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Simultaneous Scheduling and Synthesis of Industrial Water Allocation Networks

Sudha Chauhan [1] and Munawar A. Shaik [2,*]

[1] Department of Chemical Engineering, Indian Institute of Technology Delhi, New Delhi 110016, India
[2] Department of Chemical and Petroleum Engineering, College of Engineering, UAE University, Al Ain P.O. Box 15551, United Arab Emirates
* Correspondence: munawar@uaeu.ac.ae

Abstract: This work addresses integration of batch scheduling with water allocation, recycle and reuse opportunities for freshwater minimization in batch plants via sequential and simultaneous methodologies. The presented scheduling model is based on state task network representation and unit-specific event based continuous time formulation. In the production scheduling model, a three-index finish time variable has been considered for handling multiple states having different processing time durations for the same task in a processing unit. The scheduling model introduces constraints to handle storage violations for production and consumption of the same state in the same unit. In the water network model for freshwater minimization, a regeneration unit along with a central water storage tank has been included to exploit the possibility of water reuse in the washing units. Four case studies are solved with single and multiple contaminants to evaluate the performance of the proposed model, which gives better savings in terms of freshwater consumption and thus also minimizes the effluent generation. Additionally, a preliminary analysis for two-objective optimization is presented where revenue is maximized, and the total water cost is minimized simultaneously using the weighted-sum method.

Keywords: water allocation network; water recycling and reuse; industrial water use; mathematical programming; optimization; scheduling

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1. Introduction

In the chemical industry, batch plants are commonly used for their flexible nature, which allows sharing of the same vessel for production of different products in a multipurpose fashion. Sharing of equipment also leads to water usage for cleaning purposes. Water network or water allocation network (WAN) synthesis incorporates water recycle and reuse opportunities by reusing water among different units requiring cleaning. Due to the stringent environmental regulations and increasing cost of effluent treatment, the optimum use of water is necessary [1]. Water network synthesis can be done for process units, regeneration (wastewater treatment) units or as integration of both process and regeneration units [2]. The goal of such integration is to obtain a water network design that minimizes the consumption of fresh water and generation of wastewater/effluent.

Regarding batch scheduling and freshwater minimization, research works have presented many mathematical formulations to handle this problem either using sequential or simultaneous approaches, and by incorporating direct or indirect water re-use opportunities. In the sequential approach, the scheduling problem is solved first independently with the objective of maximization of profit, followed by solving the water network synthesis problem separately for the resulting solution of the scheduling problem. In the simultaneous approach, both maximization of profit and minimization of freshwater are considered simultaneously, resulting in a better overall solution relative to the sequential approach. In the water network problem, *direct water re-use* refers to consumption of used water coming from one unit directly in another unit without using any storage for used water, while *indirect water reuse* refers to use of a central storage tank with the added flexibility of being able to find a better match among different water sources and sinks. Here, a classification of literature work based on the solution approaches (sequential/simultaneous) and the type of water re-use (direct/indirect) is presented.

1.1. Sequential Methodology and Direct or Indirect Water Re-Use

Water network problems solved with the help of a sequential approach are found in the published literature mostly involving indirect usage of water through a central water tank/regeneration unit along with the direct water usage possibilities among the units. Therefore, the detailed description of the same is presented in this section.

Majozi [3] presented a model for freshwater and wastewater minimization in batch plants with and without using a water storage tank. The presented formulation was based on the predefined start and finish times for washing tasks and was solved for a single contaminant. The model was solved for two scenarios, where in the first case, the outlet concentration of the contaminant and the mass load was fixed, and in the second one, the outlet concentration varies within the given bounds. The first case results in a mixed-integer nonlinear programming (MINLP) problem that is exactly linearized; however, the second case remains nonlinear and the programming does not guarantee global optimality for large scale problems. Cheng et al. [4] incorporated three optimization problems in a single MINLP problem to generate integrated water networks. In this formulation, several design specifications such as production schedule, size and number of buffer tanks, and water flow operating policies were included.

Chen et al. [5] developed a nonlinear programming model for minimum consumption of freshwater in a batch process. They solved literature examples by taking a predefined production schedule and applied the water network model on them. In the water minimization model, direct water reuse between the washing units was taken. Further, constraints related to water tanks were included in the model to enhance the freshwater reduction. The effect of cyclic processes for water reuse was incorporated using a water tank and it was observed that cyclic behavior for the washing operation contributes significantly to reduced use of freshwater.

1.2. Simultaneous Methodology and Indirect Water Re-Use

Gouws et al. [6] presented a mathematical formulation for effluent minimization in batch processes by extending the work presented by Majozi [3]. In this work, only contaminant mass load was fixed, with variable quantities of water and outlet contaminant concentrations. A reusable water storage tank was taken to find the maximum water reuse possibilities. One objective of this MINLP problem was to maximize profit and the other was minimization of the effluent. For multiple contaminants, Majozi and Gouws [7] presented a nonlinear methodology which dealt with the wastewater minimization in batch processes by considering two scenarios: without and with storage tank. In the first case, only water reuse possibilities were considered; however, in the second case, the possibility of water storage was explored using a central water storage tank along with the water reuse opportunities. They reported better freshwater savings with water storage for multiple contaminant problems.

Zhou et al. [8] presented a systematic design methodology for simultaneous optimization of batch process schedules and water allocation networks. For batch scheduling, they adopted the unit-specific event-based model of Ierapetritou and Floudas [9], using an improved state-space superstructure to capture the structural characteristics of the integrated water-allocation network for batch process. They included the cost of splitters and mixers in their formulation, and the resulting MINLP model was solved using a hybrid optimization strategy integrating DICOPT and Genetic Algorithms. Li et al. [10] presented two novel state-space-time superstructures to capture all production schemes and WAN configurations for batch water allocation network design and combining discrete and continuous time formulations in their flexible scheduling model, based on the unit-specific event-based model of Ierapetritou and Floudas [9].

Adekola and Majozi [11] presented a methodology in which a wastewater regenerator was included for further minimization of wastewater. Along with the regenerator, central water storage tank and direct water reuse were considered in the given formulation. Chaturvedi et al. [12] provided an approach for handling of multiple water resources in a batch plant and claimed that when minimizing the water operating cost for a batch plant involving multiple water resources, the resulting production schedule can also be applied to the system involving a single water source. Li and Majozi [13] introduced a method for the synthesis of flexible batch water networks by incorporating two regeneration units and solved case studies for single as well as multiple contaminants. In this method, source and sink match priority was determined by a ranking matrix which identified the maximum reusable water recovery potential and helped to design water networks that consume minimum freshwater. Yang et al. [14] introduced several regeneration units for the design of water networks by considering fixed removal ratio as well as fixed regenerated concentrations. Li and Majozi [15] investigated the opportunity to minimize freshwater consumption for a flexible batch process with a regeneration unit using a dynamic programming method. Chaturvedi and Sinha [16] solved a bi-objective problem for minimization of fresh water and storage requirement. They generated a Pareto optimal front for the two objectives to facilitate the decision makers.

1.3. Simultaneous Methodology and Direct Water Re-Use

Most of the earlier formulated models considered indirect water re-use to target minimum effluent by using a storage tank. Hence, the relevant literature on direct water re-use is presented here.

In any batch process there are some processing units which remain idle, which may be temporarily used as storage vessels. By doing this, the size of the central storage can be reduced and the utilization of processing units can be increased. In this context, Gouws and Majozi [17] presented a methodology which dealt with the minimization of single contaminant wastewater by considering the storage possibilities in such idle units. Adekola and Majozi [18] proposed a model for minimizing wastewater in batch plant scheduling by exploring the possibility of sequence dependent changeovers in washing units for a fixed mass load of contaminant. The computational results obtained for this model reported improvement in profits as well as in freshwater usage. The case studies considered were based on the single contaminant problem.

After investigating the literature works on simultaneous scheduling and water networks, some discrepancies were observed in the results of Majozi and Gouws [7] and Adekola and Majozi [11] pertaining to real time violation for task occurrence and water mass balance violations in the central storage tank, as described in detail in Sections 3.2.1, 3.3.1 and 3.4.1. In the present work, freshwater minimization is accomplished by combining the water allocation network with batch production scheduling using the simultaneous approach. A unit-specific event-based continuous time model is adapted for scheduling which is based on state task network (STN) representation. To handle different processing time durations for more than one state in a single processing unit, a three-index finish time variable is introduced in the production scheduling model. In addition to that, a constraint is introduced to handle the storage violation for production and consumption of the same state in the same unit. In the present work, freshwater minimization opportunities are exploited by including a regeneration unit along with a central water storage tank and the impact is demonstrated through the industrial examples. A comparison between different solution approaches such as sequential and simultaneous methodology is presented. Further, a preliminary analysis for two-objective optimization is presented where revenue is maximized, and total water cost is minimized simultaneously using the weighted-sum method. The main contributions in the present work are modification of batch scheduling and water-allocation network models based on three-index unit-specific event-based continuous time representation [19] to enable efficient solution of the integrated problem, because unit-specific event-based continuous time representation has been established as an efficient approach. A detailed summary of important contributions of the proposed work is given in Section 2.3.

1.4. Problem Statement

The problem considered in the present work has been addressed by the following parameters:

- The production recipe representation using STN;
- Unit capacity and suitability of occurrence of tasks in each unit;
- Storage capacity for each material state;
- Processing time for each task (variable or constant);
- Washing time in each unit;
- Contaminant mass load (constant or batch dependent);
- Maximum inlet and outlet concentration of each contaminant for different units;
- Different costs for products, fresh water and wastewater discharge;
- Scheduling time horizon;
- Maximum capacity of the central storage tank for water storage;
- Contaminant removal ratio and regenerator flow rate.

Given the above-mentioned data, the objective is to determine the optimum production schedule for a water allocation network that minimizes consumption of freshwater by using the central water storage tank for indirect reuse of water and a regenerator for purification of wastewater.

2. Mathematical Formulation

In the present work, we consider simultaneous batch scheduling and water allocation network synthesis using unit-specific event-based time representation. The sequential methodology is also presented for comparison, where the production schedule is solved first and then the water network is identified for the fixed schedule. The three-index unit-specific event-based model of Vooradi and Shaik [19] has been adapted for scheduling with some modifications. In the water allocation network, water reuse opportunity has been incorporated by using a central water storage tank and a regenerator. In this model, storage vessel and regenerator related constraints have been adapted from [11].

Modeling Assumptions: The model is presented based on the assumption that there is no waiting in washing units (i.e., no post processing unit wait policy) which is explained in detail in Section 2.2.7. For a regenerator, it has been assumed that it remains active only when a unit requires water and operates continuously with steady inlet and outlet streams for that duration. Another assumption has been made that, at a given time, the storage tank either supplies water to the washing unit or to the regeneration unit based on practical operational requirements.

The complete formulation leads to a MINLP model, as presented below.

2.1. Production Scheduling Model

The production scheduling model of Vooradi and Shaik [19] has been adapted for the proposed work, for which the original model constraints are given in Appendix A for ready reference. The model has been extended here by modifying some constraints. A detailed description for the same is given below. The nomenclature of different indices, sets, and decision variables is given at the end.

2.1.1. Handling Multiple States Having Different Processing Time Durations for the Same Task in a Processing Unit

In a processing unit, a task producing multiple states has different processing times which are state dependent, defined by a parameter α_{is} is (as it happens in the case study presented later). The finish time of the task needs to be modeled properly to capture this feature by using three index variables instead of two index variables, i.e., the finish time will be a function of task, event, and state as well. Hence, the finish time of all the constraints is modified as follows.

2.1.2. Duration Constraints

Constraints (1)–(3) define the finish time of the task i for the state s at an event n. If Δn = 0 (which means task occurring over single event), then the finish time of a task for state s that starts at the same event is calculated from constraint (1):

$$T^f(i,s,n) = T^s(i,n) + \alpha_{is} w\ (i,n,n) + \beta_{is} b(i,n,n),\ \forall s \in \alpha_{is}, i \in I,\ n \in N,\ \Delta n = 0 \quad (1)$$

However, if Δn is nonzero (which means task occurring over multiple events), then the finish time of the task that started at an earlier event is calculated from constraints (2) and (3):

$$\begin{gathered} T^f(i,s,n') \geq T^s(i,n) + \alpha_{is} w(i,n,n') + \beta_{is} b(i,n,n'), \\ \forall s \in \alpha_{is}, i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \end{gathered} \quad (2)$$

$$\begin{gathered} T^f(i,s,n') \leq T^s(i,n) + \alpha_{is} w(i,n,n') + \beta_{is} b(i,n,n') + M(1 - w(i,n,n')), \\ \forall s \in \alpha_{is}, i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \end{gathered} \quad (3)$$

If the task is active and ending at an event, then the finish time will be equal to the sum of start time and duration of the task (constraint (3)), otherwise finish time will be greater than or equal to the sum of the start time and duration (constraint (2)).

2.1.3. Sequencing Constraints

Equations (4)–(7) define the sequencing of task i for each state s at event n for different cases including: same task in the same unit, different tasks in the same unit, and different tasks in different units, respectively.
Same Task in the Same Unit:

$$T^s(i,n+1) \geq T^f(i,s,n),\ \ \forall s \in \alpha^l_{is}, i \in I, n \in N, n < N \quad (4)$$

$$\begin{gathered} T^s(i,n+1) \leq T^f(i,s,n) + M\left(1 - \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} \ \sum_{\substack{n'' \in N \\ n \leq n'' \leq n' + \Delta n}} w(i,n',n'')\right), \\ \forall s \in \alpha^l_{is}, i \in I, n \in N, n \langle N, \Delta n \rangle 0 \end{gathered} \quad (5)$$

Different Tasks in the Same Unit:

$$T^s(i,n+1) \geq T^f\big(i',s,n\big), \forall s \in \alpha^l_{i's}, i, i' \in I_j, i \neq i', j \in J_i, n < N \quad (6)$$

Different Tasks in Different Units:

$$\begin{gathered} T^s(i,n+1) \geq T^f(i',s,n) - M\left(1 - \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n)\right), \\ \forall s \in \alpha_{i's}, i, i', j, j', n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I^c_s, i' \in I^p_s \end{gathered} \quad (7)$$

Here, α^l_{is} denotes the largest time taken by one of the produced states s from a task i.

