fw} + f_2(F_{j,2}^{Fw}) \right\} = \min\left\{ 80.5t + f_2(F_{j,2}^{Fw}) \right\}$$

Stage 2

Since no water is required in the later stages, all the water from Operation D is discharged as wastewater.

$$S_{Stage2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 0t, F_{Tank1}^{St} = 19.33t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 80.5t + \sum_{j}^{J_2} F_{j,2}^{Fw} + f_1(F_{j,1}^{Fw}) \right\} = \min\left\{ 80.5t + f_1(F_{j,1}^{Fw}) \right\}$$

Stage 1

Since this is the last stage of batch processes, water from Operation E should be discharged as wastewater.

$$S_{Stage1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0t, F_{Tank1}^{St} = 19.33t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 80.5t + \sum_{j}^{J_1} F_{j,1}^{Fw} \right\} = \min\left\{ 80.5t + 0t \right\} = 80.5t$$

Example 3 with a central buffer tank and regeneration unit

The detail process of Example 3 with a central buffer tank and regeneration unit is shown as follows.

Stage 8

The situation is similar to the reuse scenario. Operation A is fed with freshwater with a quantity of 50 t. The state of stored water is zero.

$$S_{Stage8} = \left\{ \sum_{j}^{J_8} F_{j,8}^{Fw} = 50t, F_{Tank1}^{St} = 0t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min \left\{ \sum_{j}^{J_8} F_{j,8}^{Fw} + f_7(F_{j,7}^{Fw}) \right\} = \min \left\{ 50t + f_7(F_{j,7}^{Fw}) \right\}$$

Stage 7

As in this case, the regeneration unit is employed to purify the wastewater, outlet water of process A as the only water source at this moment should be sent to Tank 1 for regeneration.

$$S_{Stage7} = \left\{ \sum_{j}^{J_7} F_{j,7}^{Fw} = 0t, F_{Tank1}^{St} = 50t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min \left\{ 50t + \sum_{j}^{J_7} F_{j,7}^{Fw} + f_6(F_{j,6}^{Fw}) \right\} = \min \left\{ 50t + f_6(F_{j,6}^{Fw}) \right\}$$

Stage 6

As in Stage 7 regeneration unit starts to purify the outlet water from process A, the available regenerated water at Stage 6 is 11.875 t. It is deficient in supplying both processes B and C. Hence; there are two states of freshwater consumption. One state is that all the regenerated water is to feed process B, the total freshwater consumption is 18.594 t (13.594 t for process B, 5 t for process C), while for process C it requires an amount of 5 t water from Tank 1. The other state is that process C is fed with regenerated water (7.5 t), the remaining regenerated water (4.375 t) is to supply process B. The freshwater consumption of process B is 19.219 t.

$$S_{Stage6}^{1} = \left\{ F_{B,6}^{Fw} = 13.594t, F_{C,6}^{Fw} = 5t, F_{B,6}^{\mathrm{Re}} = 11.875t, F_{Tank1,3}^{St} = 5t, F_{Tank1}^{St} = 33.125t \right\}$$

$$S_{Stage6}^{2} = \left\{ F_{B,6}^{Fw} = 19.219t, F_{C,6}^{\mathrm{Re}} = 7.5t, F_{B,6}^{\mathrm{Re}} = 4.375t, F_{\mathrm{Tank1}}^{St} = 38.125t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min \left\{ 50 + \sum_{j}^{J_6} F_{j,6}^{Fw} + f_5(F_{j,5}^{Fw}) \right\} = \min \begin{Bmatrix} 13.594t + 5t + 50t + f_5(F_{j,5}^{Fw}); \\ 19.219t + 50t + f_5(F_{j,5}^{Fw}) \end{Bmatrix}$$

$$= \min \left\{ 68.594t + f_5(F_{j,5}^{Fw}); \right\}$$

Stage 5

As the time gap between Stage 5 and Stage 4 is 0.5 h, the available regenerated water is 5.938 t. A quantity of 15.516 t water from Tank 1 is required to supply process D.

