Optimization of energy and water use in multipurpose batch plants using an improved mathematical formulation

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Abstract

Presented in this contribution is a formulation that addresses optimization of both water and energy,while simultaneously optimizing the batch process schedule. The scheduling framework used in this study is based on the recent and efficient formulation. This formulation has been shown to result in a significant reduction of computational time, an improvement of the objective function and leads to fewer time points. The objective is to improve the profitability of the plant by minimizing wastewater generation and utility usage. From a case study it was found that through applying only water integration the cost is reduced by 11.6%, by applying only energy integration the cost is reduced by 29.1% and by applying both energy and water integration the cost is reduced by 34.6%. This indicates that optimizing water and energy integration in the same scheduling framework will reduce the operating cost and environmental impact significantly.

Keywords: Wastewater minimization, Energy integration, Heat storage, Multipurpose batch plant

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1. Introduction

In recent years, batch processes have been getting more attention due to their suitability for the production of small volume, high value added products. The flexibility of batch plants allows the production of different products within the same facility. Batch manufacturing is typically used in the pharmaceutical, polymer, food and specialty chemical industries as demands for such products are highly seasonal and are influenced by changing markets. A common feature of many batch plants is that they utilize fossil fuels as the energy source and use water for process equipment cleaning, due to inherent sharing of equipment by different tasks. Despite the advantage of batch plants being flexible, they also pose a challenging task to operate in a sustainable way. In the past, batch industries could tolerate high inefficiencies in energy and water consumption due to the high value of final products which outstrips the production costs. However, greater public awareness of the impact of industrial pollution, more stringent environmental regulations and escalating raw materials, energy, and waste treatment costs have now motivated energy and water saving measures for more sustainable operations (Halim and Srinivasan , 2011). Since scheduling, energy and wastewater minimization for multipurpose batch plants go hand in hand, published works in those areas are reviewed.

1.1. Scheduling of batch plants

Much research has been done on developing mathematical models to improve batch plant efficiency. The substantial advancement in modern computers allows the possibility of handling large and more complex problems by using optimization techniques. Excellent reviews of current scheduling techniques based on different time representations and associated challenges have been conducted (Méndez et al , 2006; Floudas and Lin , 2004; Shaik et al., 2006). In the reviews, with regard to time representation, the models are classified as slot based, event based and precedence based (sequence-based). In the slot based models, (Pinto and Grossmann , 1994; Lim and Karimi , 2003; Liu and Karimi , 2008) the time horizon is divided into nonuniform unknown slots and tasks start and finish in the same slot. On the other hand, slot models exist that use nonuniformun known slots where tasks are allowed to continue to the next slots (Schilling and Pantelides , 1996; Karimi and McDonald , 1997; Reddy et al. , 2004; Sundaramoorthy and Karimi , 2005; Erdirik-Dogan and Grossmann , 2008; Susarla et al. , 2010). The event based models can also be categorized into those that use uniformun known events, where the time associated with the events is common across all units, (Maravelias and Grossmann , 2003; Castro et al. , 2004) and those that use unit specific events where the time associated with the events can be different across the units (Ierapetritou and Floudas , 1998; Majozi and Zhu , 2001; Janak and Floudas , 2008; Shaik et al., 2006; Shaik and Floudas , 2009; Li et al. , 2010). The heterogeneous location of events across the units gives fewer event points as compared to both the global event based and slot based models. As a result, unit specific event based models are computationally superior. The sequence-based or precedence-based representation uses either direct precedence (Méndez and Cerdá , 2000; Hui and Gupta , 2000; Liu and Karimi , 2007) or indirect precedence sequencing of pairs of tasks in units (Méndez et al. , 2000, 2001; Méndez and Cerdá , 2003; Ferrer-Nadal et al , 2008). The models do not require pre-postulation of events and slots. Seid and Majozi (2012) presented a mixed integer linear programming (MILP) formulation based on the state sequence network and unit specific time points, which can handle proper sequencing of tasks and fixed intermediate storage (FIS) policy. The model results in a reduction of event or time points required and as a result, gives better performance in terms of objective value and CPU time required when compared to previous literature models.

1.2. Energy integration in batch plants

Many heat integration techniques are applied to predefined schedules which are inherently suboptimal. Vaklieva-Bancheva et al. (1996) considered direct heat integration with the objective of minimizing total costs. The resulting overall formulation was an MILP problem, solved to global optimality, although only specific pairs of units were allowed to undergo heat integration. Uhlenbruck et al. (2000) improved OMNIUM, which is a tool developed for heat exchanger network synthesis by Hellwig and Thne (1994). The improved OM-

NIUM tool increased the energy recovery by 20%. Bozan et al. (2001) developed a single step, interactive computer program (BatcHEN) used for the determination of the campaigns i.e. the set of products which can be produced simultaneously, the heat exchange areas of all possible heat exchangers in the campaigns and the heat exchanger network. This work addressed the limitation of the graph theory method for the determination of the campaign by Bancheva et al. (1996). Krummenacher and Favrat (2001) proposed a new systematic procedure, supported by graphics, which made it possible to determine the minimum number of heat storage units. Chew et al. (2005) applied cascade analysis proposed by Kemp and Macdonald (1987) to reduce the utility requirement for the production of oleic acid from palm olein using immobilized lipase. The result obtained showed savings of 71.4% and 62.5% for hot and cold utilities respectively. Pires et al. (2003) developed the BatchHeat software, whose aim was to highlight the energy inefficiencies in the process and thereby enabling the scope for possible heat recovery to be established through direct heat exchange or storage through implementation of cascade analysis.

Boer et al. (2006) evaluated the technical and economic feasibility of an industrial heat storage system for an existing production facility of organic surfactants. Fritzson and Berntsson (2006) applied process integration methods to investigate the potential to decrease the energy usage in the slaughtering and meat processing industry. The result obtained illustrates that 30% of the external heat demand and more than 10% of the shaftwork used can be saved. Morrison et al. (2007) developed a user friendly software package known as optimal batch integration (OBI). Chen and Ciou (2008) formulated a method to design an optimization of indirect energy storage systems for batch process. Their work aimed at simultaneously solving the problem of indirect heat exchange network synthesis and its associated thermal storage policy for recirculated hot/cold heat storage medium (HEN). Most of the previous works solved this sequentially. Foo et al. (2008) extended the minimum units targeting and network evolution techniques that were developed for batch mass exchange network (MEN) into batch HEN. They applied the technique for energy integration of oleic acid production from palm olein using immobilized lipase. Halim and Srinivasan (2009) discussed a sequential method using direct heat integration. A number of optimal schedules with minimum makespan were found, and heat integration analysis was performed on each. The schedule with minimum utility requirement was chosen as the best. Later, Halim and Srinivasan (2011) extended their technique to carry out water reuse network synthesis simultaneously. One key feature of this method is its ability to find the heat integration and water reuse solution without sacrificing the quality of the scheduling solution.

Atkins et al. (2010) applied indirect heat integration using heat storage for a milk powder plant in New Zealand. The traditional composite curves have been used to estimate the maximum heat recovery and to determine the optimal temperatures of the stratified tank. Tokos et al. (2010) applied a batch heat integration technique to a large beverage plant. The opportunities of heat integration between batch operations were analyzed by a mixed integer linear programming (MILP) model, which was slightly modified by considering specific industrial circumstances. Muster-Slawitsch et al. (2011) came up with the Green Brewery concept to demonstrate the potential for reducing thermal energy consumption in breweries. Three detailed case studies where investigated. The Green Brewery concept has shown a saving potential of over 5000 t/y fossil CO_2 emissions from thermal energy supply for the 3 breweries that were closely considered. Becker et al. (2012) applied time average energy integration approach to a real case study of a cheese factory with non-simultaneous process operations. Their work addressed appropriate heat pump integration. A cost saving of more than 40% was reported.

For a more optimal solution, scheduling and heat integration may be combined into an overall problem. Papageorgiou et al. (1994) embedded a heat integration model within the scheduling formulation of Kondili et al. (1993). Opportunities for both direct and indirect heat integration were considered as well as possible heat losses from a heat storage tank. The operating policy, in terms of heat integrated or standalone, was predefined for tasks. Adonyi et al. (2003) used the S-Graph scheduling approach and incorporated one to one direct heat integration. Barbosa-Póvoa et al. (2001) presented a mathematical formulation for the detailed design of multipurpose batch process facilities with heat integration. Pinto et al. (2003) extended the work of Barbosa-Póvoa et al. (2001) with the consideration of the economic savings in utility requirements, while considering both the cost of the auxiliary structures i.e. heat-exchanger through their transfer area and the design of the utility circuits and associated piping costs. Majozi (2006) presented a direct heat integration formulation based on the state sequence network of Majozi and Zhu (2001) which uses an unevenly discretized time horizon. The direct heat integration model developed by Majozi (2006) was extended to incorporate heat storage for more flexible schedules and utility savings in the later work by Majozi (2009). However, the storage size is a parameter in his formulation which is addressed later by Stamp and Majozi (2011), where the storage size is determined by the optimization exercise. Chen and Chang (2009) extended the work of Majozi (2006) to periodic scheduling, based on the resource task network (RTN) scheduling frame work. The reader can get a more comprehensive and detail review on energy recovery for batch processes in the paper by Fernández et al. (2012).