2.1.4. Tightening Constraint

The tightening constraint is also modified and governed by Equation (8):

$$\sum_{i \in I_j} \sum_{n \in N} \sum_{\substack{n' \in N \\ n \leq n' \leq n + \Delta n}} \big(\alpha^l_{is} w\big(i,n,n'\big) + \beta_{is} b\big(i,n,n'\big)\big) \leq H,\ \forall s \in \alpha^l_{is}, j \in J \quad (8)$$

2.1.5. Storage Constraints

The modified storage constraints are given by Equations (9) and (10):

$$T^f(i',s,n) \geq T^s(i,n) - M\left[1 - \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} w(i',n',n)\right] \tag{9}$$
$$\forall s^{dfis} \in \alpha_{i's^{dfis}}, j, j' \in J, n \in N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p$$

$$T^s(i,n+1) \leq T^f(i',s,n) + M\left[2 - \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} w(i',n',n) - \sum_{\substack{n' \in N \\ n+1 \leq n' \leq n+1+\Delta n}} w(i,n+1,n')\right], \tag{10}$$
$$\forall s^{dfis} \in \alpha_{i's^{dfis}}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p$$

Equations (11) and (12) are the new constraints which are introduced in the production scheduling model. Constraint (11) states that, the excess amount stored at event n plus the amount produced at the same event cannot exceed the given storage limits when the same state is being produced and consumed in the same unit:

$$ST(s,n) + \sum_{i \in I_s^p \cap I^{pc}} \rho_{is} \sum_{n-\Delta n \leq n' \leq n} b(i,n',n) \leq ST_s^{max}, \forall s \in S^{dfis} \cap S^{pc}, n \in N \tag{11}$$

Similarly, constraint (12) imposes upper bounds to prevent storage violation for all states related to a Finite Intermediate Storage (FIS) policy, except those which are being produced and consumed in the same unit:

$$ST(s,n) \leq ST_s^{max}, \forall s \in S^{dfis} - S^{pc}, n \in N \tag{12}$$

2.2. WAN Model

2.2.1. Mass Balance of Water around Washing Unit

A superstructure for water mass balance is shown in Figure 1. The figure depicts only water using part of the batch process and unit j represents the unit where washing is taking place.

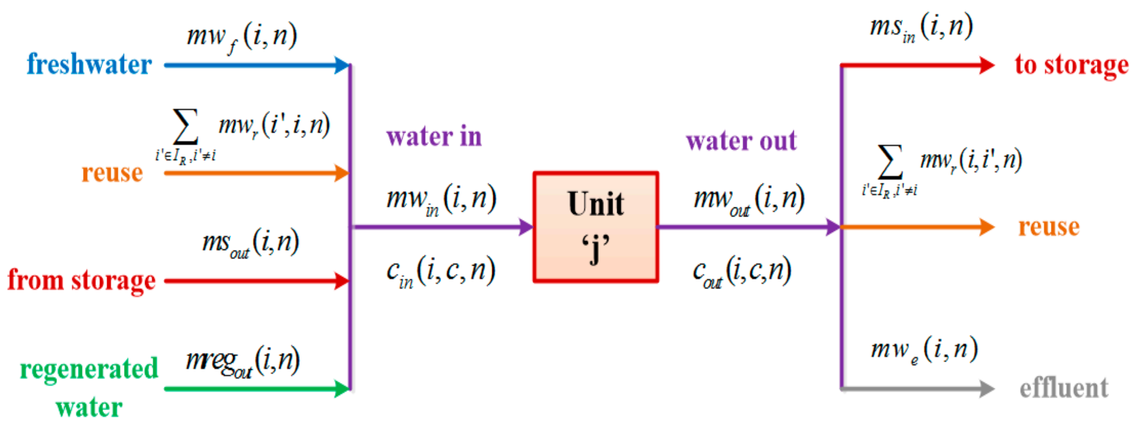

Figure 1. Superstructure for water mass balance in each unit *j*.

Constraint (13) states that total inlet water in the washing unit should be the summation of reused water from other units, freshwater requirement, water received from the central water storage tank, and water coming out from the regeneration unit:

$$mw_{in}(i,n) = \sum_{i' \in I_R, i' \neq i} mw_r(i',i,n) + mw_f(i,n) + ms_{out}(i,n) + mreg_{out}(i,n), \forall i \in I_R, n \in N \tag{13}$$

Here, $i \neq i'$ is used for reused water to avoid mixing the exit of the same unit having a higher contaminant load going back to the same unit. Constraint (14) describes that the exiting water from a unit could be sent to the other unit for reuse, into the central water storage tank, and/or directly to the effluent:

$$mw_{out}(i,n) = \sum_{i' \in I_R, i' \neq i} mw_r(i,i',n) + mw_e(i,n) + ms_{in}(i,n), \forall i \in I_R, n \in N \quad (14)$$

Constraint (15) states that the total inlet and outlet of water for each task I at each event n should be equal:

$$mw_{in}(i,n) = mw_{out}(i,n),\ \forall i \in I_R, n \in N \quad (15)$$

Constraint (16) describes the mass balance of contaminant around a washing unit for the fixed mass load of contaminant, whereas constraint (17) describes the same when the given contaminant mass load is batch-size dependent:

$$mw_{out}(i,n)c_{out}(i,c,n) = mw_{in}(i,n)c_{in}(i,c,n) + M_{i,c}^{load} yw(i,n),\ \forall i \in I_R, n \in N, c \in C \quad (16)$$

$$mw_{out}(i,n)c_{out}(i,c,n) = mw_{in}(i,n)c_{in}(i,c,n) + M_{i,c}^{load} \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} b(i,n',n),\ \forall i \in I_R, n \in N, c \in C \quad (17)$$

Constraint (18) is the contaminant balance for the mixer before the washing unit:

$$\begin{aligned} mw_{in}(i,n)c_{in}(i,c,n) = & \sum_{i' \in I_R, i' \neq i} mw_r(i',i,n)c_{out}(i',c,n) + ms_{out}(i,n)cs_{out}(c,n) \\ & + mreg_{out}(i,n)creg_{out}(c,n), \forall i \in I_R, n \in N, c \in C \end{aligned} \quad (18)$$

For multi-contaminant problems, the concentrations of individual components cannot be set to the maximum since the contaminants are not limiting simultaneously. Hence, the limiting contaminant will always be at the maximum outlet concentration and the non-limiting contaminants will be below their respective maximum outlet concentration. The maximum amount of water into a washing unit is governed by Equation (19):

$$Mw_i^U = \max_{c \in C} \left\{ \frac{M_{i,c}^{load}}{C_{i,c}^{out,U} - C_{i,c}^{in,U}} \right\}, \forall i \in I_R \quad (19)$$

which states that the maximum flow rate of water for a given task corresponds to the maximum ratio of contaminant mass load and the difference between the outlet and inlet concentration of that contaminant. Equations (20)–(23) define upper bounds on the maximum inlet and outlet contaminant concentrations, and maximum water flow requirement for a given task i at event n:

$$c_{in}(i,c,n) \leq C_{i,c}^{in,U} yw(i,n), \forall i \in I_R, n \in N, c \in C \quad (20)$$

$$c_{out}(i,c,n) \leq C_{i,c}^{out,U} yw(i,n), \forall i \in I_R, n \in N, c \in C \quad (21)$$

$$mw_{in}(i,n) \leq Mw_i^U yw(i,n), \forall i \in I_R, n \in N \quad (22)$$

$$mw_r(i',i,n) \leq Mw_i^U yw_r(i',i,n),\ \forall i,i' \in I_R, i' \neq i, n \in N \quad (23)$$

2.2.2. Water Mass Balance around the Central Water Storage Tank

Figure 2 describes the water mass balance around the central water storage tank. Constraint (24) states that the total water stored in the tank at event n is the summation of the amount stored at the previous event n–– 1, and the net difference between the water entering the storage at the previous event n–— 1 and water leaving the storage at the event n to the washing unit or to the regenerator:

$$qw_s(n) = qw_s(n-1) + \sum_i ms_{in}(i, n-1) - \sum_i ms_{out}(i, n) - \sum_{stt} mreg_{in}(stt, n), \forall i \in I_R, n \in N, n > 1 \quad (24)$$

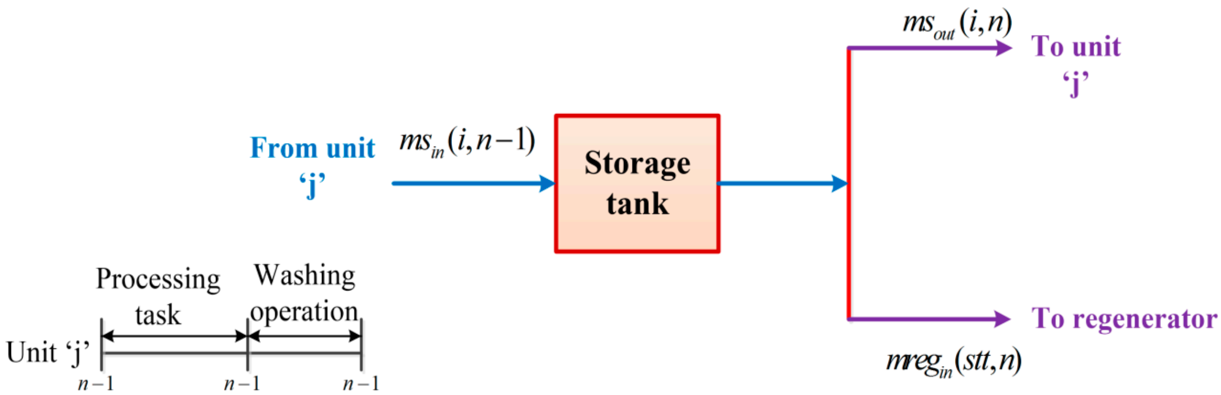

Figure 2. Superstructure for water mass balance in central water storage tank.

Constraint (25) describes the initial amount of water stored in the tank at the first event:

$$qw_s(n) = Qw_s^0 - \sum_i ms_{out}(i, n) - \sum_{stt} mreg_{in}(stt, n), \forall i \in I_R, n \in N, n = 1 \quad (25)$$

Equation (26) defines the contaminant balance around the central water storage tank based on the total balance given in Equation (24):

$$\begin{gathered} qw_s(n)cs_{out}(i, n) = qw_s(n-1)cs_{out}(i, n-1) + \sum_i ms_{in}(i, n-1)c_{out}(i, c, n-1) \\ - \sum_i ms_{out}(i, n)cs_{out}(i, n) - \sum_{stt} mreg_{in}(stt, n)cs_{out}(i, n), \ \forall i \in I_R, n \in N, n > 1 \end{gathered} \quad (26)$$

Constraint (27) limits the maximum water storage in the tank:

$$qw_s(n) \leq Qw_s^U, \forall n \in N \quad (27)$$

Constraint (28) defines the initial concentration of water coming out from the storage tank:

$$cs_{out}(c, n) = Cs_c^{out,0}, \forall c \in C, n = 1 \quad (28)$$

Constraints (29) and (30) define upper bounds on the maximum inlet water coming to the storage tank and outlet water exiting from the central storage, respectively:

$$ms_{out}(i, n) \leq Mw_i^U ys_{out}(i, n), \forall i \in I, n \in N \quad (29)$$

$$ms_{in}(i, n) \leq Mw_i^U ys_{in}(i, n), \ \forall i \in I, n \in N \quad (30)$$

Equation (31) states that there should be no accumulation of water in the storage tank at the last event point:

$$qw_s(n) = Qw_s^0, \forall n \in N, n = N \quad (31)$$

2.2.3. Water Mass Balance around Regeneration Unit

The function of a regeneration unit is to purify contaminated water so that it can be reused further in washing operations. Constraint (32) states that the inlet and outlet quantity of water in a regenerator should be equal at each event n, i.e., a regeneration unit should work in a continuous manner without any accumulation of water in the unit:

$$\sum_{stt} mreg_{in}(stt,n) = \sum_{i} mreg_{out}(i,n), \forall i \in I_R, n \in N \tag{32}$$

Constraint (33) describes the outlet contaminant concentration of water exiting from a regeneration unit based on the specified removal ratio, RR_c:

$$creg_{out}(c,n) = cs_{out}(c,n)(1 - RR_c), \ \forall c \in C, n \in N \tag{33}$$

Constraint (34) gives the contaminant mass balance around the regenerator:

$$cs_{out}(c,n) \sum_{i} mreg_{in}(stt,n) = creg_{out}(c,n) \sum_{i} mreg_{out}(i,n) + m_{dirt}(c,n), \forall i \in I_R, \ stt \in STT, n \in N \tag{34}$$

which states that for contaminant c, the total contaminant mass load entering into a regenerator is the summation of the contaminant mass load leaving the regenerator and the contaminant mass removed from the water by the regenerator, i.e., $m_{dirt}(c,n)$.

2.2.4. Sequencing Constraints for Water Reuse

Constraint (35) states that it is not necessary that water reuse will occur if a washing operation is taking place in each unit, because a unit can use water from other sources too:

$$yw_r(i,i',n) \le yw(i',n), \ \forall i \in I_R, i' \ne i, n \in N \tag{35}$$

Constraints (36) and (37) enforce equality of timings of the outlet water of a unit with that of inlet water of the other unit, if water reuse is taking place between the said units:

$$ts_{out}(i,n) \ge tw_{in}(i,n) - H(2 - ys_{out}(i,n) - yw(i,n)), \ \forall i, \in I_R, n \in N \tag{36}$$

$$tw_{out}(i,n) \ge tw_{in}(i',n) - H[1 - yw_r(i,i',n)], \forall i \in I_R, i' \ne i, n \in N \tag{37}$$

2.2.5. Sequencing Constraints for Storage Tank

Constraints (38)–(41) describe the sequencing of timings of inlet and outlet of water in washing units via storage tank. Equations (38) and (39) state that if a washing operation is being accomplished with the help of a central water storage facility, then the timings of the outlet water from storage and the inlet water to washing unit should be equal at each event n:

$$ts_{out}(i,n) \le tw_{in}(i,n) + H(2 - ys_{out}(i,n) - yw(i,n)), \ \forall i, \in I_R, n \in N \tag{38}$$

$$ts_{out}(i,n) \ge tw_{in}(i,n) - H(2 - ys_{out}(i,n) - yw(i,n)), \ \forall i, \in I_R, n \in N \tag{39}$$

Similarly, Equations (40) and (41) describe that in a washing unit, if water is entering into the storage tank after completion of washing operation, then the timing of inlet water to the storage tank should coincide with that of the outlet water from the washing unit at each event n:

$$ts_{in}(i,n) \le tw_{out}(i,n) + H(2 - ys_{in}(i,n) - yw(i,n)), \ \forall i, \in I_R, n \in N \tag{40}$$

$$ts_{in}(i,n) \ge tw_{out}(i,n) - H(2 - ys_{in}(i,n) - yw(i,n)), \ \forall i, \in I_R, n \in N \tag{41}$$

2.2.6. Sequencing Constraints Associated with Regeneration Unit

Constraint (42) defines that if there is an inlet of water in a regenerator then there must be an exit for the water at the same event, i.e., it cannot hold the water for the next event:

$$yreg_{out}(i,n) = yreg_{in}(stt,n), \ \forall i \in I_R, \ stt \in STT, \ n \in N \tag{42}$$

Constraints (43) and (44) describe that if a washing unit is receiving water from the regenerator, then the timings of inlet water in the unit and the outlet water from the regenerator should be equal at each event n:

$$treg_{out}(i,n) \geq tw_{in}(i,n) - H(2 - yreg_{out}(i,n) - yw(i,n)),\ \forall i \in I_R, n \in N \tag{43}$$

$$treg_{out}(i,n) \leq tw_{in}(i,n) + H(2 - yreg_{out}(i,n) - yw(i,n)),\ \forall i \in I_R, n \in N \tag{44}$$