$$S_{Stage5} = \left\{ \sum_{j}^{J_5} F_{j,5}^{Fw} = 0t, F_{D,5}^{\mathrm{Re}} = 5.938t, F_{Tank1,D,5}^{ind} = 15.156t, F_{\mathrm{Tank1}}^{St} = 12.032t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 68.594 + \sum_{j}^{J_5} F_{j,5}^{Fw} + f_4(F_{j,4}^{Fw}) \right\} = \min\left\{ 68.594t + + f_4(F_{j,4}^{Fw}) \right\}$$

Stage 4

As the regeneration unit is in continuous mode, it should ensure enough water sent to regeneration to operation smoothly. All the outlet water of process B (25.469 t) should be sent to the Tank 1for regeneration.

$$S_{Stage4} = \left\{ \sum_{j}^{J_4} F_{j,4}^{Fw} = 0t, F_{\mathrm{Tank1}}^{St} = 31.563t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 68.594t + \sum_{j}^{J_4} F_{j,4}^{Fw} + f_3(F_{j,3}^{Fw}) \right\} = \min\left\{ 68.594t + f_3(F_{j,3}^{Fw}) \right\}$$

Stage 3

To reduce the regenerated cost, the outlet water of process C should be sent to process E. However, if water from process C is chosen to feed process E, it is not enough to meet the requirement of regeneration. On the other hand, it has been stored enough amount of regenerated water in the tank. Therefore, all the water of process C (10 t) is selected to send to regeneration, rather than to feed the process E. The quantity of regenerated water to supply process E is identified as 16.67 t.

$$S_{Stage3} = \left\{ \sum_{j}^{J_3} F_{j,3}^{Fw} = 0t, F_{E,3}^{\mathrm{Re}} = 16.67t, F_{\mathrm{Tank1}}^{\mathrm{St}} = 17.813t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 68.594t + \sum_{j}^{J_3} F_{j,3}^{Fw} + f_2(F_{j,2}^{Fw}) \right\} = \min\left\{ 68.594t + + f_2(F_{j,2}^{Fw}) \right\}$$

Stage 2

In this stage, a quantity of 21.093 t water is generated by process D. To supply enough water for the regeneration unit, the outlet water of process D should be sent to Tank 1. As in Stage 1 it does require water any more, it can determine the optimal quantity of water allocated to Tank 1 and discharge as wastewater based on the regeneration flowrate and water utilization. Hence, a quantity of 11.875 t water is allocated to Tank 1, the remaining (9.218 t) is discharged as wastewater.

$$S_{Stage2} = \left\{ \sum_{j}^{J_2} F_{j,2}^{Fw} = 0t, F_{Tank1}^{St} = 0t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 68.594 + \sum_{j}^{J_2} F_{j,2}^{Fw} + f_1(F_{j,1}^{Fw}) \right\} = \min\left\{ 68.594t + + f_1(F_{j,1}^{Fw}) \right\}$$

Stage 1

Since Stage 1 is the final stage, the water sent to Tank 1 is enough to supply the regeneration unit, all the water of process E is discharged as wastewater. To reduce the cost of storage as possible, the water sent to Tank 1 in previous stages should equal to regenerated water and indirect water from Tank 1. In Stage 1, the stored water in Tank 1 is zero.

$$S_{Stage1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 0t, F_{Tank1}^{St} = 0t \right\}$$

$$f_8(F_{j,8}^{Fw}) = \min\left\{ 68.594t + \sum_{j}^{J_1} F_{j,1}^{Fw} \right\} = \min\left\{ 68.594t + 0t \right\} = 68.594t$$

Appendix B

The detailed processes for Example 3 in Chapter 4 are described as follows.