1.3. Wastewater minimization in batch plants

Wastewater is generated in batch plants during cleaning of multipurpose equipment and when water is used as a solvent. Tight environmental regulations and increased public awareness demand that batch plants consider rational use of water during their operation. Many researchers have developed methodologies for the efficient use of water through direct reuse, indirect reuse and regeneration of wastewater. Direct reuse consists of recycle and reuse. Recycle refers to the reuse of an outlet wastewater stream from a processing unit in the same unit, while reuse refers to the use of an outlet wastewater stream from a processing unit in another processing unit. Indirect reuse is when wastewater is temporarily stored in a storage vessel and later reused in a processing unit requiring water.

Based on the analogy of heat and mass transfer, several methodologies for synthesizing water reuse network in batch processes have also been developed. Gouws et al. (2010) reviewed these techniques based on graphical-based pinch analysis and mathematical optimization approach. The seminal work on pinch analysis application to batch water network was reported by Wang and Smith (1994). Foo et al. (2005) proposed a time-dependent water cascade analysis to obtain minimum required water flows in a process. While these graphical-based techniques are useful, they share a common drawback is that their application is limited to single contaminant cases. The mathematical optimization-based techniques, which are capable of solving multiple contaminant problems, can be differentiated into two groups, namely, those based on the schedule being known a priori i.e. sequential approach and those that simultaneously determine the process schedule and minimize the freshwater usage.

Almató et al. (1997) addressed the problem of water reuse through storage tank allocation based on the optimal schedule being known a priori. Kim and Smith (2004) proposed a more generalized method for optimal design of discontinuous water reuse network. In their approach, a production schedule was fixed and direct reuse of water between operations within the same time interval was allowed without passing through storage tanks. Most of the mathematically based models are based on a superstructure approach. Majozi and Gouws (2009) proposed a continuous-time scheduling framework to simultaneously optimize the schedule and water reuse while addressing both single and multiple contaminants. Cheng and Chang (2007) considered the optimization of the batch production schedule, water reuse schedule and wastewater treatment schedule in a single problem based on discrete time scheduling framework. At the end of optimization, the production schedule, the number and sizes of buffer tanks and the physical configuration of the pipeline network were obtained. Adekola and Majozi (2011) extended the work of Majozi and Gouws (2009) by incorporating wastewater regenerator for further improvement of water utilization.

From the review it can be seen that wastewater minimization and heat integration in batch plants are addressed separately. To the knowledge of the authors the only work presented by Halim and Srinivasan (2011) and Adekola et al. (2013) addressed this literature gap. In the work of Halim and Srinivasan (2011) the overall problem is decomposed into three parts viz. scheduling, heat integration and water reuse optimization and solved sequentially. Batch scheduling is solved first to meet an economic objective function. Next, alternate schedules are generated through a stochastic search based integer cut procedure. For each resulting schedule, minimum energy and water reuse targets are established and networks identified which might lead to suboptimal results. Adekola et al. (2013) also addressed this problem by developing a model that simultaneously optimize energy, water and production throughput. They demonstrated that the unified approach where all resources are optimized simultaneously give a better economic performance compared to the common sequential techniques for wastewater and energy integration techniques developed for multipurpose batch plants. However, the model has two basic limitations. The first drawback is the model is not based on TAM (time average model) and treats the temperature driving force based on initial and target temperatures of cold and hot streams. This assumption makes the model impossible to apply for a case where the starting and finishing time of the heat integrated units to be anywhere between the starting and finishing time of the processing tasks since it is required to calculate the intermediate temperatures to ensure for the minimum thermal driving force. The second limitation is it forces the heat integrating units to start simultaneously which results suboptimal because of restricting the flexibility of the schedule.

In this paper a contribution is made to close the literature gap by simultaneously solving energy integration and wastewater minimization problem in the same scheduling framework. The model is based on TAM and time slice model (TSM) where the time slice is a variable determined by optimization to keep the flexibility of the schedule as compared to previous models based on fixed schedule and fixed time slice for heat integration. The model also addressed the two basic limitations as discussed above in the model of Adekola et al. (2013). Additionally, the proposed model used the resent robust scheduling framework of Seid and Majozi (2012) as a plat form since the model gave better objective value as compared to previous literature models. The rest of the paper is organized as follows. Section 2 defines the problem statement. Section 3 describes the detail mathematical formulation. Section 4 describes the application of the mathematical model to literature problems. Finally conclusions are drawn from this work in Section 5.

2. Problem statement

2.1. Given

(i) The production recipe (STN or SSN representation).

(ii) The capacity of units and the type of tasks each unit can perform.

(iii) The maximum storage capacity for each material.

(iv) The task processing times.

(v) Hot duties for tasks require heating and cold duties for tasks that require cooling.

(vi) Operating temperatures of heat sources and heat sinks.

(vii) Minimum allowable temperature differences.

(viii) The material heat capacities.

(ix) The units washing time.

(x) The mass load of each contaminant.

(xi) The concentration limits of each contaminant.

(xii) The costs of raw materials, products and utilities.

(xiii) The scheduling time horizon (for profit maximization problem).

(xiv) Production demand (for makespan minimization problem).

2.2. Determine

(a) The optimum production schedule, i.e. allocation of tasks to units, timing of all tasks, and batch sizes.

(b) Optimum energy requirement and associated heat exchange configuration.

(c) Optimum water requirement and associated water-reuse network.

3. Mathematical formulation

The scheduling model by Seid and Majozi (2012) was adopted as a scheduling platform since it has proven to result in better CPU time and optimal objective value compared to other scheduling models. Uneven discretization of the time horizon so called continuous time was used.

3.1. Heat integration model

The mathematical model is based on the superstructure in Figure 1. Each task may operate using either direct or standalone mode by using only external utilities. If direct integration is not sufficient to satisfy the required duty, external utilities may make up for any deficit.

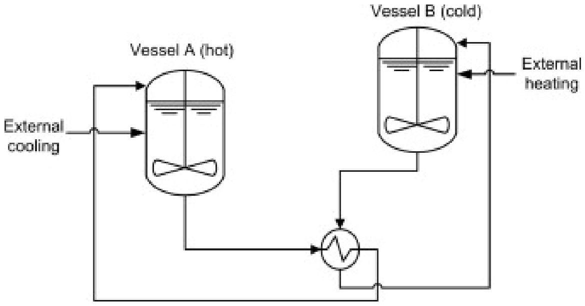

Figure 1: Superstructure for the energy integration.

$$\sum_{s_{inj_c}} x(s_{inj_c}, s_{inj_h}, p, pp) \leq y(s_{inj_h}, p),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (1)$$

$$\sum_{s_{inj_h}} x(s_{inj_c}, s_{inj_h}, p, pp) \leq y(s_{inj_c}, p),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (2)$$

Constraints (3.1) and (3.1) are active simultaneously and ensure that one hot unit will be integrated with one cold unit when direct heat integration takes place, in order to simplify operation of the process. It is worth noting that, mathematically it is also possible for one unit to integrate with more than one unit at a given time point when the summation notation is not used. However, this is practically very difficult to implement. Also, if two units are to be heat integrated at a given time point, they must both be active at that time point. For better understanding, the difference between time point p and extended time point pp is explained using Figure 2. If a unit j that is active at time point p is integrated with more than one unit in different temperature and time intervals, an extended time point pp must be defined. Unit $j1$ active at time point p can be integrated with units $j2$ and $j3$ in different time and temperature intervals. At the beginning, unit $j1$ is integrated with unit $j2$ at time point p and the extended time point pp is the same as time point p. Later $j1$ is integrated with unit $j3$ in another time interval where extended time point pp equals to $p+1$. pp is equal to or greater than time point p and less than or equal to $n+p$, where n is a parameter which is greater than or equal to zero. If n equals 2 then a unit that is active at time point p can be integrated in three different intervals. The model should be solved starting from n equals zero and adding one at a time until no better objective value is achieved.

Constraint 3.1 describes the amount of cooling load required by the hot unit from its initial temperature to its target temperature. In a situation where the temperature in the reactor unit is fixed during exothermic reaction, the heat load becomes the product of the amount of mass that under-

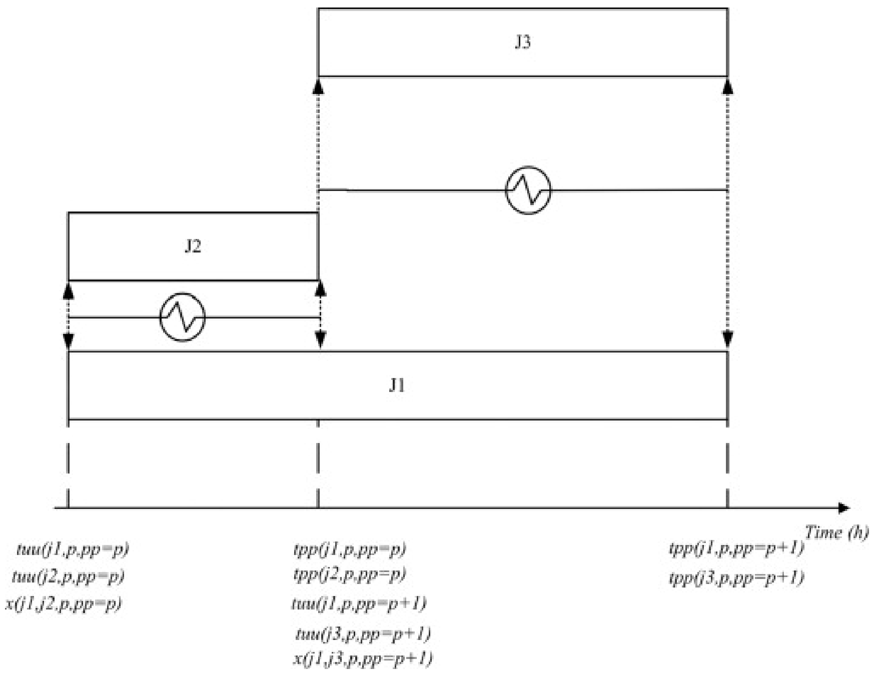

Figure 2: Differentiating time point p and extended time point pp.