Constraint (45) defines the exit time of water from the regenerator:

$$treg_{out}(i,n) = treg_{in}(stt,n) + \left[\frac{\sum_i mreg_{in}(stt,n)}{f_{reg}}\right] yreg_{in}(stt,n), \forall i \in I_R, stt \in STT, n \in N \tag{45}$$

Constraint (46) states that the storage tank cannot supply water to the regenerator and the washing unit simultaneously, at each event n:

$$yreg_{in}(stt,n) + ys_{out}(i,n) \leq 1, \forall i \in I_R, stt \in STT, n \in N \tag{46}$$

Similarly, the washing unit cannot receive water simultaneously from the regenerator and the storage tank at the same event, which is enforced by constraint (47):

$$yreg_{out}(ir,n) + ys_{out}(i,n) \leq 1,\ \forall i \in I_R, n \in N \tag{47}$$

2.2.7. Scheduling Constraints for Washing

As shown in Figure 3, the variable T^f is modified to include the finish time of the processing task plus the corresponding washing time in each washing unit. Hence, the following constraints are proposed for the case of 'no post-processing unit wait policy' for washing units. These constraints stipulate that washing must begin immediately after completion of the processing task in a washing unit. Since the duration of washing is fixed, a unit cannot hold water for longer than the stipulated duration. In constraints (48) and (49), T^f signifies the combined finish time of processing task plus washing:

$$tw_{out}(i,n) \geq T^f(i,n) - H[1 - yw(i,n)],\ \forall i \in I_R, n \in N \tag{48}$$

$$tw_{out}(i,n) \leq T^f(i,n) + H[1 - yw(i,n)],\ \forall i \in I_R, n \in N \tag{49}$$

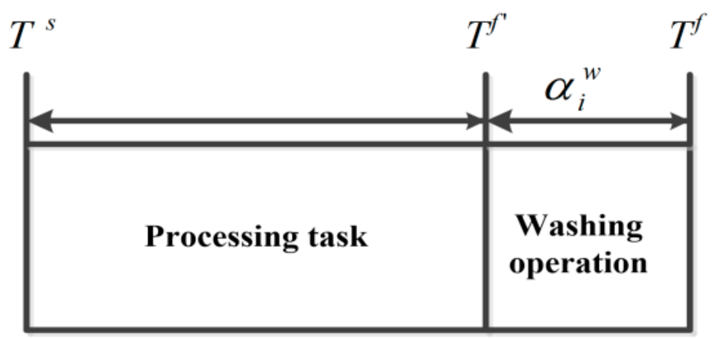

Figure 3. Washing sequence with no unit wait policy for washing units.

Constraint (50) defines the total time of washing operation:

$$tw_{out}(i,n) = tw_{in}(i,n) + \alpha_i^w yw(i,n),\ \forall i \in I_R, n \in N \tag{50}$$

Constraint (51) activates the washing operation to take place at the end of the same processing task occurring in the same unit at the same event:

$$yw(i,n) = \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i,n',n),\ \forall i \in I_R, n \in N \tag{51}$$

2.2.8. Modifications in the Scheduling Model

As finish time combines the processing time of the task and the respective washing time, changes are needed in the scheduling model to reflect the finish time of the processing tasks that require washing. Hence, the following modifications have been made in the three-index unit specific event-based production scheduling model.

Duration Constraints:

Constraints (52)–(54) are the modified duration constraints:

$$T^f(i,n) = T^s(i,n) + (\alpha_i + \alpha_i^w)w(i,n,n') + \beta_i b(i,n,n'),\ \forall i \in I, n, n' \in N, \Delta n = 0 \quad (52)$$

$$T^f(i,n') \geq T^s(i,n) + (\alpha_i + \alpha_i^w)w(i,n,n') + \beta_i b(i,n,n'), \forall i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \quad (53)$$

$$\begin{gathered} T^f(i,n') \leq T^s(i,n) + \left(\alpha_i + \alpha_i^w\right)w(i,n,n') + \beta_i b(i,n,n') + M[1 - w(i,n,n')] \\ \forall i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \end{gathered} \quad (54)$$

where washing time α_i^w has been added to the fixed processing time α_i so that the combined time may incorporate both reaction and washing time. Constraints (55)–(57) describe the duration constraints for the three-index finish time:

$$T^f(i,s,n) = T^s(i,n) + (\alpha_{is} + \alpha_{is}^w)w\ (i,n,n) + \beta_{is} b(i,n,n),\ \forall s \in \alpha_{is}, i \in I,\ n \in N,\ \Delta n = 0 \quad (55)$$

$$\begin{gathered} T^f(i,s,n') \geq T^s(i,n) + \left(\alpha_{is} + \alpha_{is}^w\right)w(i,n,n') + \beta_{is} b(i,n,n'), \\ \forall s \in \alpha_{is}, i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \end{gathered} \quad (56)$$

$$\begin{gathered} T^f(i,s,n') \leq T^s(i,n) + \left(\alpha_{is} + \alpha_{is}^w\right)w(i,n,n') + \beta_{is} b(i,n,n') + M(1 - w(i,n,n')), \\ \forall s \in \alpha_{is}, i \in I, n, n' \in N, n \leq n' \leq n + \Delta n, \Delta n > 0 \end{gathered} \quad (57)$$

Sequencing Constraints:

Constraint (58) is the modified sequencing constraint for the different tasks in different units. Similarly, constraint (59) is the modified sequencing constraint for the three-index finish time. In these constraints, washing time has been subtracted from the finish times of the processing task to capture the actual finish time of the reaction.

Different Tasks in Different Units:

$$\begin{gathered} T^s(i,n+1) \geq T^f(i',n) - \alpha_{i'}^w \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n) - M\left[1 - \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n)\right], \\ \forall s, i, i', j, j', n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p \end{gathered} \quad (58)$$

$$\begin{gathered} T^s(i,n+1) \geq T^f(i',s,n) - \alpha_{i's}^w \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n) - M\left[1 - \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n)\right], \\ \forall s \in \alpha_{i's}, i, i', j, j', n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p \end{gathered} \quad (59)$$

Storage Related Constraints

Constraints (60) and (61) are the modified FIS related constraints when washing time is combined with the finish time of the given processing task:

$$\begin{gathered} T^f(i',n) - \alpha_{i'}^w \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n) \geq T^s(i,n) - M\left[1 - \sum_{\substack{n' \in N \\ n - \Delta n \leq n' \leq n}} w(i',n',n)\right], \\ \forall s^{dfis}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p \end{gathered} \quad (60)$$

$$T^s(i,n+1) \le T^f(i',n) - \alpha^w_{i'} \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n) + M\left[2 - \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n) - \sum_{\substack{n' \in N \\ n+1 \le n' \le n+1+\Delta n}} w(i,n+1,n')\right], \tag{61}$$
$$\forall s^{dfis}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \ne i', j \ne j', i \in I^c_s, i' \in I^p_s$$

Similarly, constraints (62) and (63) will be used for handling the different processing times in the same unit for different states:

$$T^f(i',s,n) - \alpha^w_{i's} \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n) \ge T^s(i,n) - M\left[1 - \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n)\right], \tag{62}$$
$$\forall s^{dfis} \in \alpha_{i's^{dfis}}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \ne i', j \ne j', i \in I^c_s, i' \in I^p_s$$

$$T^s(i,n+1) \le T^f(i',s,n) - \alpha^w_{i's} \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n) + M\left[2 - \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n) - \sum_{\substack{n' \in N \\ n+1 \le n' \le n+1+\Delta n}} w(i,n+1,n')\right], \tag{63}$$
$$\forall s^{dfis} \in \alpha_{i's^{dfis}}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \ne i', j \ne j', i \in I^c_s, i' \in I^p_s$$

Tightening Constraints

The tightening constraints (64) and (65) state that all the production tasks corresponding to their washing operations should be completed in the given time horizon:

$$\sum_{i \in I_j} \sum_{n \in N} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} (\alpha_i + \alpha^w_i) w(i,n,n') + \beta_i b(i,n,n')) \le H \ \forall j \in J \tag{64}$$

$$\sum_{i \in I_j} \sum_{n \in N} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} \left(\alpha^l_{is} + \alpha^w_{is}\right) w(i,n,n') + \beta_i b(i,n,n')) \le H \ \forall j \in J \tag{65}$$

Bounds

The following upper bounds are placed on the various timing variables, stipulating them to be less than the specified time horizon:

$$T^f(i,s,n) \le H \ \forall i \in I, n \in N \tag{66}$$

$$tw_{in}(i,n) \le H \ \forall i \in I_R, n \in N \tag{67}$$

$$tw_{out}(i,n) \le H \ \forall i \in I_R, n \in N \tag{68}$$

$$tw_{out}(i,s,n) \le H \ \forall s \in \alpha_{is}, i \in I_R, n \in N \tag{69}$$

$$tw_r(i,i',n) \le H \ \forall i, i' \in I_R, n \in N \tag{70}$$

$$tw_r(i,i',s,n) \le H \ \forall s \in \alpha_{is}, i, i' \in I_R, n \in N \tag{71}$$

$$treg_{in}(stt,n) \le H \ \forall stt \in STT, n \in N \tag{72}$$

$$treg_{out}(i,n) \le H \ \forall i \in I_R, n \in N \tag{73}$$

$$treg_{out}(i,s,n) \le H \ \forall s \in \alpha_{is}, i \in I_R, n \in N \tag{74}$$

2.2.9. Objective Function

The objective function in Equation (75) is to maximize the net profit where the costs of freshwater and wastewater are subtracted from the total revenue obtained from sales of products:

$$\begin{aligned} Obj. = \sum_{s\in S^p} P_s \sum_{n=N} \left[ST(s,n) + \sum_{i\in I_s^p} \rho_{is} \sum_{\substack{n'\in N \\ n-\Delta n\le n'\le n}} b(i',n',n) \right] \\ -CF \sum_{i\in I_R} \sum_{n\in N} mw_f(i,n) - CE \sum_{i\in I_R} \sum_{n\in N} mw_e(i,n) \end{aligned} \tag{75}$$

2.3. Important Contributions of the Proposed Work

- A unit-specific event-based production scheduling model has been adapted from the literature [19] with several modifications including: introducing a three-index finish time variable to handle different processing times for multiple states produced by a task, new constraints for avoiding real time storage violation when the same state is being produced and consumed in the same unit, modified sequencing constraints to handle the new definition of finish time of a task by combining the washing operation to occur at the same event after the task.
- In WAN, immediate washing is considered in the processing units after completion of the processing task i.e., the washing operation takes place without post processing unit wait policy.
- Central water storage tank and wastewater regenerator are incorporated in the water network synthesis to target minimum freshwater consumption.
- Sequential and simultaneous methodologies are compared for the integrated problem of water allocation network synthesis and batch scheduling.
- A preliminary analysis for two-objective optimization is presented where revenue is maximized, and the total water cost is minimized simultaneously using the weighted-sum method.

3. Computational Results and Discussion

In order to demonstrate the performance of the proposed model, four case studies from the literature have been investigated. Case study 1 is used for comparison between the sequential and simultaneous methodologies, while case study 2 has been solved for determining the optimum WAN for multiple contaminants without considering the storage tank and regenerator. Case studies 3 and 4 have been solved for multiple contaminants by including the storage tank as well as the regenerator. All the case studies are solved using GAMS 23.9 software on a 32 GB RAM 3.10 GHz Intel Xeon processor using Linux operating system.

3.1. Case Study 1

This case study is referred to as BATCH1 in the literature [20]. The STN representation for this problem is given in Figure 4, where the first task is the heating task which is occurring in a heater. Three reaction tasks are suitable to take place in two reactors and one separator is used for the separation task, and the overall recipe produces two final products S8 and S9. After each reaction, the processing unit must be washed, which ensures the removal of any contaminants from the unit for further reactions. The presented case study is a single contaminant problem that is used to compare sequential versus simultaneous methodologies, and the impact of considering a central storage tank for each methodology is further investigated. Water reuse is allowed among the units and no accumulation of water is allowed in the central storage tank by the end of the complete time horizon.

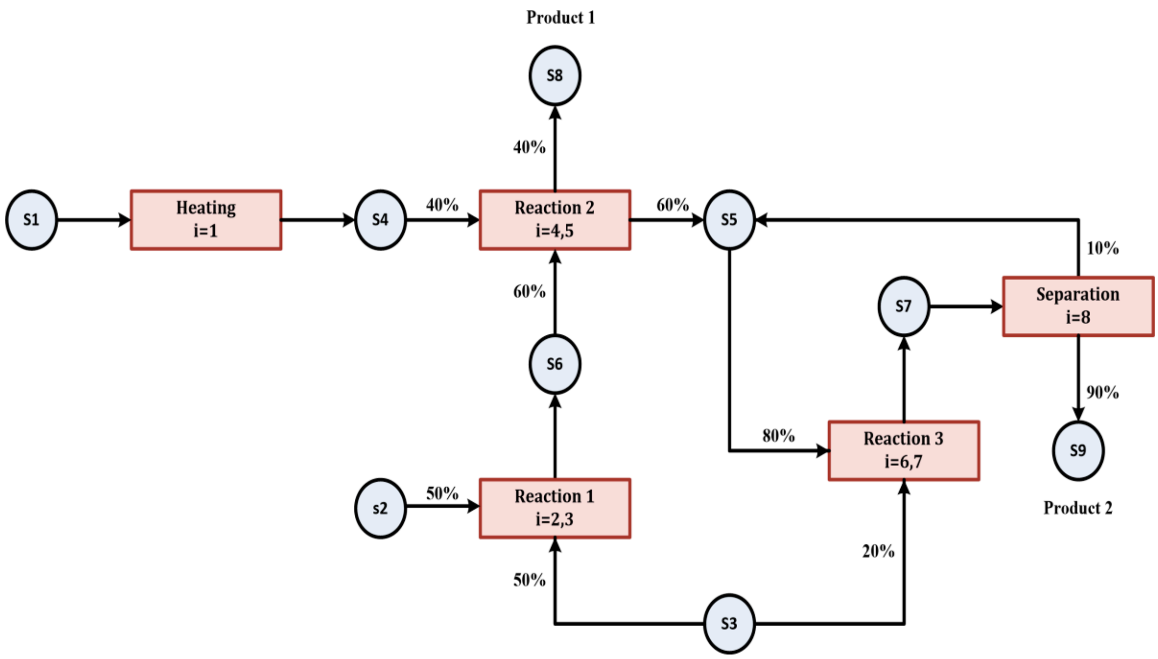

Figure 4. STN representation for case study 1.

The data related to the production scheduling and wastewater minimization has been taken from [21] as given in Appendix B. The cost of freshwater and effluent discharge has been considered as $1/t of water. It is to be noted that the cost of effluent discharge was not considered in the literature [21]. Further, the capacity of the water storage tank was not provided in the literature [21]. Hence, a central water storage tank of 100t capacity is considered in this work and the time horizon is taken as 8 h. The production scheduling data, storage capacities and washing data are given in Tables A1–A3 (in Appendix B).