Stage 4

In Stage 4, there is a single water operation P1. Because there is no water available for reuse. There is only a state of freshwater consumption in Stage 4, with a quantity of 375 kg of freshwater consumed in this stage, i.e., $F_{SK_1,4}^{Fw}$ = 375 kg. As there are no alternative water sources with its water quality higher than freshwater, the quantity of stored water is zero. The selected state and return cost for Stage 4 is shown below. This work aims to minimize freshwater consumption. Therefore, the return cost for the problem is the extent of freshwater consumption.

$$S_{Stage4} = \left\{ \sum_{j}^{J_4} F_{j,4}^{Fw} = 375\text{kg} \right\}$$

$$f_4(F_{j,4}^{Fw}) = \min \left\{ \sum_{j}^{J_4} F_{j,4}^{Fw} + f_3(F_{j,3}^{Fw}) \right\} = \min \left\{ 375\text{kg} + f_3(F_{j,3}^{Fw}) \right\}$$

Stage 3

In Stage 3, there is the operation P3 which can be fed by the mixture of reusable water from operation P1 and freshwater or only fed by freshwater. If operation P3 is fed with freshwater, the quantity is identified as 600 kg. Based on the Eqs (7)-(12), the quantity of reusable water from operation P1, and freshwater is determined as 210 kg, and 390 kg, respectively. The remaining water from operation P1 is 165 kg. Therefore, the state with minimum freshwater consumption is 390 kg. The recursive function of the problem could be updated by the state of freshwater consumption in Stage 3. The return cost is the sum of the minimum freshwater consumption in Stages 4 and 3 and the freshwater consumption over the remaining stages (Stages 1-2). It is noted that in each stage it is assumed the remaining water is stored in the specific tank. For example, water from P1 is stored in Tank 1, represented by F_{Tank1}. The water from P3 is stored in Tank 3, indicated by F_{Tank3}.

$$S^1_{Stage3} = \left\{ \sum_j^{J_3} F^{Fw}_{j,3} = 600kg, F_{\text{Tank1}} = 375kg \right\}$$

$$S^2_{Stage3} = \left\{ \sum_j^{J_3} F^{Fw}_{j,3} = 390kg, F_{\text{P1},P3,3} = 210kg, F_{\text{Tank1}} = 165kg \right\}$$

$$f_4(F^{Fw}_{j,4}) = \min \left\{ 375kg + \sum_j^{J_3} F^{Fw}_{j,3} + f_2(F^{Fw}_{j,2}) \right\} = \min \left\{ 765\text{kg} + f_2(F^{Fw}_{j,2}) \right\}$$

Stage 2

In this stage, there exists an operation P4. Because the remaining water from operation P1 is 165 kg, which is insufficient to supply P4. Therefore, the mixture of reusable water from P1 and P3 is used. There are two states, i.e., freshwater only and the mixture of freshwater and water from P1 and P3. In the first state, it is to supply freshwater to P4; the quantity of freshwater is 1166.67 kg, as shown in S^1_{Stage2}. The second state is that operations P1 and P3 are used to feed operation P4, and the deficit is complemented by freshwater. This state consumes a quantity of 838.33 kg freshwater. Because wastewater from operation P1 can be reused by P2 in stage 1, only part of this amount of water is reused by P4. The freshwater consumption is 955 kg, and the quantity of water from operations P1 and P3 are determined as 48.33 kg, and 163.33 kg, respectively, as shown in S^3_{Stage2}.

$$S^1_{Stage2} = \left\{ \sum_j^{J_2} F^{Fw}_{j,2} = 1166.67\text{kg}, F_{\text{Tank1}} = 165kg \right\}$$

$$S^2_{Stage2} = \left\{ \sum_j^{J_2} F^{Fw}_{j,2} = 838.34kg, F_{\text{P1,P4,2}} = 165kg, F_{\text{P1,P4,2}} = 163.33kg, F_{\text{Tank3}} = 436.67kg \right\}$$

$$S^3_{Stage3} = \left\{ \begin{array}{l} \sum_j^{J_2} F^{Fw}_{j,2} = 955kg, F_{P1,P4,2} = 48.33kg, \; F_{P3,P4,2} = 163.33\text{kg}, \\ F_{\text{Tank1}} = 116.67\text{kg}, \; F_{\text{Tank3}} = 436.67kg \end{array} \right\}$$

$$f_4(F^{Fw}_{j,4}) = \min \left\{ 765kg + \sum_j^{J_2} F^{Fw}_{j,2} + f_1(F^{Fw}_{j,1}) \right\} = \min \left\{ 1603.34kg + f_1(F^{Fw}_{j,1}) \right\}$$