goes reaction and the heat of reaction.

$$\begin{aligned} &cl(s_{inj_h}, p) \\ &\quad = mu(s_{inj_h}, p) cp(s_{inj_h}) (T^{in}_{s_{inj_h}} - T^{out}_{s_{inj_h}}), \\ &\qquad \forall p \in P,\ s_{inj_h} \in S_{inJ_h} \end{aligned} \tag{3}$$

Constraint 3.1 describes the amount of heating load required by the cold unit from its initial temperature to its target temperature. In a situation where the temperature in the reactor unit is fixed during endothermic reaction, the heat load becomes the product of the amount of mass that undergoes reaction and the heat of reaction.

$$\begin{aligned} &hl(s_{inj_c}, p) = \\ &\quad mu(s_{inj_c}, p) cp(s_{inj_c}) (T^{out}_{s_{inj_c}} - T^{in}_{s_{inj_c}}), \\ &\qquad \forall p \in P,\ s_{inj_c} \in S_{inJ_c} \end{aligned} \tag{4}$$

Constraints 3.1 and 3.1 describe the average heat flow for the hot and cold unit, respectively during the processing time which is the same as time average (TAM) model to address the energy balance during heat integration properly.

$$\begin{aligned} &cl(s_{inj_h}, p) = \\ &\quad avcl(s_{inj_h}, p)(tp(s_{inj_h}, p) - (s_{inj_h}, p)), \\ &\qquad \forall p \in P,\ s_{inj_h} \in S_{inJ_h} \end{aligned} \tag{5}$$

$$\begin{aligned} &hl(s_{inj_c}, p) = avhl(s_{inj_c}, p)(tp(s_{inj_c}, p) - tu(s_{inj_c}, p)), \\ &\qquad \forall p \in P,\ s_{inj_c} \in S_{inJ_c} \end{aligned} \tag{6}$$

Constraints 3.1 and 3.1 define the heat load at time point p and extended time point pp for the hot and cold unit.

$$hlp(s_{injc}, p, pp) = avhl(s_{injc}, p)(tpp(s_{injc}, p, pp) - tuu(s_{injc}, p, pp)), \quad \forall p, pp \in P,\ s_{injc} \in S_{inJ_c} \tag{7}$$

$$clp(s_{injh}, p, pp) = avcl(s_{injh}, p)(tpp(s_{injh}, p, pp) - tuu(s_{injh}, p, pp)), \quad \forall p, pp \in P,\ s_{injh} \in S_{inJ_h} \tag{8}$$

Constraints 3.1 and 3.1 are used to calculate the temperature of the hot and cold unit at the intervals.

$$clp(s_{injh}, p, pp) = mu(s_{injh}, p)cp(s_{injh}) (T^{in}(s_{injh}, p, pp) - T^{out}(s_{injh}, p, pp)), \quad \forall p, pp \in P,\ s_{injh} \in S_{inJ_h} \tag{9}$$

$$hlp(s_{injc}, p, pp) = mu(s_{injc}, p)cp(s_{injc}) (T^{out}(s_{injc}, p, pp) - T^{in}(s_{injc}, p, pp)), \quad \forall p, pp \in P,\ s_{injc} \in S_{inJ_c} \tag{10}$$

Constraint 3.1 states that the amount of heat exchanged by the hot unit with the cold units should be less than the cooling load required by the hot unit during the interval.

$$\sum_{s_{injc}} qe(s_{injc}, s_{injh}, p, pp) \leq clp(s_{injh}, p, pp), \quad \forall p, pp \in P,\ s_{injh} \in S_{inJ_h},\ s_{injc} \in S_{inJ_c} \tag{11}$$

Constraint 3.1 states that the amount of heat exchanged by the cold unit with the hot units should be less than the heat load required by the cold unit during the interval.

$$\sum_{s_{injh}} qe(s_{injc}, s_{injh}, p, pp) \leq hlp(s_{injc}, p, pp), \quad \forall p, pp \in P,\ s_{injh} \in S_{inJ_h},\ s_{injc} \in S_{inJ_c} \tag{12}$$

Constraints 3.1 and 3.1 state that the temperature of the unit at the start of an interval should be equal to the temperature at the end of the previous interval.

$$T^{in}(s_{injh}, p, pp) = T^{out}(s_{injh}, p, pp-1), \quad \forall p, pp \in P,\ s_{injh} \in S_{inJ_h} \tag{13}$$

$$T^{in}(s_{injc}, p, pp) = T^{out}(s_{injc}, p, pp-1), \quad \forall p, pp \in P,\ s_{injc} \in S_{inJ_c} \tag{14}$$

Constraints 3.1 and 3.1 state that the temperature at the start of the first interval, which is time point p, which is also pp, should be equal to the initial temperature of the task.

$$T^{in}(s_{injh}, p, pp) = T^{in}_{s_{injh}}, \quad \forall p, pp \in P,\ p = pp,\ s_{injh} \in S_{inJ_h} \tag{15}$$

$$T^{in}(s_{injc}, p, pp) = T^{in}_{s_{injc}}, \quad \forall p, pp \in P,\ p = pp,\ s_{injc} \in S_{inJ_c} \tag{16}$$

Constraints 3.1 and 3.1 ensure that the minimum thermal driving forces are obeyed when there is direct heat integration between a hot and a cold unit.

$$T^{in}(s_{inj_h}, p, pp) - T^{out}(s_{inj_c}, p, pp) \geq \\ \triangle T - \triangle TU(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (17)$$

$$T^{out}(s_{inj_h}, p, pp) - T^{in}(s_{inj_c}, p, pp) \geq \\ \triangle T - \triangle TU(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (18)$$

Constraints 3.13.1 ensure that the times at which units are active are synchronized when direct heat integration takes place.

$$tuu(s_{inj_h}, p, pp) \geq \\ tuu(s_{inj_c}, p, pp) - M(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (19)$$

$$tuu(s_{inj_h}, p, pp) \leq \\ tuu(s_{inj_c}, p, pp) + M(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (20)$$

$$tpp(s_{inj_h}, p, pp) \geq \\ tpp(s_{inj_c}, p, pp) - M(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (21)$$

$$tpp(s_{inj_h}, p, pp) \leq \\ tpp(s_{inj_c}, p, pp) + M(1 - x(s_{inj_c}, s_{inj_h}, p, pp)), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (22)$$

Constraints 3.1 and 3.1 stipulate that the starting time of the heating load required for the cold unit and cooling load required for the hot unit at the first interval should be equal to the starting time of the hot and cold unit.

$$tuu(s_{inj_h}, p, pp) = tu(s_{inj_h}, p), \\ \forall p, pp \in P,\ p = pp,\ s_{inj_h} \in S_{inJ_h} \quad (23)$$

$$tuu(s_{inj_c}, p, pp) = tu(s_{inj_c}, p), \\ \forall p, pp \in P,\ p = pp,\ s_{inj_c} \in S_{inJ_c} \quad (24)$$

Constraints 3.1 and 3.1 state that the starting time of heating and cooling in an interval should be equal to the finishing time at the previous interval.

$$tuu(s_{inj_h}, p, pp) = tpp(s_{inj_h}, p, pp - 1), \\ \forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h} \quad (25)$$

$$tuu(s_{inj_c}, p, pp) = tpp(s_{inj_c}, p, pp - 1), \\ \forall p, pp \in P,\ s_{inj_c} \in S_{inJ_c} \quad (26)$$

Constraint 3.1 ensures that if heat integration occurs, the heat load should have a value that is less than the maximum amount of heat exchangeable. When the binary variable associated to heat integration takes a value of zero, no heat integration occurs and the associated heat load is zero.

$$qe(s_{inj_c}, s_{inj_h}, p, pp) \leq Q^U x(s_{inj_c}, s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (27)$$

Constraints 3.1 and 3.1 state that if the binary variable associated with heat integration is active, then the binary variable associated with heating and cooling must be active at that interval.

$$x(s_{inj_c}, s_{inj_h}, p, pp) \leq y_{int}(s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (28)$$

$$x(s_{inj_c}, s_{inj_h}, p, pp) \leq y_{int}(s_{inj_c}, p, pp),$$
$$p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (29)$$

Constraints 3.1 and 3.1 state that the heating and cooling loads take on a value for a certain duration when the binary variables associated with heating and cooling is active.

$$tpp(s_{inj_h}, p, pp) - tuu(s_{inj_h}, p, pp) \leq$$
$$H y_{int}(s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h} \quad (30)$$

$$tpp(s_{inj_h}, p, pp) - tuu(s_{inj_h}, p, pp) \leq$$
$$H y_{int}(s_{inj_h}, p, pp),$$
$$\forall p, pp \in P, s_{inj_h} \in S_{inJ_h} \quad (31)$$

Constraints 3.1 and 3.1 state that temperatures change in the heating and cooling unit when the binary variables associated with heating and cooling are active.

$$T^{in}(s_{inj_h}, p, pp) - T^{out}(s_{inj_h}, p, pp) \leq$$
$$\triangle TU(s_{inj_h}) y_{int}(s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h} \quad (32)$$

$$T^{out}(s_{inj_c}, p, pp) - T^{in}(s_{inj_c}, p, pp) \leq$$
$$\triangle TU(s_{inj_c}) y_{int}(s_{inj_c}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_c} \in S_{inJ_c} \quad (33)$$

Constraint 3.1 states that the cooling of a hot unit will be satisfied by direct heat integration and external cooling utility if required.

$$cl(s_{inj_h}, p) = cw(s_{inj_h}, p) + \sum_{s_{inj_c}} qe(s_{inj_c}, s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (34)$$

Constraint 3.1 states that the heating of a cold unit will be satisfied by direct heat integration and external heating utility if required.

$$hl(s_{inj_c}, p) = st(s_{inj_h}, p) + \sum_{s_{inj_h}} qe(s_{inj_c}, s_{inj_h}, p, pp),$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c} \quad (35)$$

3.2. Wastewater minimization model

The superstructure on which the wastewater minimization model is based is depicted in Figure 3. Only the water using operations which are part of a complete batch process are depicted. Unit j represents a water using operation in which the water used can consist of freshwater, reuse water or reuse and freshwater. Water from unit j can be reused elsewhere or sent to effluent treatment.