In the sequential approach, the optimum production schedule is independently determined using five events as shown in Figure 5, followed by the solution of the WAN model for the obtained production schedule.

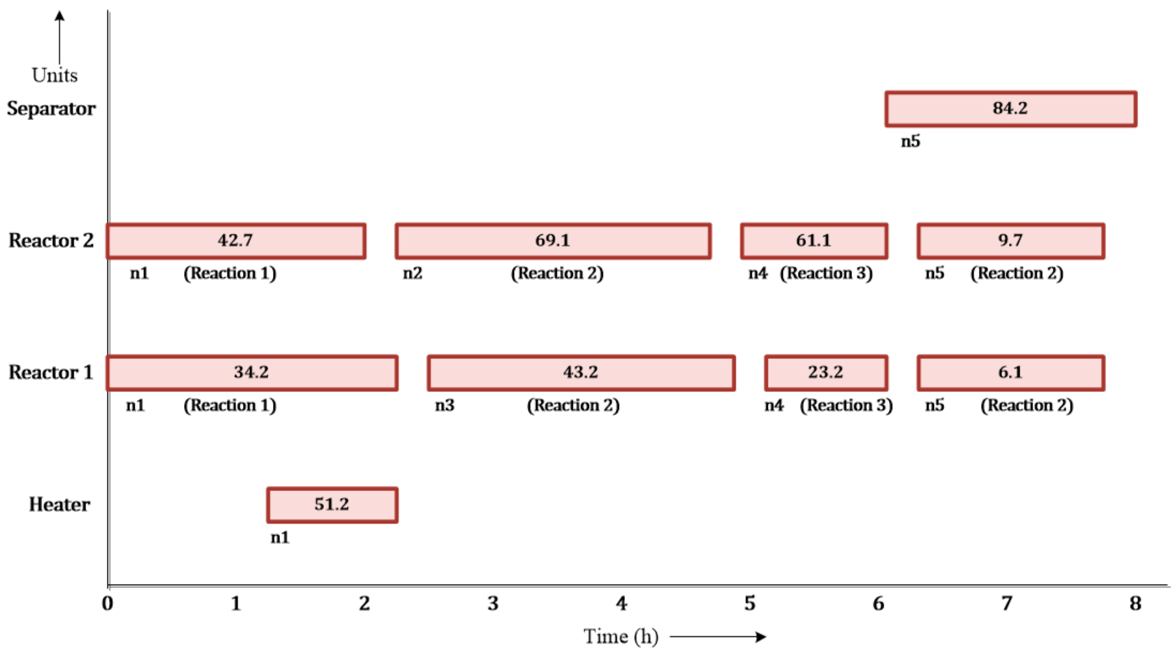

Figure 5. Production schedule obtained for the sequential approach.

By applying the WAN model on the fixed schedule shown in Figure 5, the total freshwater consumption determined is 370.392 t. Further, when the same WAN model is solved by including a central water storage tank, the resulting freshwater consumption is reduced to 341.176 t. Figures 6 and 7 represent the Gantt chart obtained for the above cases, where x- and y-axes represent time horizon and the processing units, respectively.

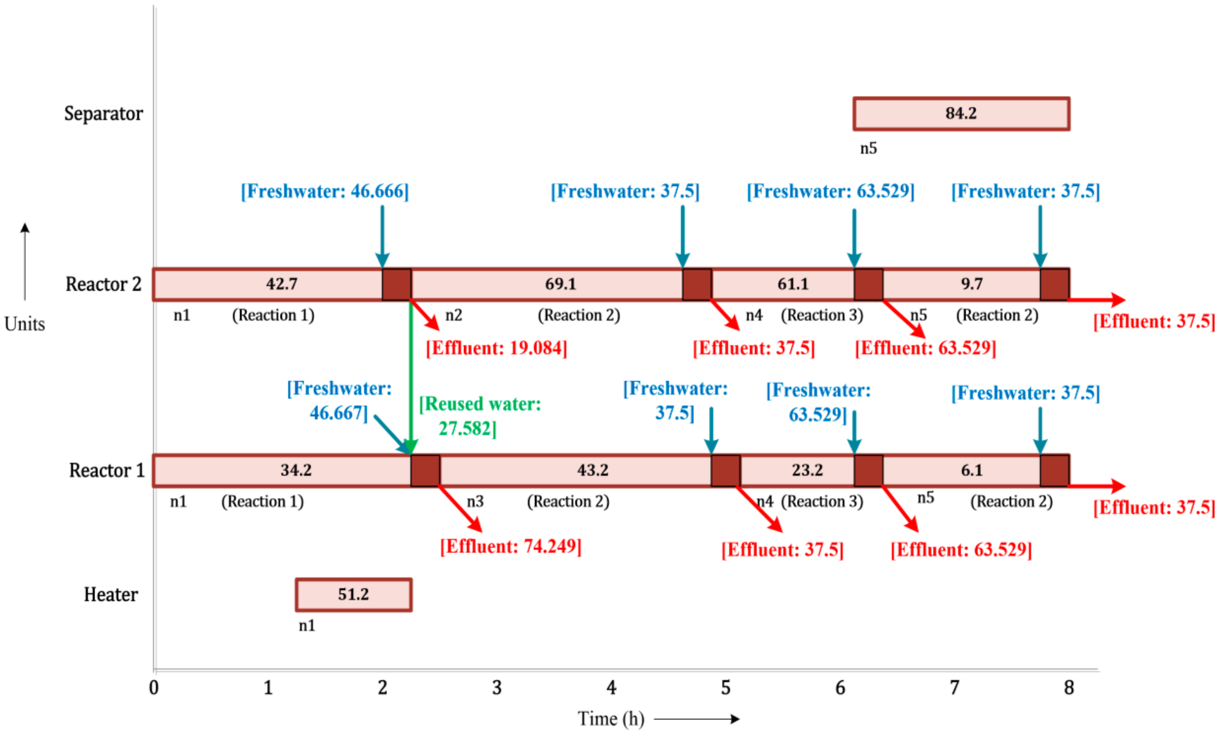

Figure 6. Gantt chart for the sequential approach without using water storage tank for case study 1.

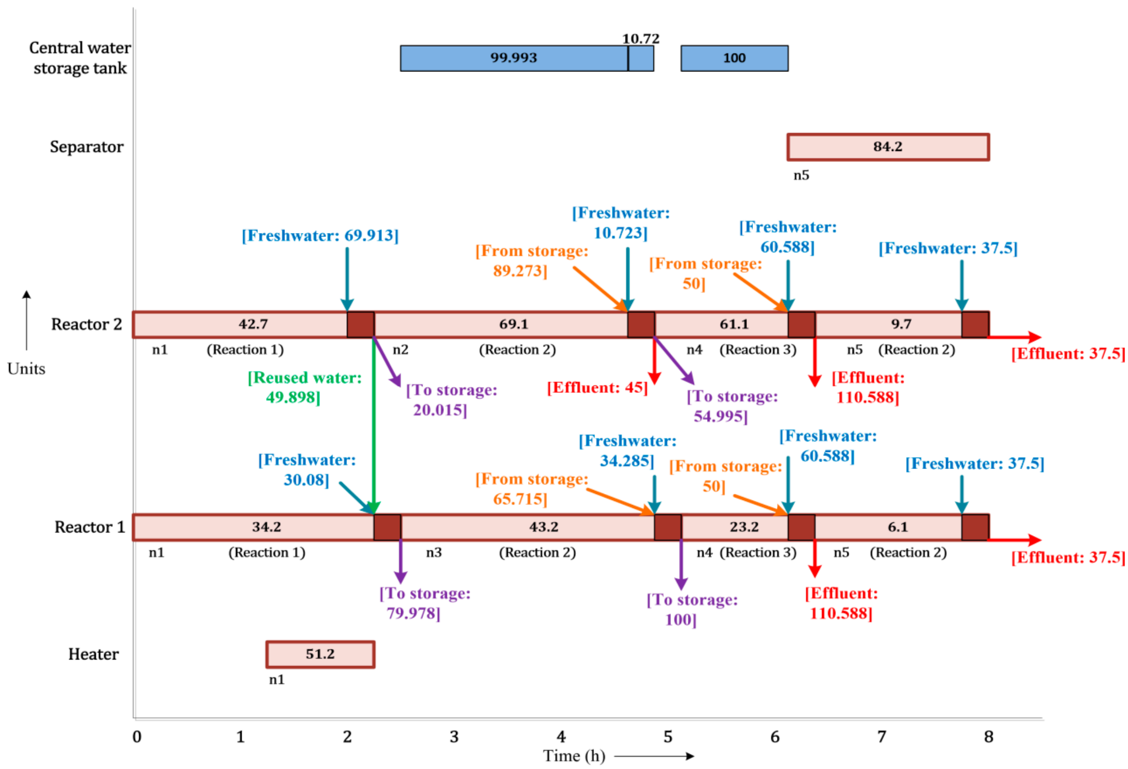

Figure 7. Gantt chart for the sequential approach using a water storage tank for case study 1.

In the depicted Gantt charts, the rectangular boxes represent the processing tasks in the units and the dark shaded boxes represent the washing operation in the processing unit after completion of the reaction. The numbers written inside the rectangular boxes indicate the amount of material processed in the unit. In Figures 6 and 7, reactor 1 is receiving reused water from reactor 2 at the end of event *n*1 because the finish time of washing in reactor 2 coincides with the start time of washing in reactor 1 at event *n*1. Figure 7 depicts reactor 1 using water from the storage tank along with the freshwater at the end of events *n*3 and *n*4, respectively. Similarly, reactor 2 is also using stored water along with some freshwater at the end of events *n*2 and *n*4, respectively. Hence, it can be concluded from the above Gantt charts that the central water storage tank contributes to reduction in the freshwater requirement in the washing units, as expected, by supplying the stored water for further reuse.

Simultaneous methodology optimizes production schedule and WAN simultaneously unlike the sequential methodology. The combined model of production scheduling and WAN results in a MINLP model, which is solved in GAMS software using SCIP solver. In this case, the total freshwater consumption obtained is 269.362 t when the water reuse opportunities are accommodated without a storage tank. However, the water usage is further reduced to 242.5 t when a central water storage tank of given capacity is included. Figures 8 and 9 represent the Gantt charts obtained for the simultaneous case without using a water storage tank and with use of a water storage tank, respectively.

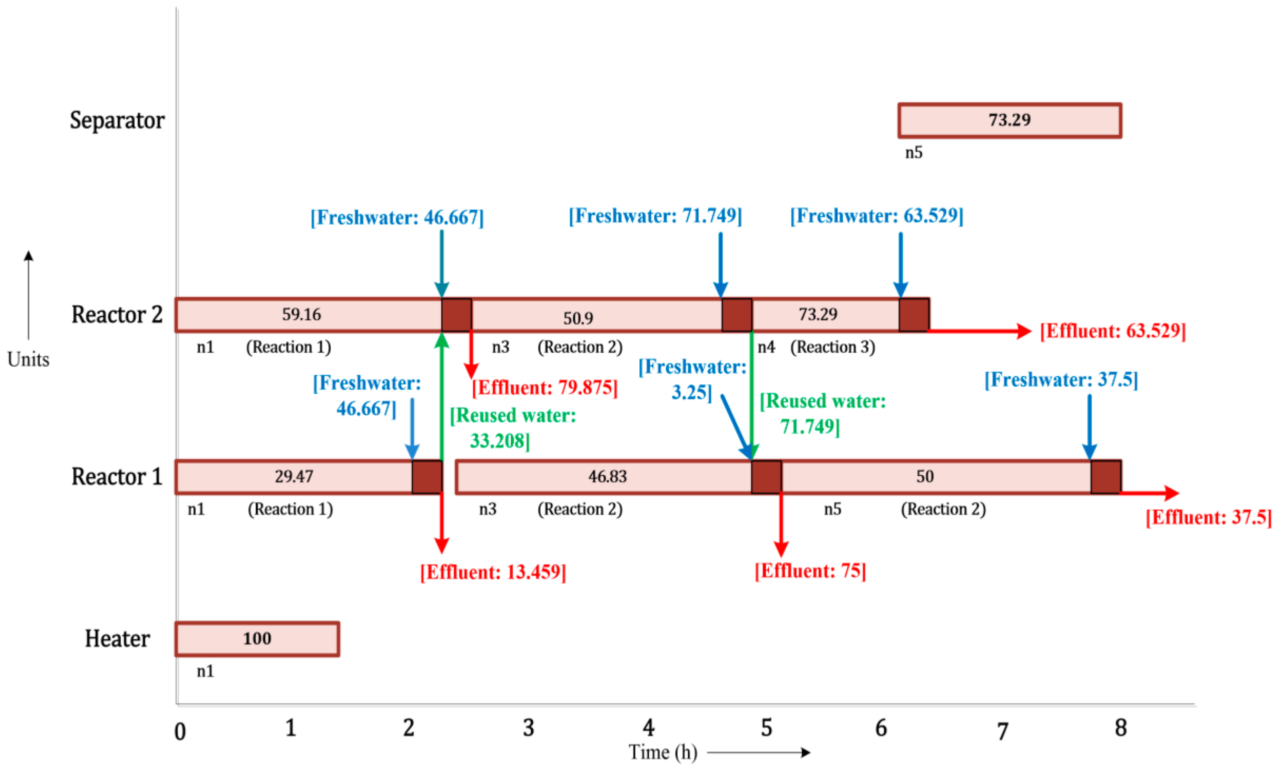

Figure 8. Gantt chart for the simultaneous approach without a water storage tank for case study 1.

From the Gantt chart in Figure 8, it is clearly seen that reactor 2 is receiving water from reactor 1 at the end of event *n*1, and reactor 1 is receiving water from reactor 2 at the end of event *n*3, which is enabled for direct re-use due to the alignment of start and finish times of washing operation in the respective units. On the other hand, from Figure 9 it can be observed that reactions 2 and 3 occurring in reactors 1 and 2 are re-using water from the central water storage facility along with freshwater at the end of events *n*3 and *n*4, respectively, which leads to a reduction in the total freshwater requirement.