Stage 1

In this stage, operation 2 can be feed with freshwater, and the mixture of freshwater and reusable water from previous operations, such as operations P1, P3. Because the outlet concentration of P4 is far more than the inlet concentration of P2, it is not suitable to be reused by P2. For the first state, operation P2 is fed with freshwater, i.e., 333.33 kg. As for the second state, if operation P2 is fed by the reusable water from operation P3, the freshwater and reusable water from operation P3 are 46.67 kg and 286.67 kg, respectively. For the third state, operation P2 is fed by the mixture of freshwater and reusable water from operations P1 and P3. The freshwater and reusable water from operations P1 and P3 are determined as 170 kg, 116.67 kg, and 46.67 kg, respectively. According to the results of these states, the state with freshwater consumption of 170 kg is chosen to update the recursive function of the problem. However, this state has nothing to do with the stage in the previous stage. Thus, it should go back to the previous stage to choose the state again.

$$S_{Stage1}^{1} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 333.33kg \right\}$$

$$S_{Stage1}^{2} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 286.33kg, F_{P3,P2,1} = 46.67kg, F_{\mathrm{Tank3}} = 390kg \right\}$$

$$S_{Stage1}^{3} = \left\{ \sum_{j}^{J_1} F_{j,1}^{Fw} = 170kg, F_{\mathrm{P1,P2,1}} = 116.67kg, F_{\mathrm{P1,P2,1}} = 46.67kg, F_{\mathrm{Tank3}} = 390kg \right\}$$

$$f_4(F_{j,4}^{Fw}) = \min \left\{ 1603.34kg + \sum_{j}^{J_1} F_{j,1}^{Fw} \right\} = 1890kg$$

If going back to Stage 2, the total freshwater consumption for this process is 1890 kg. These two paths have the same result. However, when the remaining wastewater from P1 is reused by P4 and operation P2 is only fed by the mixture of freshwater and reusable water from P3, the resultant water network has less connection.

Appendix C

The detailed process for Chapter 5 is as follows:

5.4.1 Example 1

The example illustrated in Section 5.3 in Chapter 5 is revisited here. In water reuse/recycle scenario, a buffer tank is used to store reuse water for reuse. In regeneration scenario, the regenerator with fixed outlet concentration is considered. During the processes, the capacity of tanks deployed in the water network is restricted to 70 t.

5.4.1.2 Consideration of Regeneration

The same procedure of reuse scenario is repeated for the regeneration scenario. Step 1 of data extraction is not repeated here. The remaining steps are described as follows.

Step 2. Establishment of the match matrix: A 7 × 6 matrix is constructed to represent the source-sink match matrix, as shown in Table S1. It is similar to the reuse/recycle scenario. The difference is that in this scenario, a water source of regenerated water is added into the matrix. In column 6, the value of reuse water for the regeneration unit is the limiting water quantity of each water source.

Table S1 The matching matrix for reuse scenario (unit: t)

	A	B	C	D	E	Re
A	(0,0)	(7.5, 22.5)	(5, 5)	(21, 3)	(33.33, 0)	(50, 0)
B	(0, 50)	(0,0)	(5, 5)	(21, 3)	(33.33, 0)	(22.5, 0)
C	(0, 50)	(6, 24)	(0,0)	(16.8, 7.2)	(36, 4)	(10, 0)
D	(0, 50)	(5, 25)	(3.33, 6.67)	(0,0)	(30, 10)	(24, 0)
E	(0, 50)	(4.29, 29.71)	(2.86, 7.14)	(12, 12)	(0,0)	(33.33,0)
Re	(0, 50)	(30, 0)	(7.5, 0)	(12, 0)	(16.67, 0)	(0, 0)
Fr	(0, 50)	(0, 22.5)	(0, 6)	(0, 10)	(0, 14.28)	(0, 0)

Step 3. Obtaining the match ranking matrix: Next, the match ranking matrix is established by sorting all the source-sink matches in ascending order of freshwater consumption. Because the outlet concentration of regenerator is lower than most of the operations, the regenerated water can be reused by all processes except process A. The ranking results are shown in Table S2.