Constraint 3.2 defines the amount of water entering the unit as the sum of freshwater and reuse water from other units.

$$mwin(s_{inj},p) = mfw(s_{inj},p) + \sum_{s'_{inj}} mrw(s'_{inj},s_{inj},p), \quad \forall p \in P,\ s_{inj},s'_{inj} \in S_{inJ} \tag{36}$$

Constraint 3.2 states that the amount of water leaving the unit is equal to the sum of reuse water sent to other units and water sent to effluent treatment.

$$mwout(s_{inj},p) = \sum_{s'_{inj}} mrw(s_{inj},s'_{inj},p) + mew(s_{inj},p), \quad \forall p \in P,\ s_{inj},s'_{inj} \in S_{inJ} \tag{37}$$

Constraint 3.2 is the water balance around the unit and states that the amount of water entering the unit equals the amount of water leaving the unit.

$$mwin(s_{inj},p) = mwout(s_{inj},p), \quad \forall p \in P,\ s_{inj} \in S_{inJ} \tag{38}$$

Constraint 3.2 defines the inlet contaminant load as the mass of contaminant, entering with reuse water.

$$cin(s_{inj},c,p)mwin(s_{inj},p) = \sum_{s'_{inj}} cout(s'_{inj},c,p)mrw(s'_{inj},s_{inj},p), \quad \forall p \in P,\ s_{inj},s'_{inj} \in S_{inJ},\ c \in C \tag{39}$$

Constraint 3.2 states that the amount of contaminant leaving the unit equals the sum of the contaminant entering into the unit and the contaminant removed from the process.

$$mwout(s_{inj},p)cout(s_{inj},c,p) = SMC(s_{inj})mu(s_{inj},p)+cin(s_{inj},c,p)mwin(s_{inj},p), \quad \forall p \in P,\ s_{inj} \in S_{inJ},\ c \in C \tag{40}$$

Constraint 3.2 ensures that the amount of reused water from unit j to other units does not exceed the maximum allowable water in the receiving units. It also indicates whether water from unit j is reused or not.

$$mrw(s_{inj},s'_{inj},p) \leq W^{U}_{in}(s'_{inj})y_{re}(s_{inj},s'_{inj},p), \quad \forall p \in P,\ s_{inj},s'_{inj} \in S_{inJ} \tag{41}$$

Constraint 3.2 ensures that the reuse of water from unit j in other units can occur only if the units are active.

$$y_{re}(s_{inj},s'_{inj},p) \leq y)(s'_{inj},p), \quad \forall p \in P,\ s_{inj},s'_{inj} \in S_{inJ} \tag{42}$$

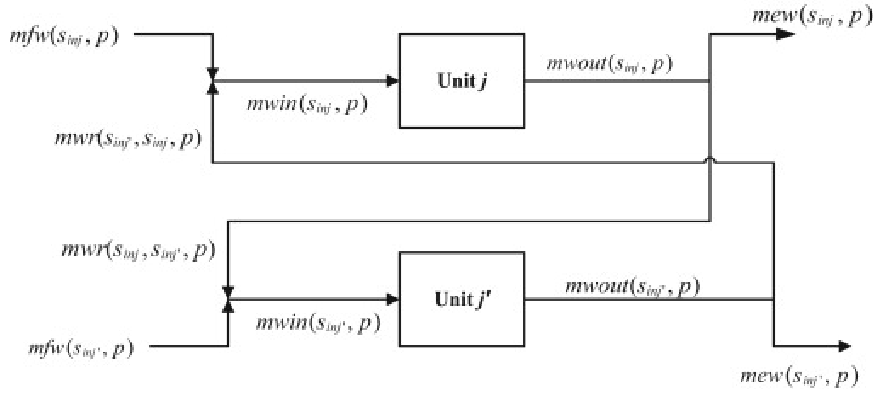

Figure 3: Superstructure for water usage.

Constraint 3.2 gives the upper bound on the water entering into unit j. It also ensures that water enters into the unit only if it is active.

$$mwin(s_{inj}, p) \leq W_{in}^{U}(s_{inj}) y(s_{inj}, p), \quad \forall p \in P,\ s_{inj} \in S_{inJ} \tag{43}$$

In Constraints 3.2 and 3.2, wastewater can only be directly reused if the finishing time of the unit producing wastewater and the starting time of the unit receiving wastewater coincide.

$$tuw(s_{inj}, p) \geq tpw(s'_{inj}, p) - M * y_{re}(s_{inj}, s'_{inj}, p), \quad \forall p \in P,\ s_{inj},\ s'_{inj} \in S_{inJ} \tag{44}$$

$$tuw(s_{inj}, p) \leq tpw(s'_{inj}, p) + M * y_{re}(s_{inj}, s'_{inj}, p), \quad \forall p \in P,\ s_{inj}, s'_{inj} \in S_{inJ} \tag{45}$$

Constraint 3.2 defines the finishing time of the washing operation as the starting time of the washing operation added to the duration of washing.

$$tpw(s_{inj}, p) \geq tuw(s_{inj}, p) + \tau w(s_{inj}) y(s_{inj}, p), \quad \forall p \in P,\ s_{inj} \in S_{inJ} \tag{46}$$

Constraint 3.2 ensures that the staring time of a task in a unit is greater than the finishing time of the washing operations.

$$tu(s_{inj}, p) \geq tpw(s'_{inj}, p1), \quad \forall p \in P,\ s_{inj}, s'_{inj} \in S_{inJ}, S^{*}_{inj} \tag{47}$$

Constraint 3.2 stipulates that the starting time of the washing operation in a unit occurs after the completion of the task in the unit.

$$tuw(s_{inj}, p) \geq tp(s_{inj}, p), \forall p \in P, s_{inj} \in S_{inJ} \tag{48}$$

Constraints 3.2 and 3.2 ensure that the inlet and outlet concentrations do not exceed the maximum allowable concentration.

$$cin(s_{inj}, c, p) \leq cin^{U}(s_{inj}, c), \quad \forall p \in P,\ s_{inj} \in S_{inJ},\ c \in C \tag{49}$$

$$cout(s_{inj}, c, p) \leq cout^U(s_{inj}, c), \quad \forall p \in P,\ s_{inj} \in S_{inJ},\ c\ inC \quad (50)$$

Constraint 3.2 is the objective function in terms of profit maximization, with profit defined as the difference between revenue from product, cost of utility, raw material cost, freshwater cost and effluent treatment cost.

$$\max \left(\begin{array}{l} \sum_{s^p} price(s^p) d(s^p) - \\ \sum_p \sum_{s_{inj_h}} \cos tcw * cw(s_{inj_h}, p) - \\ \sum_p \sum_{s_{inj_c}} costst * st(s_{inj_c}, p) - \\ \sum_p \sum_{s_{inj}} costfw * mfw(s_{inj}, p) - \\ \sum p \sum s_{inj} costew * mew(s_{inj}, p) \end{array} \right)$$
$$\forall p, \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c},\ s_{inj} \in S_{inJ} \quad (51)$$

Constraint 3.2 defines minimization of energy and wastewater if the product demand is known.

$$\min \left(\begin{array}{l} \sum_p \sum_{s_{inj_h}} costcw * cw(s_{inj_h}, p) + \\ \sum_p \sum_{s_{inj_c}} \cos tst * st(s_{inj_c}, p) + \\ \sum_p \sum_{s_{inj}} costfw * mfw(s_{inj}, p) + \\ \sum_p \sum_{s_{inj}} \cos tew * mew(s_{inj}, p) \end{array} \right)$$
$$\forall p, pp \in P,\ s_{inj_h} \in S_{inJ_h},\ s_{inj_c} \in S_{inJ_c},\ s_{inj} \in S_{inJ} \quad (52)$$

4. Case studies

Case studies from published literature were selected to demonstrate the application of the proposed model. The results from the proposed models were obtained using CPLEX 9 as MILP solver and CONOPT 3 as NLP solver in DICOPT interface of GAMS 22.0 and were solved using a 2.4 GHz, 4 GB of RAM, Acer TravelMate 5740G computer.