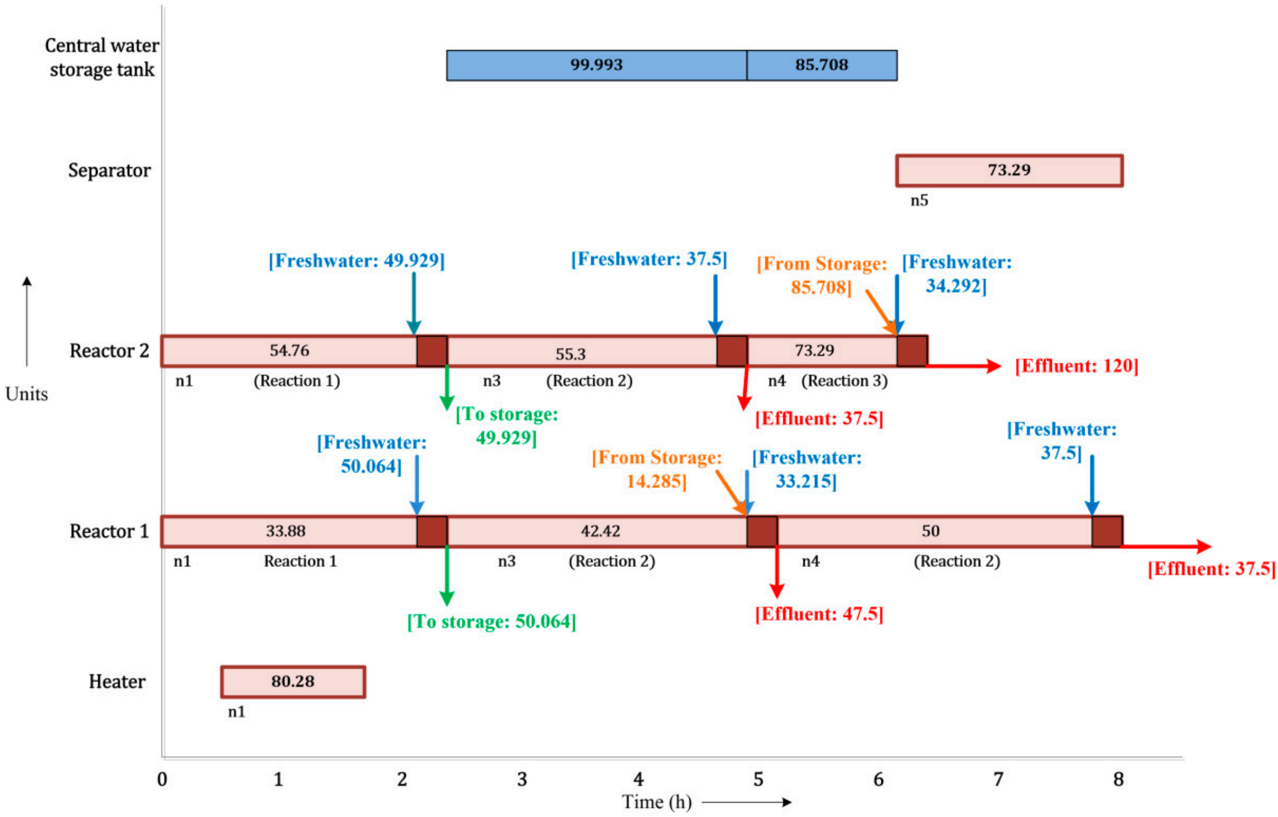

Figure 9. Gantt chart for the simultaneous approach with water storage tank for case study 1.

Hence, from the given case study 1, it can be concluded that the simultaneous methodology gives less freshwater consumption relative to the sequential methodology, as expected, since it optimizes both the production schedule and freshwater demand simultaneously. In addition, the inclusion of a central water storage tank offers a further reduction in freshwater consumption as it provides a temporary water storage option for improved re-use. Tables 1 and 2 provide a comparison of the results for the cases of without and with a storage tank for the sequential and simultaneous approaches, respectively. The net profit obtained when a central storage tank is used is higher compared to the net profit obtained when no storage tank is used, in both Tables 1 and 2. Similarly, the net profits obtained for the simultaneous approach in Table 2 are higher than those of for the sequential approach in Table 1 due to higher flexibility. The model statistics including the number of variables and constraints are higher when a central storage tank is used due to the relevant modeling of storage related issues.

Table 1. Results obtained for the sequential approach for case study 1.

	Without Central Storage Tank	With Central Storage Tank
Total freshwater (t)	370.392	341.176
Cost of fresh water and effluent ($)	740.784	682.42
Net profit ($)	529.644	588.076
Binary variables	180	234
Continuous variables	501	571
No. of constraints	1321	1390

Table 2. Results obtained for the simultaneous approach for case study 1.

	Without Central Storage Tank	With Central Storage Tank
Total freshwater (t)	269.362	242.5
Cost of fresh water and effluent ($)	538.724	485
Net profit ($)	711.798	765.522
Binary variables	250	310
Continuous variables	729	797
No. of constraints	1810	2419

3.2. Case Study 2

This case study from Majozi and Gouws [7] corresponds to a multiple contaminant problem with three contaminants over a time horizon of 10 h. The STN representation is the same as in the previous case study 1, and the production scheduling data, water requirement data, and contaminants related data are provided in Tables A4–A8 (in Appendix B). The objective of this case study is to maximize the net profit with minimum freshwater usage.

Case study 2 has been solved using the simultaneous approach for the case of not using a central water storage tank. The resulting MINLP problem is solved using SCIP solver in GAMS software. Figure 10 shows the resulting Gantt chart, where it can be observed that water is being re-used from reactor 2 to reactor 1 at the end of events $n1$ and $n3$, along with the freshwater.

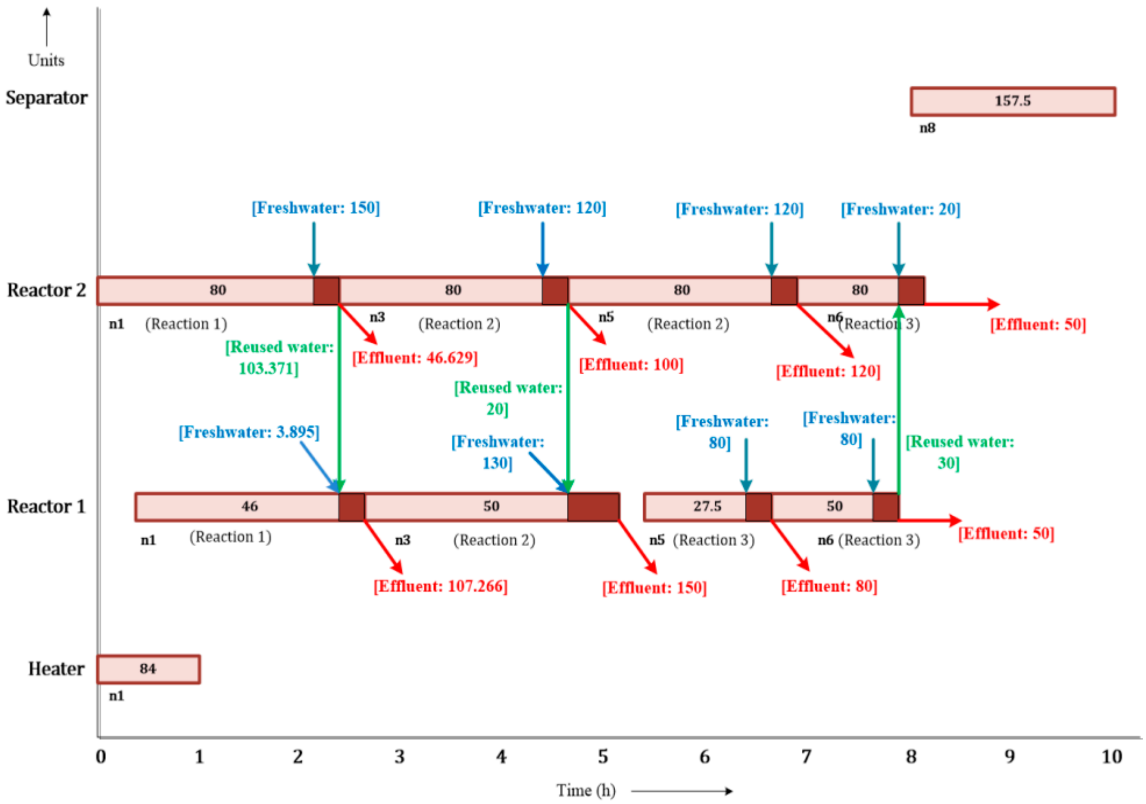

Figure 10. Gantt chart for the simultaneous approach for case study 2.

Similarly, the used water from reactor 1 is reused in reactor 2 at the end of event $n6$. However, the rest of the units are consuming only fresh water for washing purposes. The total profit for this MINLP problem turns out to be $19,055.524 with zero integrality gap. The corresponding total freshwater requirement is 703.9 kg approximately. Table 3 summarizes a comparison of the results obtained from the proposed work with the literature [7]. Although the reported objective value in the literature [7] is higher, there are some violations in their results as explained below.

Table 3. Comparison of results for case study 2 with the literature.

	Proposed Work	Majozi and Gouws [7]
Objective value ($)	19,055.524	21,187.5
Revenue from products ($)	22,575	24,800
Freshwater consumption (kg)	703.895	722.5
Total cost of freshwater and effluent ($)	3519.475	3612.5
Binary variables	3088	-
Continuous variables	5300	-
No. of Constraints	16,301	-

3.2.1. Limitations of the Literature Gantt Chart from Majozi and Gouws

Figure 11 shows the Gantt chart for case study 2 as reported in the literature [7], which has some limitations that directly affect the reported profit value. As per the information provided for the given case study, three reactions are suitable to occur in two reactors. Hence, it is obvious that no two reactions can take place in the same reactor at the same time. From the reported Gantt chart in Figure 11, it is evident that the total finish time of reaction 1 is 7.3 h (including washing operation time) in reactor 1, but reaction 2 started in the same reactor at 7.05 h. This violation is marked using a red colored oval shape in Figure 11. Similarly, the total finish time of reaction 3 is 5.8 h in reactor 2, but reaction 2 has already started at 4.8 h. Hence, it can be concluded that the reported results in [7] show more production with higher profit due to these violations.

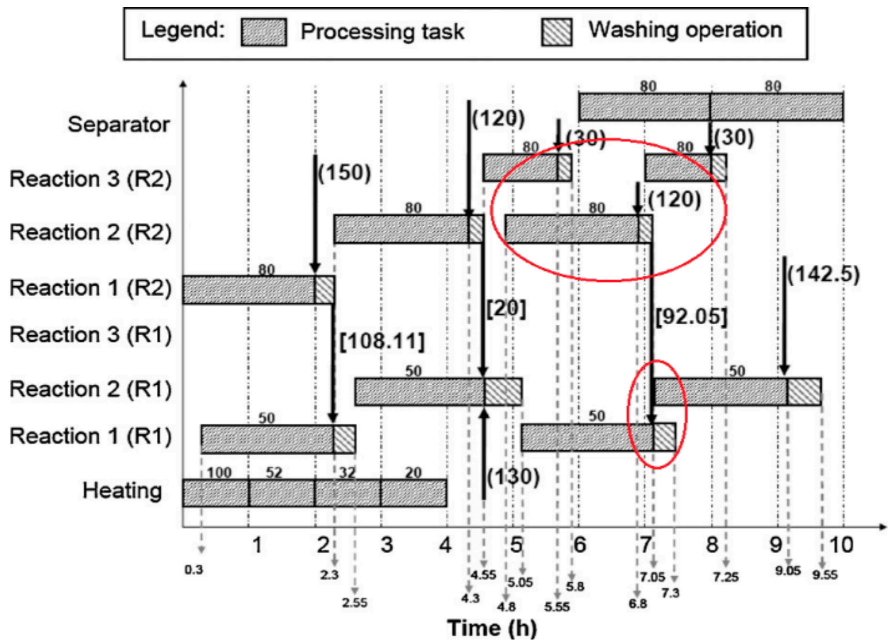

Figure 11. Reported Gantt chart from Majozi and Gouws [7] with overlapping time violation shown using red colored oval.

3.3. Case Study 3

This case study has been taken from Adekola and Majozi [11] with the same STN representation as in the previous two case studies. It is a multi-contaminant problem with three contaminants, and a central water storage tank of 200 kg capacity is used for temporary storage of the used water. A regeneration unit is also used to purify the contaminated water and this purified water is further used in other washing units. The regenerator flowrate is given as 100 kg/h and the time horizon considered for the case study is 10 h. The data for production scheduling and water requirement is the same as in case study 2, whereas the contaminant removal ratio is given in Table A9 (in Appendix B). The objective of the given problem is to maximize the net profit by incorporating minimum freshwater usage. The integrated production scheduling and WAN model is solved in GAMS software using SCIP solver with 0.09% integrality gap in the specified CPU time of 4 h.

First, the given problem is solved using a central water storage tank. The Gantt chart obtained along with the resulting water network is shown in Figure 12, where the units are using only freshwater for washing purposes in reactor 2, at the end of events $n1$, $n2$ and $n5$, while reaction 3 is using water only from the storage tank at the end of event $n7$.

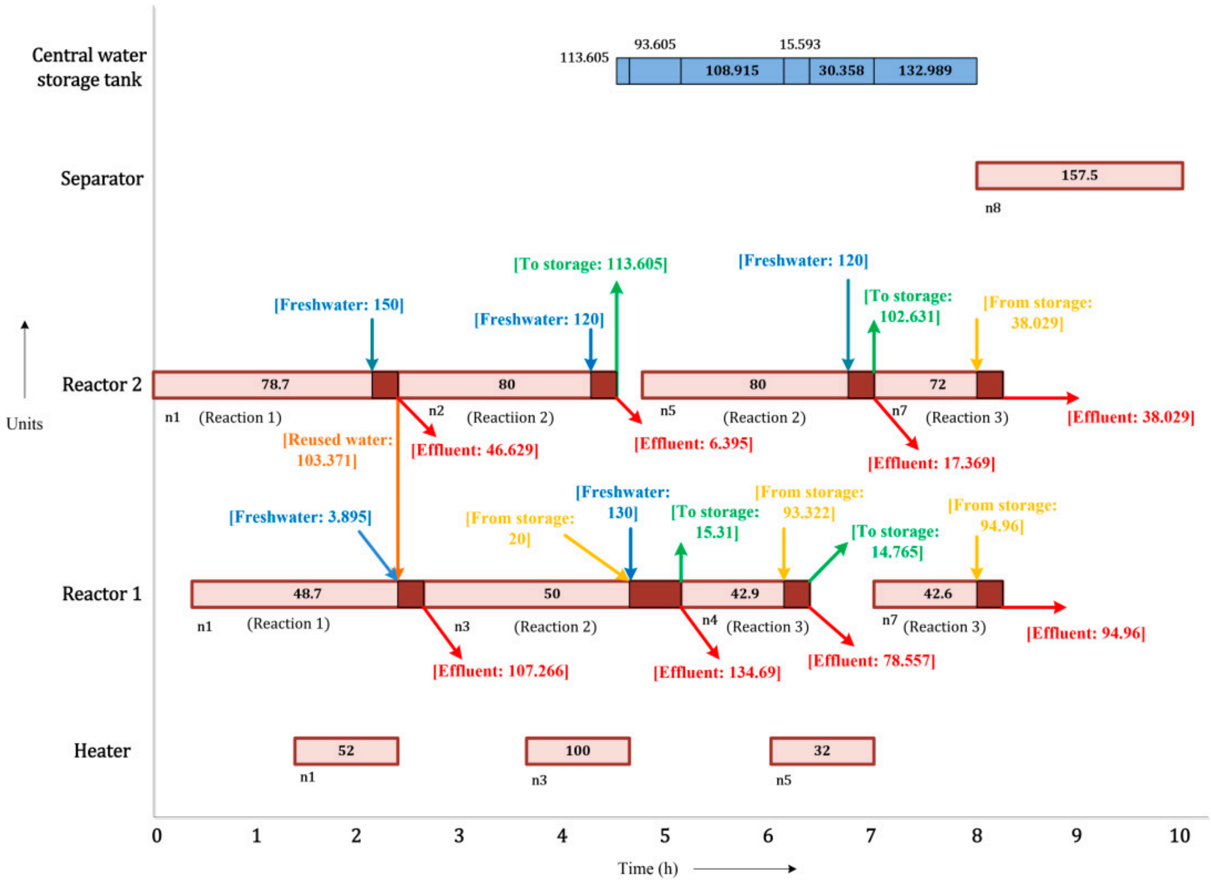

Figure 12. Gantt chart obtained for the simultaneous approach for case study 3 with water storage tank.