Table S2 The match ranking matrix for Example 1 (regeneration)

	A	B	C	D	E	Re
A	-	3	2	2	2	-
B	-	-	2	2	2	-
C	-	4	-	3	3	-
D	-	5	4	-	4	-
E	-	6	5	5	-	-
Re	-	1	1	1	1	-
Fr	1	2	3	4	5	-

Step 4. Identification of potentially optimal match: Based on the results of Table S2, the potentially optimal matches can be identified, as shown in Table S3. For simplicity, not all the rankings are listed. This is because the presented ranking is enough to provide sufficient water quantity for the sinks.

The same procedure described in previous sections is repeated until the water demand of water sink is satisfied. The results are shown in Table S4. Except for Operation E, it is straightforward to determine the water utilization for the remaining operations. However, because Operation E has a higher inlet concentration, it can be fed by wastewater from Operations A or B without freshwater requirements, as shown in the shaded area. Whether to choose the regenerated water or wastewater from Operations

A and B is dependent on the availability of these two sources. Hence, at this stage, it is not possible to determine which source should be sent to Operation E.

Table S3 The potentially optimal match between sources and sinks

Ranking	A	B	C	D	E
1	Fr-A	Re-B	Re-C	Re-D	Re-E
2		Fr-B	A-C; B-C	A-D; B-D	A-E; B-E
3			Fr-C	C-D	C-E

Table S4 The initial potentially optimal match between sources and sinks

	A	B	C	D	E	Re
A					(33.33, 0)	(50, 0)
B					(33.33, 0)	(30, 0)
C						(7.5, 0)
D						(12, 0)
E						(33.33, 0) or (16.67, 0)
Re		(30, 0)	(7.5, 0)	(12, 0)	(16.67, 0)	
Fr	(0, 50)					

Step 5. Design of the initial batch water network: The same procedure of reuse scenario is carried out to design an initial batch water network based on the insight obtained from Table S3. Operation A has a zero inlet concentration so that it is tackled first. The first ranking match for this operation is the source of freshwater. The quantity required for the operation is 50 t.

As shown in Table S1, regenerated water is located at the first place for all the operations excluding Operation A, implying that regenerated water should be considered preferentially as compared to other water sources. Because the regenerated water comes from the effluent of other operations, the constraint of reuse of regenerated water is the availability. To achieve the minimum freshwater consumption, the system should consume freshwater as less as possible to minimize the freshwater consumption if the regenerated water is not available. It implies that the operation with higher inlet concentration should be placed in the early sequence before regenerated water is available. Therefore, Operation E is a suitable process satisfying the criterion above. Operation E is the second operating process in the batch operation.

Since Operation E has the choice of utilizing reusable water from Operations A and B or regenerated water, there exist three alternatives. If Operation E is fed with regenerated water, the actual time horizon of interest exceeds the given value, i.e., 8.5 h. This is because the regenerator requires time to purify the wastewater. Consequently, this solution is infeasible. Similarly, the alternative scenario, in which the wastewater from Operation B is used by Operation E, is also eliminated. If the water requirement of Operation E is only fed with the outlet water of Operated A, the remaining water is insufficient to meet the demand of the regeneration unit. Furthermore, there is no regenerated water at this point. Therefore, only partial wastewater from Operation A can be sent to Operation E; the deficit of Operation E is supplied with freshwater. The remaining wastewater from Operation A is sent to the regeneration unit. The specific quantity of reuse water consumed in Operation E depends on the water requirement of the regenerator.

Because the remaining operations preferentially choose the regenerated water, the availability of regenerated water is the primary constraint. The less freshwater requirement, the earlier the process is. This is because regenerated water can supply these operations without any freshwater. The sequence of remaining operations is C, D, and B. Operation B is the last operation, whose finish time should be 8.5 h. According to the water requirement of each process, and the requirement of regeneration unit, the timing of other operations and quantity of wastewater sent to regenerator is determined.