4.1. Case study I

This case study has been investigated extensively in published literature Halim and Srinivasan (2011). It is a simple batch plant requiring only one raw material to yield a product as depicted in the state task network (STN) representation in Figure 4. The plant comprises of 5 units and two intermediate storage units. The conversion of the raw material into product is achieved through three sequential processes. The first task can be performed in two units ($j1$ and $j2$), the second task can be performed only in unit $j3$ and the third task can be performed in units $j4$ and $j5$. Tasks 1 and 2 require cooling during their operation, while task 3 requires heating. The cooling and heating demands are satisfied by external utilities and heat integration. The operational philosophy requires that the units are cleaned before the next batch is processed. Both freshwater and reuse water can be used as cleaning agents. Table 1 gives the capacities of the units, durations of processing and washing tasks, initial availability of states, storage capacities and selling prices and costs for the states. Table 2 gives data pertaining to initial and target temperatures for the tasks, specific heat capacities for the states, maximum inlet and outlet contaminant concentrations which are unit dependent and the specific contaminant loads.

4.1.1. Results and discussion

The computational results for case study I using the proposed model for the different

Table 1: Scheduling data for case study I.

Task(i)	Unit(j)	Max batch size(kg)	Total operation time(h)	Washing time(h)	Material state(m)	Initial inventory(kg)	Max storage(kg)	Revenue or cost (\$/kg or \$/MJ)
Task 1	Unit 1	100	1.5	0.25	A	1000	1000	0
	Unit 2	150	2	0.3	B	0	200	0
Task 2	Unit 3	200	1.5	0	C	0	250	0
Task 3	Unit 4	100	1	0.25	D	0	1000	5
	Unit 5	150	1.5	0.3	Wash water			0.1
					Waste water			0.05
					Cooling water			0.02
					Steam			1

Note: Total operation time includes processing time and washing time.

Table 2: Energy and cleaning requirements for case study I.

Task(i)	T^{in}(°C)	T^{out}(°C)	Unit(j)	C$_p$(kJ/kg°C)	Max inlet concentration (ppm)	Max outlet concentration (ppm)	Contaminant loading (g contaminant/ kg batch)
Task 1	140	60	Unit 1	4	500	1000	0.2
			Unit 2	4	50	100	0.2
Task 2	60	40	Unit 3	3.5	-	-	0.2
Task 3	40	80	Unit 4	3	150	300	0.2
			Unit 5	3	300	2000	0.2
Cooling water	20	30					
Steam	170	1600					

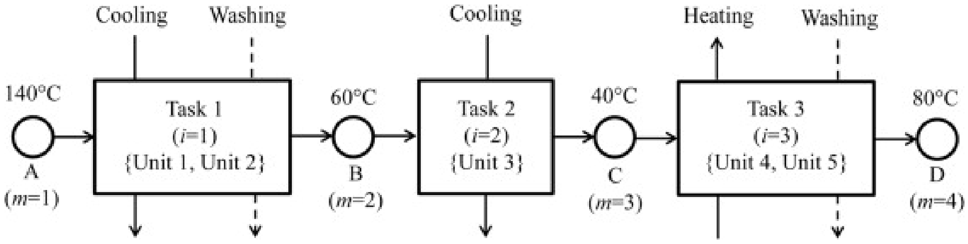

Figure 4: STN representation of a simple batch plant producing one product.

scenarios and results obtained from literature are presented in Table 3. For the scenario without energy and water integration, the total cost of utilities was \$293.5. Applying only water integration, the total cost obtained was \$259.5, which is an 11.6% reduction, compared to the standalone operation without energy and water integration. For the scenario with energy integration only, a total cost of \$208 was obtained, which is a 29.1% reduction compared to the standalone operation. The fifth column shows the results obtained with combined energy and water integration solved simultaneously giving a total cost of \$191.8, which is a 34.6% saving compared to the standalone operation. These results show that in order to achieve the best economic performance, the scheduling problem has to be solved simultaneously considering both water and energy integration.

The performance of the proposed model was compared to the sequential optimization technique by Halim and Srinivasan (2011) which resulted in an overall cost of \$239.5, which is an 18.4% saving, much less than the 34.6% saving obtained by the proposed model. This work also give much better result compared to the resent simultaneous optimization technique of Adekola et al. (2013) with a cost saving of 23.4% compared to 34.6% saving obtained by the proposed model. The suboptimality results of the method by Adekola et al. (2013) are attributed to two basic drawbacks. The first drawback is due to restricting the flexibility of the schedule by forcing the heat integrated units to start at the same time. The second drawback is the model is not based on TAM and the possibility of heat integration between pairs of tasks as well as possible $\triangle T$ violations was investigated for each pair of hot and cold tasks before optimization using the initial and target temperatures of the heat integrated tasks. This limits the chance a unit to be integrated in multiple intervals with different intermediate temperatures with other units. Using the proposed model we keep the schedule flexibility by allowing the heat integrated units to start anywhere between the starting and finishing time of the heat integrated tasks. This benefit can be demonstrated in Figure 5, for example Unit 2 during processing a task from 3.2 h to 4.9 h is integrated to exchange heat with Unit 4 during processing a task from 4.25 h to 5 h. These two units are integrated from 4.25 h to 4.9 h to exchange heat which is not possible by the method of Adekola et al. (2013). Consequently, this work reduce the steam requirement by 40.9% compared to technique by Adekola et al. (2013). The efficiency of the proposed model can be attributed to solving the scheduling problem while incorporating water and energy integration in the

Table 3: Computational results for case study I.

	Proposed formulation without water and energy integration	Proposed formulation with water integration	Proposed formulation with energy integration	Proposed formulation with water and energy integration	Halim and Srinivasan(2011) with water and energy integration	Adekola et al.(2013) with water and energy integration
Profit($)	4706.5	4740.5	4791.5	4808.2	4764.1	4777.3
Steam(MJ)	120	120	36.63	39	43.9	66
Cooling water(MJ)	390	390	281.2	309	313.9	336
Total freshwater(kg)	1105	878.2	1105	977.7	1238.4	1013.3
Revenue from product($)	5000	5000	5000	5000	5000	5000
Cost of steam($)	120	120	36.63	39	43.9	66
Cost of cooling water($)	7.8	7.8	5.623	6.2	6.3	6.72
Cost of freshwater($)	110.5	87.8	110.5	97.7	123.8	101.3
Cost of waste water($)	55.25	43.9	55.2	48.9	61.9	50.7
Total Cost($)	293.5	259.5	208	191.8	23.9	224.72
CPU time(s)	2.3	5000	5000	5000	Not reported	28,797

same framework and also using the recent efficient scheduling technique by Seid and Majozi (2012). Figure 5 details the possible amount of energy integration between the cold and hot units and the time intervals during which energy integration occurred.

The energy requirements of unit $j2$ and unit $j4$ during the interval 3.25 h is emphasized to elaborate on the application of the proposed model. The cooling load of unit $j2$ between 3.2 h and 4.9 h was 32 MJ. This is partly satisfied through energy integration with unit $j4$ in the same time interval, resulting in an external cooling requirement of 26.8 MJ rather than 32 MJ if it operated in standalone mode. At the beginning of the operation of unit $j2$ from 3.2 h to 4.25 h, the cooling requirement was 19.76 MJ. This value was obtained using the time average model by multiplying the duration (4.25 h3.2 h) and the energy demand per hour (32 MJ/1.7 h (total duration of the task)=18.823 MJ) where the cooling requirement is fully satisfied by external cooling. For the rest of its operation between 4.25 h and 4.94 h, the cooling requirement was 12.24 MJ, satisfied partly with energy integration (5.2 MJ) and the difference by external cooling. The heating requirement of unit $j4$ when it is operated during the interval 4.255 h was 6 MJ. From 4.25 h to 4.9 h the steam requirement was 5.2 MJ obtained from the time average model. This heating requirement was fully satisfied during the interval, by integrating with the hot unit $j2$. The rest of the heating, 0.8 MJ, required during its operation between 4.9 h and 5 h was satisfied by external steam.

Figure 6 shows the amount of contaminant removed, freshwater usage, amount of reused water and wastewater produced from washing the necessary units. The washing operation of unit $j2$ between 4.9 h and 5.2 h required 200 kg of freshwater to remove a contaminant load of 20 g, producing water with a contaminant concentration of 100 ppm. Part of this water produced from unit $j2$, 50 kg, was used for cleaning unit $j4$ to remove a contaminant load of 10 g. This was possible because the outlet concentration from unit $j2$ (100 ppm) was lower than the maximum inlet contaminant concentration (150 ppm) for unit $j4$. From Figure 6 the total amount of reused water was 358.23 kg, thereby reducing the water usage from 1105 kg (without water integration) to 977.7 kg (with water integration). This resulted in a saving of 11.5% freshwater usage and wastewater produced.

The amount of material produced, the starting and finishing times of the processes and washing tasks are shown in Figure 7 in the form of a Gantt chart.