Further, there is a direct water reuse from reactor 2 to reactor 1 at the end of event $n1$. In reactor 1, reaction 2 uses water from the storage tank along with the freshwater at the end of event $n3$; however, at the end of events $n4$ and $n7$, reaction 3 uses water only from the central water storage tank. Thus, the Gantt chart indicates the significance of the use of the central water storage tank which decreases the requirement of freshwater, as expected. The optimum number of event points is eight for the obtained production schedule. The net profit is $19,955.524 and the freshwater consumption is approximately 524 kg while using the central water storage tank. The net profit obtained is $21,805.524 for the case when the water storage tank as well as the regenerator are used, which is higher than the net profit value obtained by using only the storage tank. The freshwater consumption in this case is 153.9 kg approximately.

Figure 13 represents the Gantt chart for WAN obtained by using the water storage tank and the regeneration unit, where the production schedule is the same as that of the previous case.

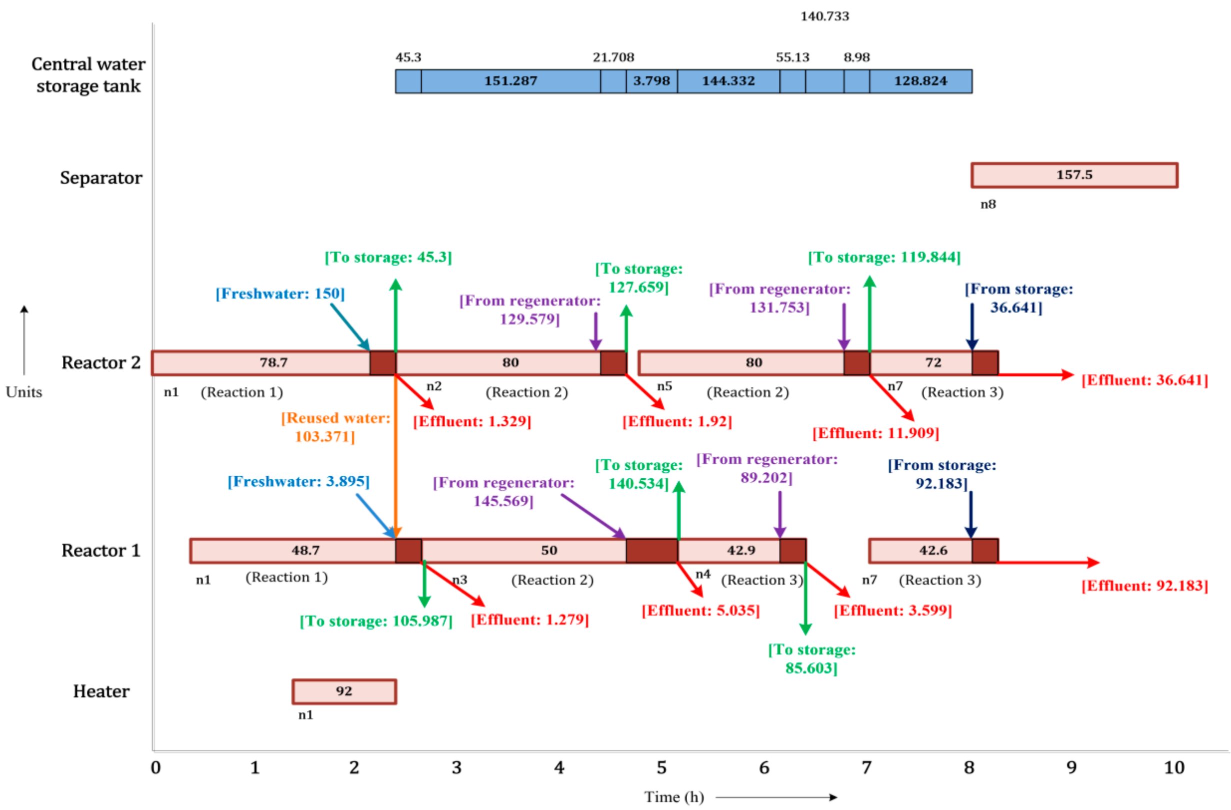

Figure 13. Gantt chart obtained for the simultaneous approach for case study 3 with water storage tank and regenerator.

From the Gantt chart, it can be observed that freshwater is being used among all the reactions in both the reactors, but only at the end of event $n1$; most of the washing tasks are using regenerated water, unlike in the previous case when the water storage tank was used without regeneration. Therefore, inclusion of the regenerator offers less freshwater requirement, as expected, which results in less effluent generation. A comparison of results with the literature [11] is shown in Table 4 for both cases, i.e., with and without regenerator. The literature [11] reported a higher objective value for the case when no regenerator is used, but there is a mass balance violation in their results as explained below.

Table 4. Comparison of results for case study 3.

	Using Storage Tank without a Regenerator		Using Storage Tank along with a Regenerator	
	Proposed Work	**Adekola and Majozi [11]**	**Proposed Work**	**Adekola and Majozi [11]**
Objective value ($)	19,955.524	20,180	21,805.524	21,129
Revenue from products ($)	22,575	22,575	22,575	23,137.5
Freshwater consumption (kg)	523.895	479	153.895	401.7
Total cost of freshwater and effluent ($)	2619.48	2395	769.475	2008.5
Binary variables	3906	-	4392	532
Continuous variables	6192	-	6528	-
No. of constraints	25,936	-	28,370	-

3.3.1. Limitations of the Literature Gantt Chart from Adekola and Majozi

Figure 14 shows the Gantt chart as reported in the literature [11] for case study 3, where there is a violation of mass balance of water around the water storage tank. From reactor 2, 150 kg of water is going to the storage tank at 2.25 h, and 145.5 kg of water is drawn out into the reactor 1 at time 4.25 h, thus 4.5 kg of water is left in the tank. But reactor 2 is using 7.5 kg of water from the storage tank at 4.5 h, which is clearly violating the mass balance. Similarly, it is violating the storage capacity of the water storage tank when it receives 265.5 kg (120 + 145.5) of water from reactors 1 and 2 at time 4.75 h, which is greater than the specified maximum capacity (200 kg) for the storage tank.

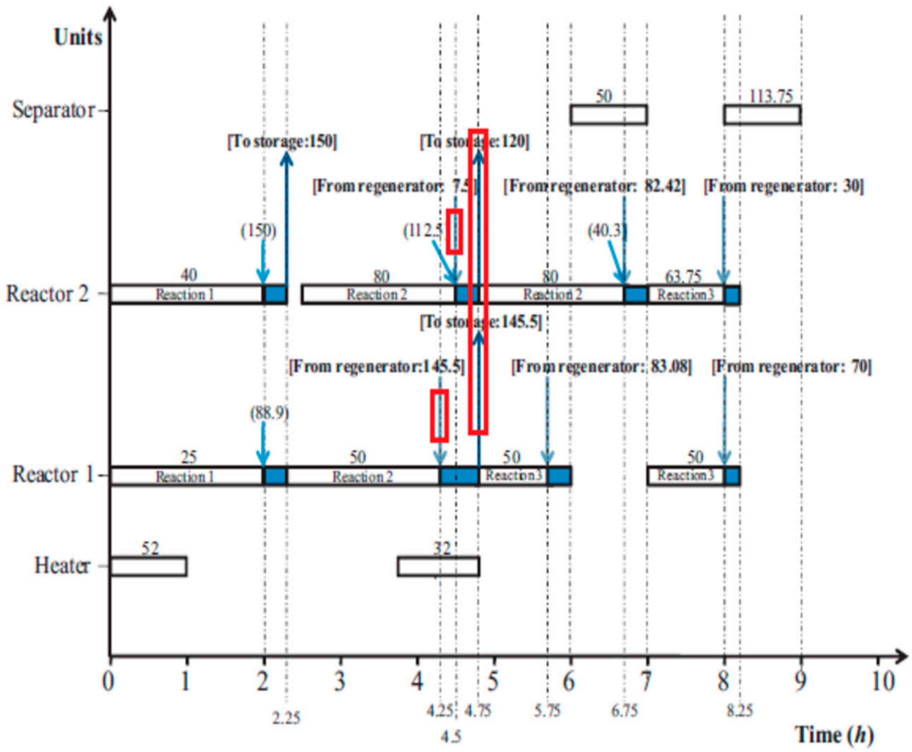

Figure 14. Reported Gantt chart from Adekola and Majozi [11] with mass balance violation shown in red box.

Additionally, when the storage tank is considered along with a regenerator, the separation unit time was taken as 1 h, while it was taken as 2 h for the case when the storage tank is used without a regenerator in the literature [11], which is inconsistent. Hence, the obtained freshwater consumption cannot be directly compared in these two cases due to different production schemes. In the original problem, the processing time was given as 1 h for the product and 2 h for the intermediate in the separation unit as shown in Table A4 (in Appendix B). In this study, the three-index finish time variable was introduced precisely to handle this issue; hence it gives an accurate result compared with the literature [11].

3.4. Case Study 4

This case study has also been taken from Adekola and Majozi [11] which comprises four pharmaceutical products suitable for production in four mixers. Each mixer is assigned to a specific product. Mixer 1 is dedicated to shampoos, mixer 2 is dedicated to deodorants, mixer 3 is dedicated to lotions and mixer 4 is dedicated to creams. Each mixer needs to be washed after performing the operation. There is adequate storage available for each product and the given time horizon is 24 h. The production and wastewater minimization related data are given in Tables A10–A13 (in Appendix B). The capacity of the central water storage tank is given as 10 t, and the washing time of each mixer is 30 min. To purify the contaminated water, a regeneration unit with a flowrate of 466 kg/h is included in the case study. The combined MINLP model of batch scheduling and WAN for freshwater minimization is solved using SCIP solver in GAMS with zero integrality gap. Figure 15 shows the Gantt chart obtained for the given case study. Freshwater consumption turns out to be 3206.735 kg when both central water storage tank and regenerator are included.

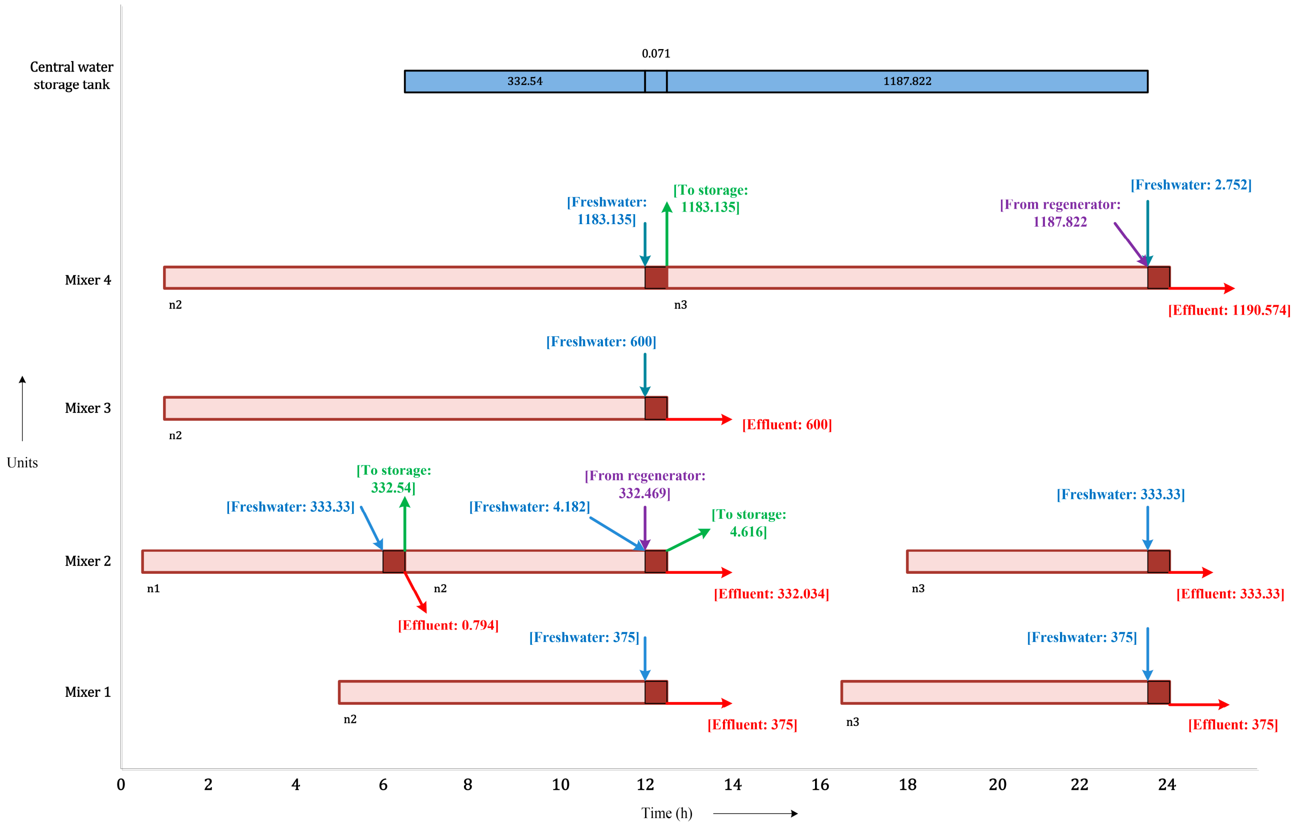

Figure 15. Gantt chart for the simultaneous approach for case study 4 with water storage tank and regenerator.

The literature [11] reported 2653 kg of freshwater requirement; however, a discrepancy has been observed in the contaminant concentration balance in the Gantt chart in the literature [11] as explained below.

3.4.1. Limitations of Literature Gantt Chart from Adekola and Majozi

Figure 16 depicts the Gantt chart as reported in Adekola and Majozi [11] for case study 4, which shows a violation of contaminant mass balance around the mixing units as shown with red colored ovals, when water is being used in other units, i.e., from mixer 1 to mixer 3 and from mixer 4 to mixers 2 and 1.

The contaminant concentration in the water entering the mixer is calculated as follows:

- Contaminant mass balance for water reuse from mixer 1 to mixer 3: $(375 + 225) \times C_{in} = 375 \times 0.04 + 225 \times 0$
- Hence, $C_{in} = 0.025$, which is greater than 0.014, the maximum allowed inlet concentration of shampoo in mixer 3.