4.2 Example 2

In the previous section, a batch plant with a single contaminant is introduced to explain the application of the proposed method. In this example, multiple contaminants problems are considered.

4.2.1 Reuse/recycle scenario

The details are explained as follows.

Step 2: Establishment of the match matrix

In this example, a 5 × 4 matrix is set up based on the water recovery potential determined by the limiting data, as shown in Table S5.

Table S5 The matching matrix for reuse scenario of Example 2 (unit: t)

	P1	P2	P3	P4
P1	(0,0)	(116.66, 216.67)	(210, 390)	(408.33, 758.34)
P2	(0, 0)	(0,0)	(0, 0)	(0, 0)
P3	(52.5, 322.5)	(46.67, 286.66)	(0,0)	(163.33, 1003.34)
P4	(21.88, 353.12)	(38.89, 294.44)	(35, 565)	(0,0)
Fr	(0, 375)	(0, 333.33)	(0, 600)	(0, 1166.67)

Step 3: Obtaining of match ranking matrix

Once the match matrix is constructed, it is easy to rank the matches based on the ascending order of freshwater consumption. The match ranking matrix is then obtained, as shown in Table S6.

Step 4: Identification of potentially optimal match

Based on the match ranking matrix, the potentially optimal matches can be determined based on these rankings. The insight can be used to select the potential optimal water sources to satisfy the water requirements of water sinks. The possible matches of the example are shown in Table S7.

Table S6 The ranking matrix for water source and sink of Example 2

	Ranks			
	P1	P2	P3	P4
P1	-	1	1	1
P2	-	-	-	-
P3	1	2	-	2
P4	2	3	2	-
Fr	3	4	3	3

Table S7 The potentially optimal matches

Rank	P1	P2	P3	P4
1	P3-P1	P1-P2	P1-P3	P1-P4
2	P4-P1	P3-P2	P4-P3	P3-P4
3	Fr-P1	P4-P2	Fr-P3	Fr-P4
4		Fr-P2		

Based on the insight of Table S7, the priority of water sources to feed the water sinks can be determined. The same procedure explained in previous sections is repeated until the water demand of water sink is satisfied. It is noted that this is an initial ranking to choose which source should be sent to the sink preferentially. The final matches between sources and sinks should consider the quantity of freshwater consumed in the processes, the availability of reusable water, and the number of the storage tank.

As shown in row 1 of Table S5, if wastewater generated from Operation P1 is reused by other operations, the requirement of freshwater consumption is the least compared to other water sources. Furthermore, Operation P1 is ranking in the first place, as shown in row 1 of Table S6. It means the outlet stream of P1 has a high quality. Therefore, Operation P1 should come first, as the first operation. The next step is to determine which operation should be supplied by Operation P1 should supply. The freshwater consumption index can be determined by the results of Table S5. It is defined as the ratio of freshwater required for diluting reuse water to meet the requirements of the maximum reuse water. For example, freshwater consumption index of 1.8573 indicates if 1 t of wastewater is recovered, 1.8573 t of freshwater should be used to dilute the wastewater. The lower the value, the less freshwater it will consume. If wastewater from P1 is reused by P2, P3, and P4, the freshwater consumption index is determined as 1.8573, 1.8571, and 1.8572, respectively. Therefore, wastewater from P1 should preferentially be sent to P3. As the quantity of wastewater from P1 is insufficient to supply P2 and P4, the water deficiency can be satisfied by the reusable water from P3. This is because P3 is ranked at the second place, as shown in Table S6. Based on the freshwater consumption index of P2 and P4, i.e., 1.8573 and 1.8572, respectively, the reusable water from P1 should supply to P4 in order to minimize the freshwater consumption. Therefore, P2 supplied by reuse water from P3, while P4 recovers the reusable water from P1 and P3.