4.2. Case study II

This case study obtained from Kondili et al. (1993) has become one of the most commonly used examples in literature. However, this case study has been adapted by Halim and Srinivasan (2011) to include energy and water integration. The batch plant produces two different products sharing the same processing units, where Figure 8 shows the plant flowsheet. The unit operations consist of preheating, three different reactions and separation. The plant accommodates many common features of multipurpose batch plants such as units performing multiple tasks, multiple units suitable for a task and dedicated units for specific tasks. The STN and SSN representations of the flowsheet are shown in Figure 9. Table 4 and Table 5 give the required data to solve the scheduling problem. The production recipe is as follows:

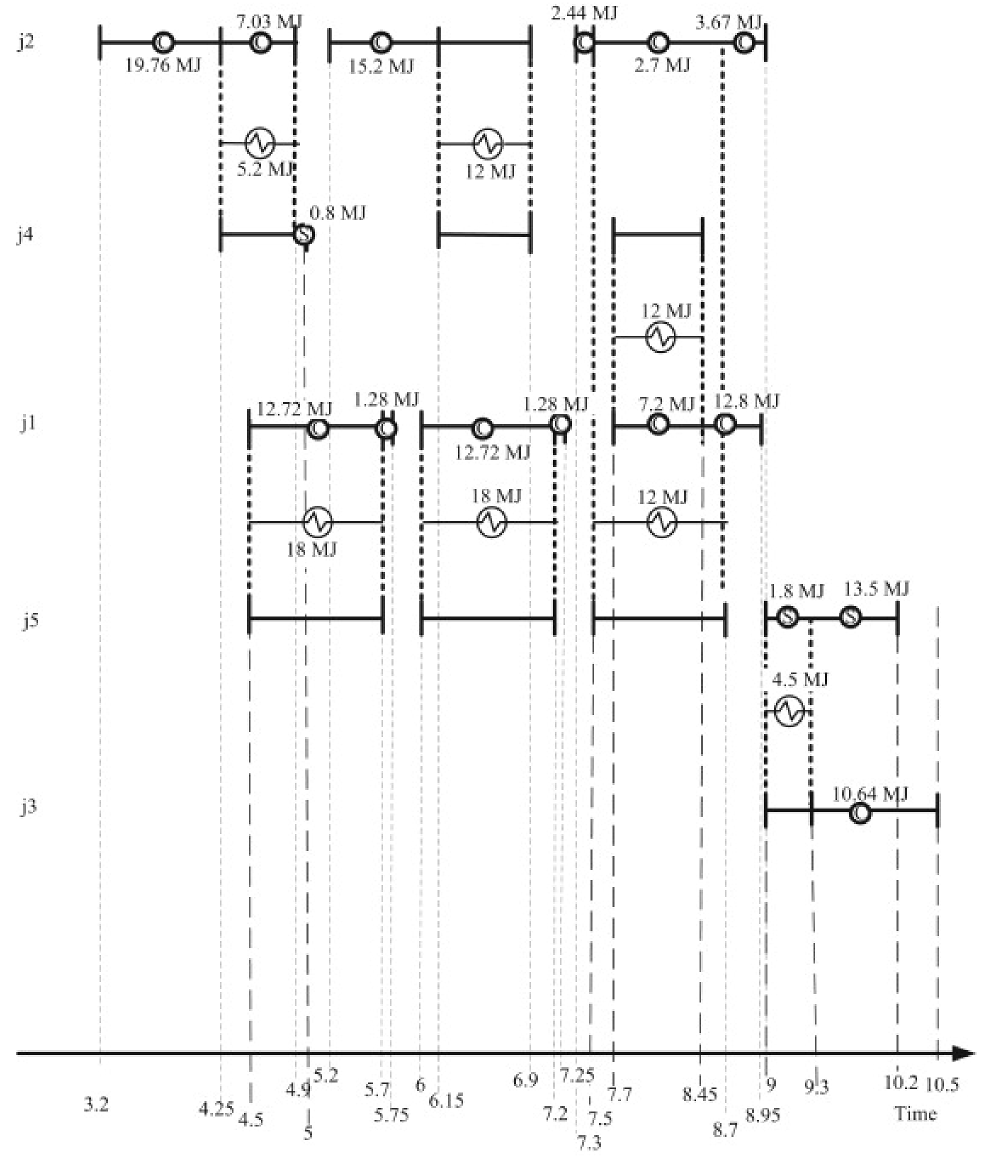

Figure 5: Possible energy integration within the time horizon of 12 h for case study I.

(a) Raw material, Feed A, is heated from 50°C to 70°C to form HotA used in reaction 2.

(b) Reactant materials, 50% Feed B and 50% Feed C are used in reaction 1 to produce IntBC. During the reaction the material has to be cooled from 100°C to 70°C.

(c) 60% of the intermediate material, IntBC, and 40% of HotA are used in reaction 2 to produce product 1 and IntAB. The process needs to be heated from 70°C to 100°C during its operation.

(d) 20% of the reactant, Feed C, and 80% of intermediate, IntAB, from reaction 2 are used in reaction 3 to produce ImpureE. The reaction needs its tempera-

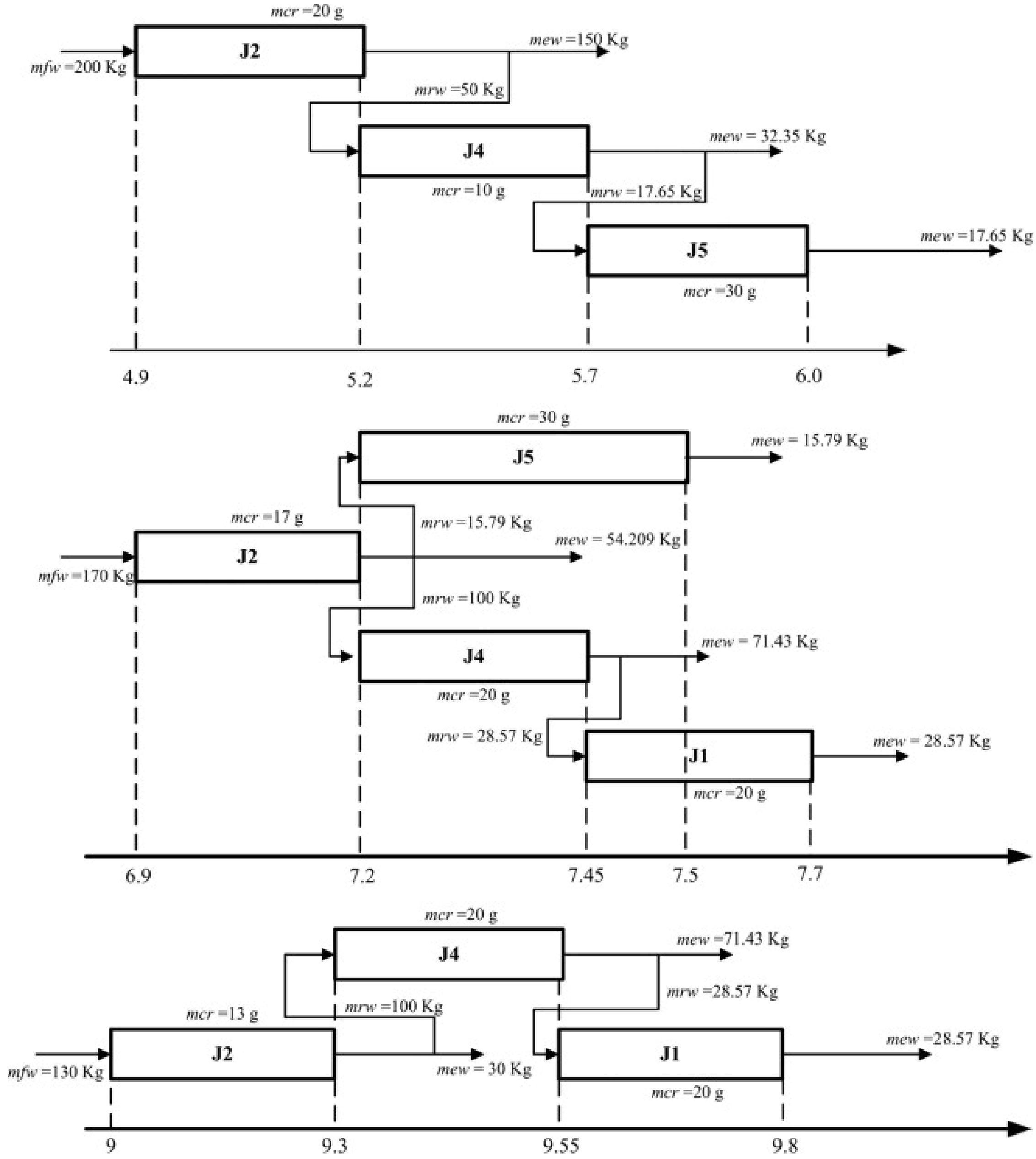

Figure 6: Water network with water integration within the time horizon of 12 h for case study I. *Note:* mfw=freshwater, mcr=contaminant removed, mrw=recycled water, mew=water sent to effluent.

ture to be raised from 100°C to 130°C during its operation.

(e) The separation process produces 90% product 2 and 10% IntAB from Impure E. Cooling water is used to lower its temperature from 130°C to 100°C.

The processing time of a task i in unit j is assumed to be linearly dependent on its batch size B, i.e. $\alpha i + \beta i B$. Where αi is a constant term of the processing time of task i and βi is a coefficient of variable processing time of task i. The batch dependent

Table 4: Scheduling data for case study II.