Contaminant mass balance for water reuse from mixer 4 to mixer 2:

- $(114.4 + 218.9) \times C_{in} = 114.4 \times 0.06 + 218.9 \times 0$
- Hence, $C_{in} = 0.0205$, which is greater than 0.007, the maximum allowed inlet concentration of cream in mixer 2.
- Contaminant mass balance for water reuse from mixer 4 to mixer 1:
- $(105.9 + 269.1) \times C_{in} = 105.9 \times 0.06 + 269.1 \times 0$
- Hence, $C_{in} = 0.0169$, which is greater than 0.0035, the maximum allowed inlet concentration of cream in mixer 1.

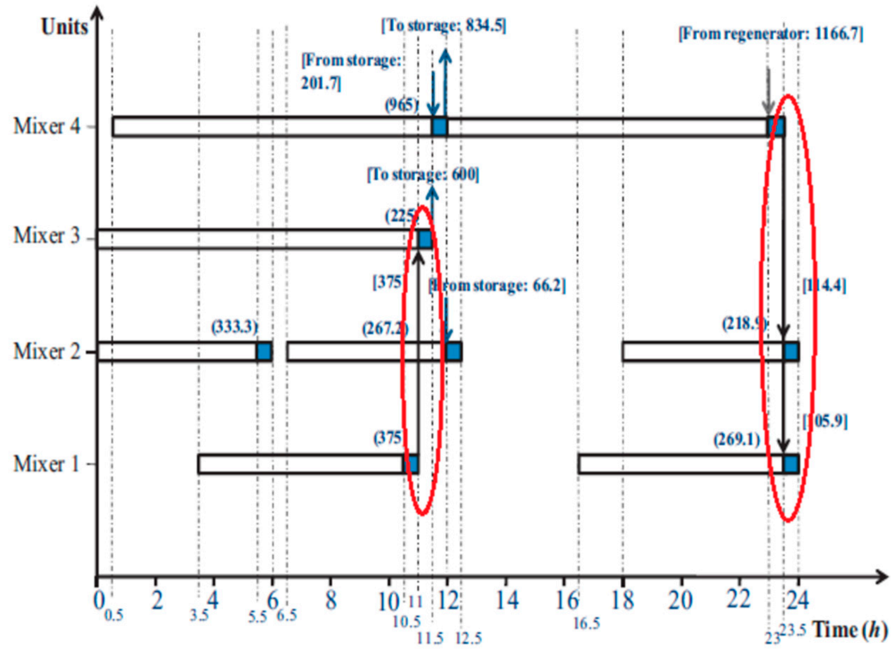

Figure 16. Reported Gantt chart for case study 4 from Adekola and Majozi [11] with contaminant mass balance violation shown in red colored oval.

Hence, from the above calculations it can be observed that the reported freshwater requirement in [11] is not accurate when compared to the results from the proposed work.

3.5. Two-Objective Optimization Using Weighted-Sum-Method

The combined model of production scheduling and water network simultaneously maximizes the product revenue and minimizes the freshwater and effluent cost. Since the objective function involves simultaneous optimization of two objectives, a preliminary Pareto optimal analysis is presented in this section. The Pareto set is generated using the weighted-sum method just for a quick initial analysis as the weighted-sum method does not guarantee generation of complete Pareto optimal front.

In Equation (75), weight w_1 is considered for the revenue term, and weight w_2 is considered for the cost of freshwater and effluent, as shown in Equation (76):

$$\begin{aligned} Max\ Obj. = w_1 \left\{ \sum_{s \in S^p} P_s \sum_{n=N} \left[ST(s,n) + \sum_{i \in I_s^P} \rho_{is} \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} b(i', n', n) \right] \right\} \\ -w_2 \left\{ CF \sum_{i \in I_R} \sum_{n \in N} mw_f(i,n) + CE \sum_{i \in I_R} \sum_{n \in N} mw_e(i,n) \right\} \end{aligned} \quad (76)$$

In a real process, the relative cost of freshwater is not significant compared to the revenue or expenses; however, from an environmental and sustainability perspective conservation of water is important. The range of weight factors w_1 and w_2 is taken as [0, 1] for each, and the Pareto graph for the two-objective optimization is generated by varying these weights with increments of 0.1 starting from $\{w_1, w_2\}$ = {0, 1} which effectively corresponds to the minimization of the single objective for the water network; this is followed by $\{w_1, w_2\}$ = {0.1, 0.9}, and so on up to $\{w_1, w_2\}$ = {1, 0}, which corresponds to the maximization of the single objective of revenue generation.

The obtained Pareto plots for the case studies 1, 2 and 3 are shown in Figure 17a–c, respectively. In case study 4, the only objective is to minimize the freshwater and effluent cost, hence it is not considered. Figure 17a,b depict that the total cost of freshwater and effluent increases as the product revenue increases. In Figure 17a, the extreme points for the total water cost are \$265 and \$1128.5 which are obtained using $\{w_1, w_2\} = \{0, 1\}$ and $\{w_1, w_2\} = \{1, 0\}$, respectively. Similarly, in Figure 17b, the corresponding extreme points are \$2100 and \$5737, respectively. The trend in Figure 17c is steeper for case study 3 relative to the plots (a) and (b). Here, the same water cost of \$769.48 is obtained for the combinations of $\{w_1, w_2\}$ with weight factors varying from $w_1 = 0.1$ to 0.3 and $w_2 = 0.9$ to 0.7. For the combination of $\{w_1, w_2\} = \{0, 1\}$, the water cost mentioned in Figure 17c is \$1015.87, which should have been less than the water cost obtained for $\{w_1, w_2\} = \{0.1, 0.9\}$ because of the decreasing value of product revenue. However, the same is not observed here due to non-convergence (69.3% integrality gap) of the weighted objective function in the reasonable CPU time of 24 h.

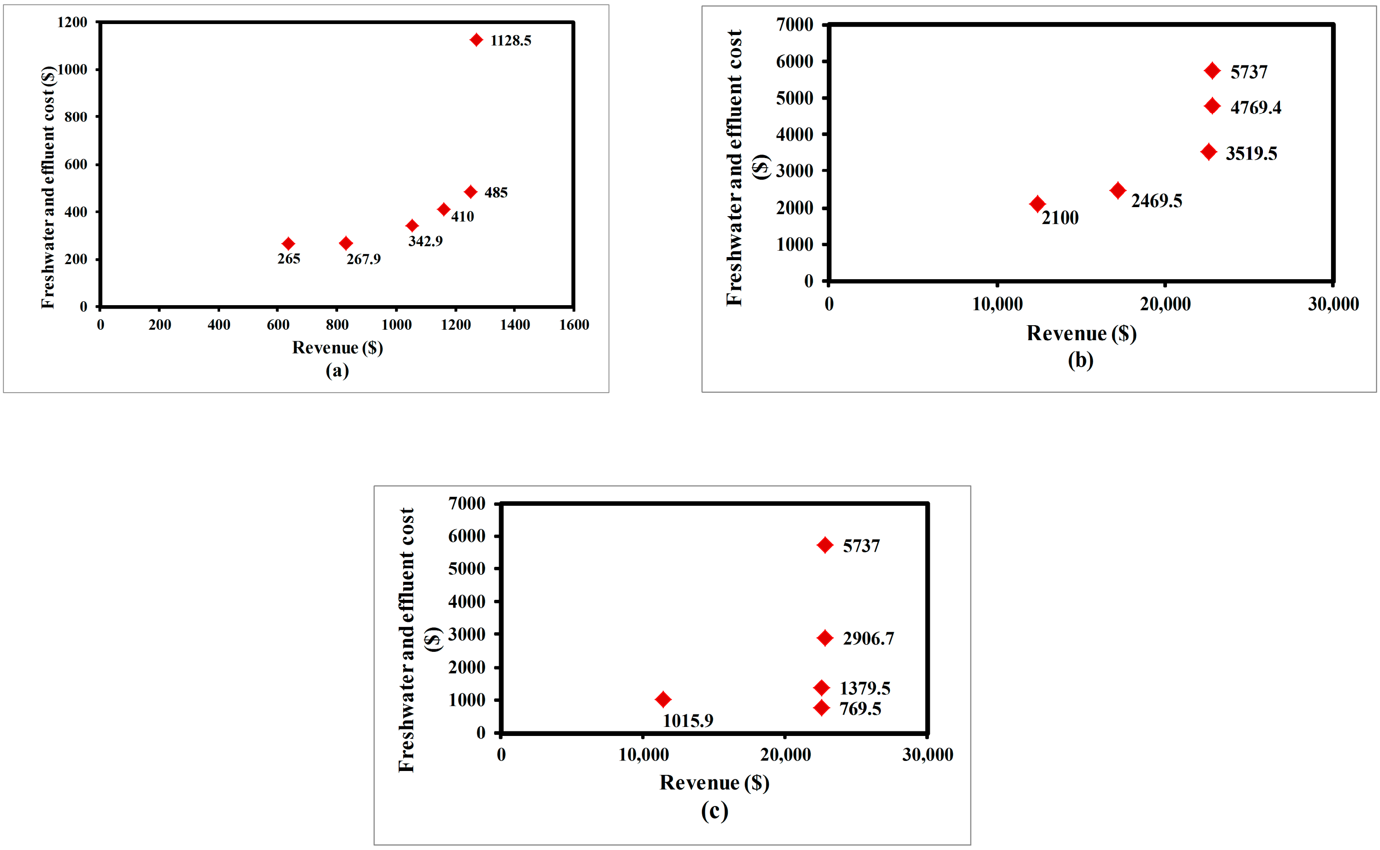

Figure 17. Pareto plots (**a**–**c**) for case studies 1, 2 and 3, for the two-objective optimization.

4. Conclusions

In this study, we consider the integrated problem of batch scheduling and water al-location network synthesis via sequential and simultaneous approaches. A unit-specific event-based model from the literature has been extended with several modifications including: introducing a three-index finish time variable to handle the case when different processing times exist for multiple states produced by a task, new constraints for avoiding real time storage violation when the same state is being produced and consumed in the same unit, modified sequencing constraints to handle the new definition of finish time of a task by combining the washing operation to occur at the same event after the task. The performance of the proposed integrated model is evaluated through four case studies from the literature. As expected, the simultaneous approach gives better savings in freshwater requirement and a higher net profit compared to the sequential approach, and so does the use of a central water storage tank and a regenerator. The proposed model gives better objective values in comparison to the reported values in the literature, i.e., net profit and freshwater minimization. This work also identified a few discrepancies in the reported Gantt charts from the literature. Further, a preliminary analysis for two-objective optimization is presented where revenue is maximized, and the total water cost is minimized simultaneously using the weighted-sum method. However, a detailed multi-objective optimization will be carried out in the future to generate comprehensive Pareto plots.

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Nomenclature

Indices:	
i, i'	tasks
j, j'	units
n, n'	events
s	states
c	contaminants
stt	storage tanks
Scheduling	
Sets:	
I	tasks
I_j	tasks that can be performed in unit j
I^{PC}	tasks that produce and consumes same state
J	units
N	total number of event points
S	states
S^{dfis}	intermediates states with dedicated finite intermediate storage
S^{PC}	states that are being produced and consumed in the same unit
C	contaminants species
Parameters	
B_i^{min}	minimum batch size of task i
B_i^{max}	maximum batch size of task i
α_{is}	fixed term of processing time of task i for state s
α_{is}^{l}	largest fixed term of processing time of task i for state s
β_{is}	variable term of the processing time of task i for state s
H	short-term scheduling horizon
P_s	price of state s
Δn	limit on the maximum number of events over which a task is allowed to continue
M	large positive number in big-M constraints
Binary Variables	
$w(i,n,n')$	binary variable for task i that starts at event n and ends at event n'
Positive Variables	
$T^s(i,n)$	start time of task i at event n
$T^f(i,n)$	finish time of task i at event n
$T^f(i,s,n)$	finish time of task i for state s at event n
Water Allocation Network	

Parameters	
CF	cost of fresh water
CE	cost of effluent water treatment
$M_{i,c}^{load}$	mass load of contaminant c added from task i to the water stream
Mw_i^U	maximum inlet water mass to task i
$C_{i,c}^{in,U}$	maximum inlet concentration of contaminant c for task i
$C_{i,c}^{out,U}$	maximum outlet concentration of contaminant c for task i
α_i^w	time required for washing after task i
Qw_s^0	initial amount of water in storage tank
Qw_s^U	maximum storage capacity of the tank
$Cs_c^{out,0}$	initial concentration of contaminant c in the storage vessel
RR_c	contaminant removal ratio
$freg$	regenerator flow rate
Binary Variables	
$yw(i,n)$	binary variable signifies the occurrence of washing task i at event n
$yw_r(i,i',n)$	binary variable shows the transfer of water from task i to task i' at event n
$ys_{in}(i,n)$	binary variable shows the transfer of water to the storage tank from task i at event n
$ys_{out}(i,n)$	binary variable shows the transfer of water from storage tank to task i at event n
$yreg_{in}(stt,n)$	binary variable shows the transfer of water from storage tank to regenerator at event n
$yreg_{out}(i,n)$	binary variable shows the transfer of water from the regenerator to task i at event n
Positive Variables	
$mw_{in}(i,n)$	mass of water consumed for washing unit for task i at the end of event n
$mw_{out}(i,n)$	mass of water exiting after washing unit for task i at the end of event n
$mw_f(i,n)$	mass of fresh water used for washing unit for task i at the end of event n
$mw_e(i,n)$	mass of effluent water produced after washing the unit for task i at the end of event n
$mw_r(i,i',n)$	mass of water recycled from task i to task i' at event n
$ms_{in}(i,n)$	mass of water to storage from task i at event n
$ms_{out}(i,n)$	mass of water coming from storage to task i at event n
$mreg_{in}(stt,n)$	mass of water coming to regenerator from storage at event n
$mreg_{out}(i,n)$	mass of water coming out from regenerator to task i at event n
$c_{in}(i,c,n)$	inlet concentration of contaminant c, entering task i at event n
$c_{out}(i,c,n)$	outlet concentration of contaminant c, exiting task i at event n
$cs_{in}(c,n)$	inlet concentration of contaminant c, entering storage at event n
$cs_{out}(c,n)$	outlet concentration of contaminant c, exiting from storage at event n
$creg_{out}(c,n)$	outlet concentration of contaminant c, exiting from regenerator at event n
$tw_{in}(i,n)$	inlet time of water used for task i, at event n
$tw_{out}(i,n)$	outlet time of water used for task i, at event n
$tw_r(i,i',n)$	water recycle time from task i to task i', at event n
$treg_{in}(stt,n)$	inlet time of water in regenerator from storage tank at event n
$treg_{out}(i,n)$	outlet time of water from regenerator to task i at event n

Appendix A

The production scheduling model of Vooradi and Shaik [19] is given here for ready reference.