For the second batch of operation P1, the first place in the ranking results is Operation P4, indicating P4 is the supplier of P1. Although this example is for multiple contaminants, in each operation, only an amount of mass load of a specific contaminant is generated. If the reusable water from one operation is used by another operation, this reusable water can be used to dilute the water from other processes to some extent. Hence, a combination of two sources could consume less freshwater than a single source. This results in the matches at the first and second place selected to meet the requirement of water sinks if the quantity of wastewater is available. The results are shown in Table S8.

Table S8 The optimal match between sources and sinks

	P1(1)*	P3	P2(1)	P4(1)	P2(2)	P1(2)	P4(2)	P2(3)
P1		210		165			368.12	
P2								
P3			46.67	163.33	41.22	52.5	114.9	41.22
P4					38.89	21.88		38.89
Fr	375	390	286.66	838.34	253.22	398.98	683.65	253.22

*Note that the value in the bracket is the sequence of batch operations, e.g., P1(1) is the first batch of Operation P1

Since the information on water flow in the network is determined, the water network can be designed. For example, the effluent of P1 is reused by P3, the finishing time of P1, and the starting time of P3 should be at the same time point.

4.2.2 Consideration of Regeneration scenario

In the regeneration scenario, a regeneration unit with given removal ratios is considered. The regenerator has a flowrate of 466 kg/h. The removal ratio of C1, C2, C3, and C4 are 0.95, 0.99, 0.96 and 0.98, respectively. The procedure is briefly introduced blow.

Table S9 The optimal matches for Example with regeneration scenario

	P1(1)	P3	P2(1)	P4(1)	P2(2)	P1(2)	P4(2)	P2(3)
P1		210		165			376.05	
P2								
P3			46.67	163.33	41.22			38.89
P4					38.89			38.89
Re(P3)*							62.7	286.08
Re(P4)*						376.05	751.73	
Fr	375	390	286.66	838.34	253.22		683.65	8.36

* Note that Re(P3) indicates the regenerated water comes from Operation P3

As shown in row 1 of Table S6, P1 is the first ranking for all other operations. This observation implies that the effluent of Operation P1 can be preferentially selected to meet the water requirement of other operations to reduce freshwater consumption. For Operation P2, the effluent cannot be reused by other operations, as shown in row 2 in Table S6. Based on the information of row 3 and 4 of Table S6, we can find that Operation P3 has a first ranking and two second rankings, while Operation P4 has two second rankings and a third ranking. This indicates that Operation 3 should be considered preferentially for indirect reuse to consume less freshwater if this source has enough flowrate. Operation 4 can be sent to the regeneration unit. The first batch of Operations P1, P2, and P4 are the same as the reuse scenario. This is because the regenerated water is not available without wastewater entering the regeneration facility. For the second batch of these operations, the amount of reusable water and regenerated water can be determined based on the ranking information by trial and error method or mathematical programming. The optimal results are shown in Table S9.

4.3 Example 3

To extend the method to fixed flowrate problem, an example adopted from Majozi et al. (2006) is considered. Based on the scenarios introduced in section of Methodology, the freshwater for all the matches is determined. The matching matrix of Example 3 is shown in Table S10. Based on the results of Table S10, the ranking results are shown in Table S11.

Table S10. The matching matrix for Example 3 (unit: t)

	1	2	3	4	5
1	(0, 0)	(280, 0)	(400, 0)	(280, 0)	(400, 0)
2	(0, 1000)	(0,0)	(0, 400)	(0,280)	(0, 400)
3	(0, 1000)	(0, 280)	(0, 0)	(280, 0)	(400, 0)
4	(0, 1000)	(0, 280)	(0, 400)	(0, 0)	(0, 400)
5	(0, 1000)	(0, 280)	(400, 0)	(280, 0)	(0, 0)
Fr	(0, 1000)	(0, 280)	(0, 400)	(0, 280)	(0, 400)

Table S11. The ranking match matrix of Example 3 (unit: t)

	1	2	3	4	5
1	-	1	1	1	1
2	2	-	2	3	2
3	2	3	-	1	2
4	2	3	2	-	1
5	2	3	1	1	-
Fr	1	2	2	2	2