Task (i)	Unit (j)	Max batch size (kg)	$\alpha(s_{inj})$	$\beta(s_{inj})$	Washing time	Material state (s)	Initial inventory	Max storage (kg)	Revenue or cost (\$/kg or \$/MJ)
Heating(H)	HR	100	0.667	0.007	0	Feed A	1000	1000	10
Reaction-1 (R1)	RR1	50	1.334	0.027	0.25	Feed B	1000	1000	10
	RR2	80	1.334	0.01770.3	Feed C	1000	1000	10	
Reaction-2 (R2)	RR1	50	1.334	0.027	0.25	HotA	0	100	0
	RR2	80	1.334	0.017	0.3	IntAB	0	200	0
Reaction-3 (R3)	RR1	50	0.667	0.013	0.25	IntBC	0	150	0
	RR2	80	0.667	0.008	0.3	ImpureE	0	200	0
Separation (S)	SR	200	1.334	0.007	0	Prod1	0	1000	20
						Prod2	0	1000	20
						Wash water			0.1
						Waste water			0.05
						Cooling water			0.02
						Steam			1

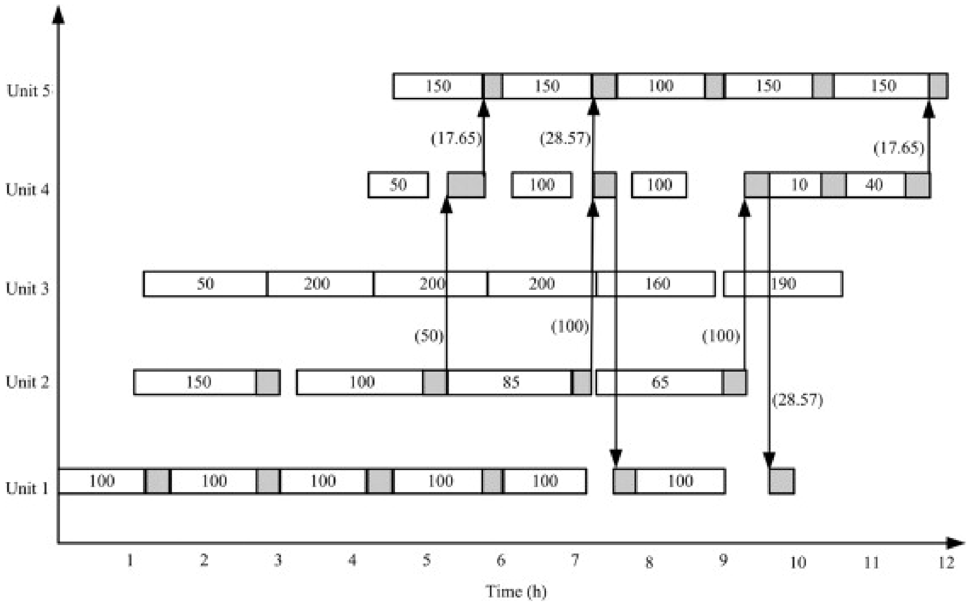

Figure 7: Gantt chart for the time horizon of 12 h incorporating energy and water integration for case study I.

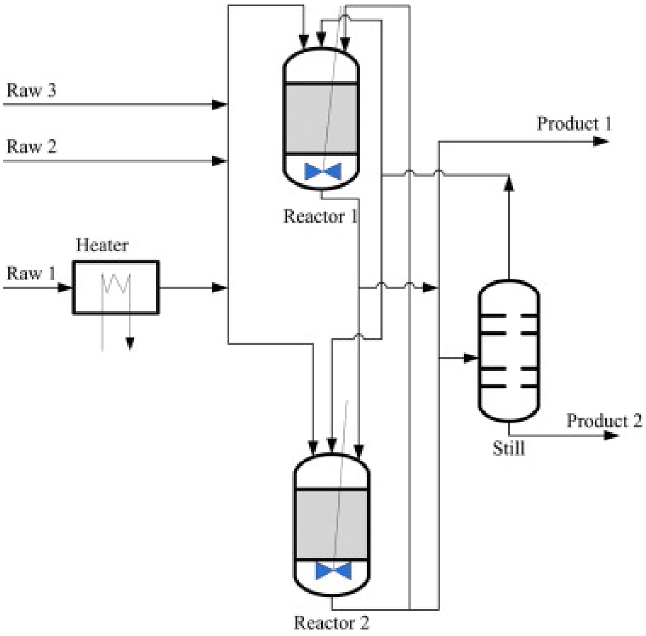

Figure 8: Flowsheet for case study II.

processing time makes this case study more complex. Table 4 gives the relevant data on coefficients of processing times, the capacity of the processing units, duration of washing, initial inventory of raw materials, storage capacity and relevant costs. Four contaminants are considered in the case study. The maximum inlet and outlet concentrations are given in Table 5. The production demand is given as 200 kg for both Prod1

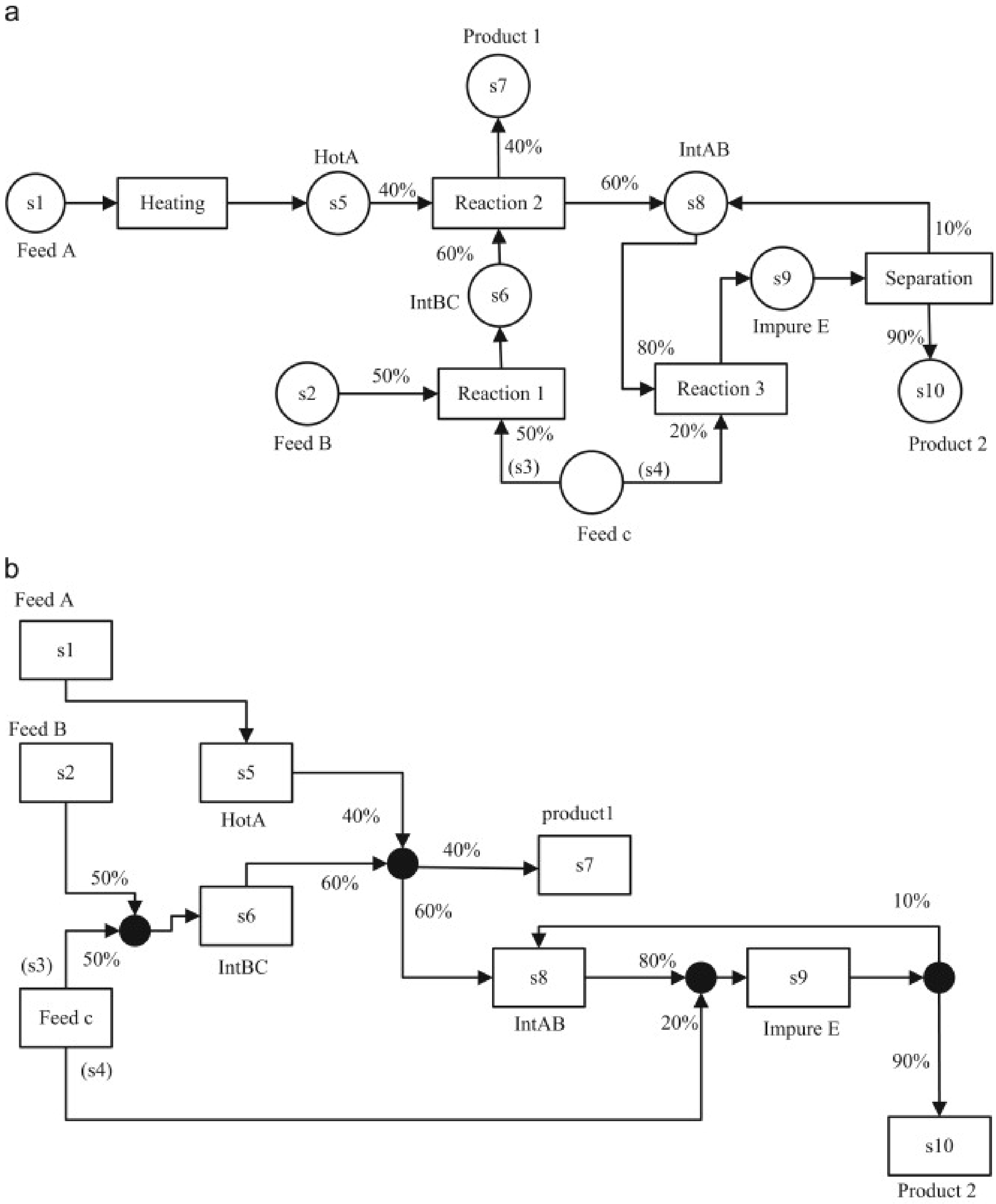

Figure 9: STN (a) and (b) SSN representation for case study II.

and Prod2. The objective here is to optimize with respect to makespan, energy and water consumption.

4.2.1. Results and discussions

The computational statistics for this case study using the proposed model and results obtained from literature are presented in

Table 5: Data required for energy and water integration.

Task (i)	T^{in} (°C)	T^{out} (°C)	Unit (j)	C_p (kJ/kg°C)	Max inlet concentration (ppm)				Max outlet concentration (ppm)				Contaminants (ar,br,cp and dw) loading(g contaminant /Kg batch)
					ar	br	cp	dw	ar	br	cp	dw	
Heating(H)	50	70	HR	2.5									
Reaction-1	100	70	RR1	3.5	300	500	800	400	700	800	1200	900	0.2
			RR2	3.5	300	500	800	400	700	800	1200	900	0.2
Reaction-2	70	100	RR1	3.2	700	600	300	400	1200	1000	600	800	0.2
			RR2	3.2	700	600	300	400	1200	1000	600	800	0.2
Reaction-3	100	130	RR1	2.6	500	200	400	300	800	500	700	900	0.2
			RR2	2.6	500	200	400	300	800	500	700	900	0.2
Separation	130	100	SR	2.8									
Cooling water	20	30											
Steam	170	160											

Table 6. For makespan minimization an objective value of 19.5 h was obtained using the proposed model, which is better than 19.96 h obtained by Halim and Srinivasan (2011) and 19.93 obtained by Adekola et al. (2013). Using the makespan obtained, the case study was solved using the different scenarios for water minimization, energy minimization and the simultaneous minimization of energy and water by setting customer requirement for Product 1 and Product 2. The total energy and freshwater required for the standalone operation were 125.5 MJ and 357.94 kg, respectively.