Appendix A.1. Allocation Constraint

$$\sum_{i\in I_j}\ \sum_{\substack{n'\in N\\ n-\Delta n\le n'\le n}}\ \sum_{\substack{n''\in N\\ n\le n''\le n'+\Delta n}} w(i,n',n'') \le 1\ ,\ \forall j\in J,\ n\in N \tag{A1}$$

Appendix A.2. Capacity Constraint

$$B_i^{min} w(i,n,n') \le b(i,n,n') \le B_i^{max} w(i,n,n'), \forall i \in I, n, n' \in N, n \le n' \le n + \Delta n \tag{A2}$$

Appendix A.3. Material Balance

$$\begin{aligned} ST(s,n) = ST(s,n-1) + \sum_{i \in I_s^P} \rho_{is} \sum_{\substack{n' \in N \\ n-1-\Delta n \le n' \le n-1}} b(i,n',n-1) \\ + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} b(i,n,n'),\ \forall s \in S, n \in N, n > 1 \end{aligned} \tag{A3}$$

$$ST(s,n) = ST_o(s) + \sum_{i \in I_S^C} \rho_{is} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} b(i,n,n'), \forall s \in S^R, n \in N, n = 1 \tag{A4}$$

$$ST(s,n) = ST_0^s + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} b(i,n,n'), \forall s \in S^I, s \in S^P, n \in N, n = 1 \tag{A5}$$

Appendix A.4. Duration Constraint

$$T^f(i,n) = T^s(i,n) + \alpha_i w\ (i,n,n) + \beta_i(i,n,n), \forall\ i \in I,\ n \in N,\ \Delta n = 0 \tag{A6}$$

$$\begin{gathered} T^f(i,n') \ge T^s(i,n) + \alpha_i w(i,n,n') + \beta_i b(i,n,n'), \\ \forall i \in I, n, n' \in N, n \le n' \le n + \Delta n, \Delta n > 0 \end{gathered} \tag{A7}$$

$$\begin{gathered} T^f(i,n') \le T^s(i,n) + \alpha_i w(i,n,n') + \beta_i b(i,n,n') + M(1 - w(i,n,n')), \\ \forall i \in I, n, n' \in N, n \le n' \le n + \Delta n, \Delta n > 0 \end{gathered} \tag{A8}$$

Appendix A.5. Sequencing Constraint

Same Task in Same Unit

$$T^s(i,n+1) \ge T^f(i,n),\ \forall i \in I, n \in N, n < N \tag{A9}$$

$$\begin{gathered} T^s(i,n+1) \le T^f(i,n) + M\left(1 - \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} \sum_{\substack{n'' \in N \\ n \le n'' \le n'+\Delta n}} w(i,n',n'')\right), \\ \forall i \in I, n \in N, n\langle N, \Delta n\rangle \end{gathered} \tag{A10}$$

Different Tasks in Same Unit

$$T^s(i,n+1) \ge T^f(i',n),\ \forall i,i' \in I_j, i \ne i', j \in J_i, n < N \tag{A11}$$

Different Tasks in Different Units

$$T^s(i,n+1) \ge T^f(i',n) - M\left(1 - \sum_{\substack{n' \in N \\ n-\Delta n \le n' \le n}} w(i',n',n)\right), \tag{A12}$$

Appendix A.6. Tightening Constraint

$$\sum_{i \in I_j} \sum_{n \in N} \sum_{\substack{n' \in N \\ n \le n' \le n+\Delta n}} (\alpha_i w(i,n,n') + \beta_i b(i,n,n')) \le H,\ \forall j \in J \tag{A13}$$

Appendix A.7. Storage Constraint

$$T^f(i',n) \geq T^s(i,n) - M\left[1 - \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} w(i',n',n)\right],$$
$$\forall s^{dfis}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p \quad \text{(A14)}$$

$$T^s(i,n+1) \leq T^f(i',n) + M\left[2 - \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} w(i',n',n) - \sum_{\substack{n' \in N \\ n+1 \leq n' \leq n+1+\Delta n}} w(i,n+1,n')\right],$$
$$\forall s^{dfis}, j, j' \in J, n \in N, n < N, i \in I_j, i' \in I_{j'}, i \neq i', j \neq j', i \in I_s^c, i' \in I_s^p \quad \text{(A15)}$$

Appendix A.8. Bounds

$$w(i,n,n') = 0, \ \forall i \in I, n' < n \quad \text{(A16)}$$

$$b(i,n,n') = 0, \ \forall i \in I, n' < n \quad \text{(A17)}$$

$$T^s(i,n) \leq H, \ \forall i \in I, n \in N \quad \text{(A18)}$$

$$T^f(i,n) \leq H, \ \forall i \in I, n \in N \quad \text{(A19)}$$

$$ST(s,n) \leq ST_s^{max}, \forall s \in S^{dfis}, n \in N \quad \text{(A20)}$$

Appendix B

The data for the case studies are given here, which are taken from the literature [7,8,18].

Table A1. Input data for production scheduling for case study 1 [21].

Tasks	i	Unit (j)	α_i (h)	β_i (h/kg)	B_i^{min} (kg)	B_i^{max} (kg)
Heating	1	Heater	0.667	0.00667	0	100
Reaction 1	2	Reactor 1	1.334	0.02664	0	50
	3	Reactor 2	1.334	0.01665	0	80
Reaction 2	4	Reactor 1	1.334	0.02664	0	50
	5	Reactor 2	1.334	0.01665	0	80
Reaction 3	6	Reactor 1	0.667	0.01332	0	50
	7	Reactor 2	0.667	0.008325	0	80
Separation	8	Separator	1.3342	0.00666	0	200

Table A2. Storage limits and the selling price of various states for case study 1 [21].

State	Storage Capacities (kg)	Selling Price ($/kg)
S1	UL	NA
S2	UL	NA
S3	UL	NA
S4	100	NA
S5	200	NA
S6	150	NA
S7	200	NA
S8	UL	10
S9	UL	10

UL: unlimited; NA: Not applicable.

Table A3. Input data for washing of the reactor units for case study 1 [21].

Tasks	i	Unit (j)	Washing Time (h)	Max. Contaminant (ppm) Inlet	Max. Contaminant (ppm) Outlet	Max. Flow (t)
Heating	1	Heater	NA	NA	NA	NA
Reaction 1	2	Reactor 1	0.2	250	600	80
	3	Reactor 2	0.2	250	600	80
Reaction 2	4	Reactor 1	0.2	500	800	100
	5	Reactor 2	0.2	500	800	100
Reaction 3	6	Reactor 1	0.2	400	850	120
	7	Reactor 2	0.2	400	850	120
Separation	8	Separator	NA	NA	NA	NA

NA: Not applicable.

Table A4. Input data for production scheduling for case study 2 [7].

Tasks	i	Unit (j)	α_i (h)	B_i^{min} (kg)	B_i^{max} (kg)
Heating	1	Heater	1	0	100
Reaction 1	2	Reactor 1	2	0	50
	3	Reactor 2	2	0	80
Reaction 2	4	Reactor 1	2	0	50
	5	Reactor 2	2	0	80
Reaction 3	6	Reactor 1	1	0	50
	7	Reactor 2	1	0	80
Separation	8	Separator	1 for product 2 2 for int.AB	0	200

Table A5. Storage limits and the selling price of various states for case study 2 [7].

State	Storage Capacities (kg)	Selling Price (c.u./kg)
S1	UL	NA
S2	UL	NA
S3	UL	NA
S4	100	NA
S5	200	NA
S6	150	NA
S7	200	NA
S8	UL	100
S9	UL	100

UL: unlimited; NA: Not applicable.

Table A6. Input data for washing of the reactor units for case study 2 [7].

Task (Unit)		Max. Contaminant Concentration (g contaminant/kg water) Contaminant 1	Contaminant 2	Contaminant 3
Reaction 1 (Reactor 1)	Max inlet	0.5	0.5	2.3
	Max outlet	1	0.9	3
Reaction 2 (Reactor 1)	Max inlet	0.01	0.05	0.3
	Max outlet	0.2	0.1	1.2
Reaction 3 (Reactor 1)	Max inlet	0.15	0.2	0.35
	Max outlet	0.3	1	1.2
Reaction 1 (Reactor 2)	Max inlet	0.05	0.2	0.05
	Max outlet	0.1	1	12
Reaction 2 (Reactor 2)	Max inlet	0.03	0.1	0.2
	Max outlet	0.075	0.2	1
Reaction 3 (Reactor 2)	Max inlet	0.3	0.6	1.5
	Max outlet	2	1.5	2.5

Table A7. Mass loads of various contaminants for case study 2 [7].

Task (*i*)	Unit (*j*)	Mass Load (g) Contaminant 1	Contaminant 2	Contaminant 3
Reaction 1	Reactor 1	4	80	10
	Reactor 2	15	24	358
Reaction 2	Reactor 1	28.5	7.5	135
	Reactor 2	9	2	16
Reaction 3	Reactor 1	15	80	85
	Reactor 2	22.5	45	36.5

Table A8. Washing duration of various reactor units for case study 2 [7].

Unit/Task	Duration of Washing (h) Reaction 1	Reaction 2	Reaction 3
Reactor 1	0.25	0.5	0.25
Reactor 2	0.3	0.25	0.25

Table A9. Contaminant removal ratio for case study 3 [11].

Contaminants	Removal Ratio, (RR_c)
Contaminant 1	0.98
Contaminant 2	0.97
Contaminant 3	0.96

Table A10. Production data for case study 4 [11].

Mixer	Product	No. of Batches	Time (h)
1	Shampoo	2	7
2	Deodorant	3	5.5
3	Lotion	1	11
4	Cream	2	11

Table A11. Wastewater minimization data for case study 4 [11].

Mixer	Contaminant	Residue Mass (kg)	Limiting Water (kg)	Maximum Outlet Contaminant Concentration (kg/kg)
1	Shampoo	15	576.9	0.04
2	Deodorant	15	361.4	0.045
3	Lotion	30	697.6	0.05
4	Cream	70	1238.9	0.06

Table A12. Maximum allowed inlet contaminant concentration for case study 4 [11].

Mixer	Shampoo (kg product/kg water)	Deodorant (kg product/kg water)	Lotion (kg product/kg water)	Cream (kg product/kg water)
1	0.014	0	0.007	0.0035
2	0.014	0.0035	0.007	0.007
3	0.014	0	0.007	0.0035
4	0.014	0	0.007	0.0035

Table A13. Contaminant removal ratio for case study 4 [11].

Contaminant	Removal Ratio, (RR_c)
Shampoo	0.95
Deodorant	0.99
Lotion	0.96
Creams	0.98

References

1. Halim, I.; Srinivasan, R. Sequential methodology for integrated optimization of energy and water use during batch process scheduling. *Comput. Chem. Eng.* **2011**, *35*, 1575–1597. [CrossRef]
2. Ahmetovic, E.; Ibric, N.; Kravanja, Z.; Grossmann, I.E. Water and energy integration: A comprehensive literature review of non-isothermal water network synthesis. *Comput. Chem. Eng.* **2015**, *82*, 144–171. [CrossRef]
3. Majozi, T. Wastewater minimisation using central reusable water storage in batch plants. *Comput. Chem. Eng.* **2005**, *29*, 1631–1646. [CrossRef]
4. Cheng, K.F.; Chang, C.T. Integrated water network designs for batch processes. *Ind. Eng. Chem. Res.* **2007**, *46*, 1241–1253. [CrossRef]
5. Chen, C.L.; Lee, J.Y.; Tang, J.W.; Ciou, Y.J. Synthesis of water-using network with central reusable storage in batch processes. *Comput. Chem. Eng.* **2009**, *33*, 267–276. [CrossRef]
6. Gouws, J.F.; Majozi, T.; Gadalla, M. Flexible mass transfer model for water minimization in batch plants. *Chem. Eng. Process.* **2008**, *47*, 2323–2335. [CrossRef]
7. Majozi, T.; Gouws, J.F. A mathematical optimisation approach for wastewater minimisation in multipurpose batch plants: Multiple contaminants. *Comput. Chem. Eng.* **2009**, *33*, 1826–1840. [CrossRef]
8. Zhou, R.J.; Li, L.J.; Xiao, W.; Dong, H.G. Simultaneous optimization of batch process schedules and water-allocation network. *Comput. Chem. Eng.* **2009**, *33*, 1153–1168. [CrossRef]
9. Ierapetritou, M.G.; Floudas, C.A. Effective continuous-time formulation for short-term scheduling: 1. *Multipurpose batch processes, Ind. Eng. Chem. Res.* **1998**, *37*, 4341–4359. [CrossRef]
10. Li, L.J.; Zhou, R.J.; Dong, H.G. State-Time-Space Superstructure-Based MINLP Formulation for Batch Water-Allocation Network Design. *Ind. Eng. Chem. Res.* **2010**, *49*, 236–251. [CrossRef]
11. Adekola, O.; Majozi, T. Wastewater minimization in multipurpose batch plants with a regeneration unit: Multiple contaminants. *Comput. Chem. Eng.* **2011**, *35*, 2824–2836. [CrossRef]
12. Chaturvedi, N.D.; Manan, Z.A.; Alwi, S.R.W.; Bandyopadhyay, S. Effect of multiple water resources in a flexible-schedule batch water network. *J. Clean. Prod.* **2016**, *125*, 245–252. [CrossRef]
13. Li, Z.; Majozi, T. Optimal design of batch water network with a flexible scheduling framework. *Ind. Eng. Chem. Res.* **2019**, *58*, 9500–9511. [CrossRef]
14. Yang, F.; Fan, X.Y.; Jia, X.; Klemes, J.J.; Liu, Z.Y. An iterative design approach for water networks with multiple regeneration units. *J. Clean. Prod.* **2020**, *271*, 122483. [CrossRef]
15. Li, Z.; Majozi, T. Synthesis of flexible batch water networks using dynamic programming. *Ind. Eng. Chem. Res.* **2020**, *59*, 13175–13189. [CrossRef]
16. Chaturvedi, N.D.; Sinha, R.K. Simultaneous minimization of minimum resource and storage requirements in batch process. *Comput. Aided Chem. Eng.* **2021**, *50*, 1741–1746. [CrossRef]
17. Gouws, J.F.; Majozi, T. Usage of inherent storage for minimization of wastewater in multipurpose batch plants. *Chem. Eng. Sci.* **2009**, *64*, 3545–3554. [CrossRef]
18. Adekola, O.; Majozi, T. Wastewater minimization in batch plants with sequence dependent changeover. *Comput. Chem. Eng.* **2017**, *97*, 85–103. [CrossRef]
19. Vooradi, R.; Shaik, M.A. Improved three-index unit-specific event-based model for short-term scheduling of batch plants. *Comput. Chem. Eng.* **2012**, *43*, 148–172. [CrossRef]
20. Kondili, E.; Pantelides, C.C.; Sargent, R.W.H. A general algorithm for short-term Scheduling of batch operations-I. MILP formulation. *Comput. Chem. Eng.* **1993**, *17*, 211–227. [CrossRef]
21. Chaturvedi, N.D.; Bandyopadhyay, S. Optimization of multiple freshwater resources in a flexible schedule batch water network. *Ind. Eng. Chem. Res.* **2014**, *53*, 5996–6005. [CrossRef]