For the scenario of water integration only allowing the use of reuse water the total cost was \$112, resulting in 12.2% saving when compared to the standalone operation which had a total cost of \$127.52. By using only energy integration the total energy requirement was reduced from 125.5 MJ in standalone operation to 64.56 MJ, resulting in a 48.6% energy saving and a total cost saving of 24.4%. For the case of simultaneous optimization of energy and water, a significant total cost saving was obtained compared to energy integration alone and water integration alone. A total cost saving of 29.4% was obtained, compared to the standalone operation. The performance of the proposed model was also compared to the technique by Halim and Srinivasan (2011), a total cost of \$103 was found using their technique which is significantly higher than \$94.3 obtained using the proposed model. Furthermore, the proposed technique is very easy to adopt as opposed to their approach which required to solve 3500 MILP scheduling problem to find the best schedule compared to only 3 MILP major iterations of the MINLP problem. Each MILP problem is solved in a specified CPU time of 2000

Table 6: Computational results for case study II.

	Proposed formulation without water and energy integration	Proposed formulation with water integration	Proposed formulation with energy integration	Proposed formulation with water and energy integration	Halim and Srinivasan(2011) with water and energy integration	Adekola et al.(2013) with water and energy integration
Makespan (h)	19.5	19.5	19.5	19.5	19.96	19.93
Objective($)	127.5	112	96.4	94.3	103.3	96.4594
Steam(MJ)	75.3	75.3	44.9	43.3	61.4	44.88
Cooling water(MJ)	50.2	50.2	19.7	18.1	35.4	19.72
Total freshwater (kg)	357.94	238.1	341.3	337.7	275.1	341.2
Revenue from product ($)	8000	8000	8000	8000	8000	8000
Cost of steam($)	75.3	75.3	44.9	43.3	61.4	44.88
Cost of cooling water($)	1	1	0.4	0.36	0.7	0.3994
Cost of freshwater ($)	35.8	23.8	34.1	33.8	27.5	34.12
Cost of wastewater ($)	17.9	11.9	17.1	16.9	13.8	17.06
Number of time points/ slots	11	11	11	11	N/A	17
CPU time(s)	5000	5000	5000	6074	Not reported	24,532

s. This complex case study was solved in a reasonable CPU time of 6074 s, which is less than 2 h, using the proposed model. When this work compared to the model by Adekola et al. (2013) the number of event points required reduced considerably from 17 to 11 which have a direct effect on reducing CPU time required. Additionally, the usage of hot and cold utilities, freshwater and wastewater are also improved.

Figure 10 shows the Gantt chart related to the optimal usage of energy and water. It also indicates the types of tasks performed in each equipment, the starting and finishing times of the processes and washing tasks and the amount of material processed in each batch.

5. Conclusions

In the presented method, wastewater minimization and heat integration are both embedded within the scheduling framework and solved simultaneously, thus leading to a truly flexible process schedule. Results from case studies show that addressing profit maximization together with heat integration and wastewater minimization gives much better overall economic performance. From the case studies a better objective value was achieved using the proposed model compared to previous literature models. Forthcoming communications will address the usage of heat storage, wastewater storage and wastewater regenerator with the consideration of capital investment to investigate further improvement in energy and water usage. Although this invariably complicate the model formulation. Additionally, this work only addressed short-term scheduling problem. Extending this work to medium-term scheduling problem using a cyclic approach will be reported in future communication.

Nomenclature

	Sets
S_{inJ_h}	$\{s_{inj_h} \mid s_{inj_h}$ task which needs cooling$\}$
S_{inJ_c}	$\{s_{inj_c} \mid s_{inj_c}$ task which needs heating$\}$
S_{inJ}	$\{s_{inj} \mid s_{inj}$ any task$\}$
P	$\{p \mid p$ time point$\}$
S_{inJ_w}	$\{ s_{inj_w} \mid s_{inj_w}$ task which needs washing afterwards$\}$
C	$\{c \mid c$ contaminant$\}$
	Parameters
$cp(s_{inj_h})$	specific heat capacity for the heating task
$cp(s_{inj_c})$	specific heat capacity for the cooling task
$T^{in}_{s_{inj_h}}$	inlet temperature of the heating task
$T^{out}_{s_{inj_h}}$	outlet temperature of the heating task
$T^{in}_{s_{inj_c}}$	inlet temperature of the cooling task
$T^{out}_{s_{inj_c}}$	outlet temperature of the cooling task
$\triangle T^U$	maximum thermal driving force
$\triangle T^U(s_{inj})$	maximum temperature change for a task
$\triangle T$	minimum thermal driving force
M	big-M mostly equivalent to the time horizon
Q^U	maximum heat requirement from the heating and cooling task
$SMC(s(inj))$	specific contaminant load produced by a task
$W^U_{in}(s_{inj})$	maximum water inlet to a processing task
$\tau w(s_{inj})$	minimum duration required for a washing task

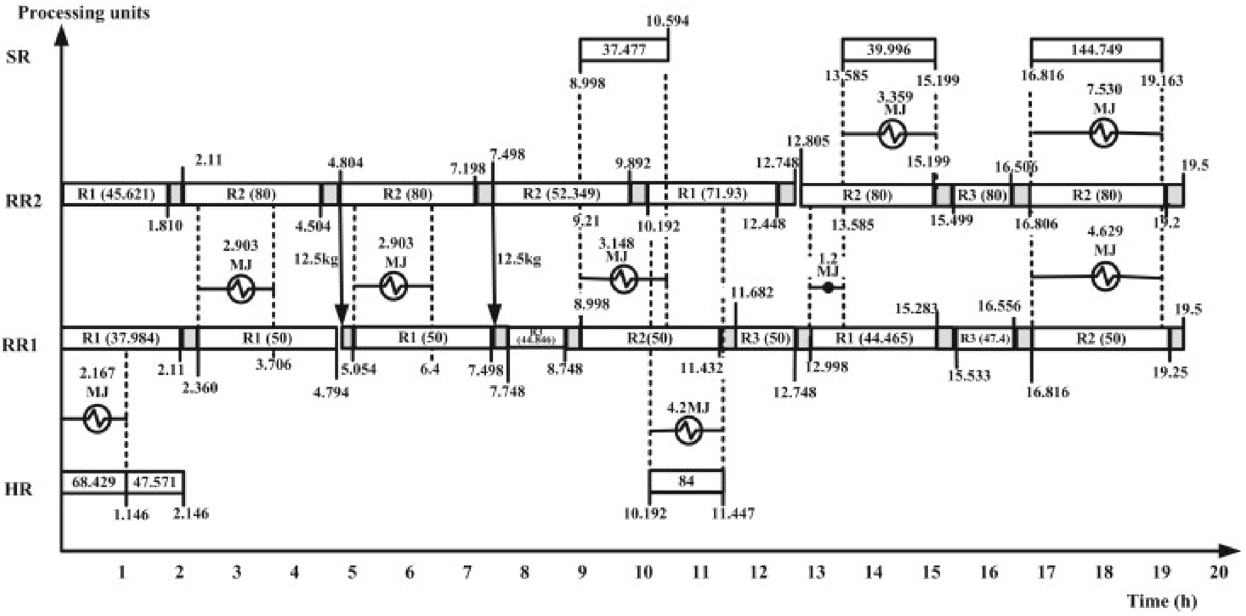

Figure 10: Resulting production schedule for case study II with direct heat integration and direct water reuse.

$cin^U(s_{inj}, c)$	maximum inlet contaminant concentration allowed for contaminant c
$cout^U(s_{inj}, c)$	maximum outlet contaminant concentration allowed for contaminant c
$price(s^p)$	price of a product
$d(s^p)$	amount of product produced at the end of the time horizon
H	time horizon of interest
$costfw$	cost of freshwater
$costew$	cost of effluent water
$costst$	cost of steam
$costcw$	cost of cooling water
	Variables
$x(s_{inj_c}, s_{inj_h}, p, pp)$	binary variable signifying whether heat integration occurs between the hot and cold unit
$y(s_{inj_h}, p)$	binary variable associated to whether the hot state is active at time point p or not
$y(s_{inj_c}, p)$	binary variable associated to whether the cold state is active at time point p or not
$y_{int}(s_{inj}, p, pp)$	binary variable associated to whether the hot and cold states are active at time point p and extended time point pp
$y_{re}(s_{inj}, s'_{inj}, p)$	binary variable associated with reuse of water from unit j to j at time point p
$cl(s_{inj_h}, p)$	cooling load required by the hot task at time point p
$hl(s_{inj_c}, p)$	heating load required by the cold task at time point p
$avcl(s_{inj_h}, p)$	average cooling load required by

	the hot task at time point p using time average model
$avhl(s_{inj_c}, p)$	average heating load required by the cold task at time point p using time average model
$mu(s_{inj_h}, p)$	amount of material processed by the hot task
$mu(s_{inj_c}, p)$	amount of material processed by the cold task
$tp(s_{inj}, p)$	end time of a heat flow for a task
$tu(s_{inj}, p)$	starting time of a heat flow for a task
$clp(s_{inj_h}, p, pp)$	cooling load required by the hot task active at time point p and extended time point pp
$hlp(s_{inj_c}, p, pp)$	heating load required by the cold task active at time point p and extended time point pp
$tuu(s_{inj}, p, pp)$	starting time of a heat flow for a task active at time point p and extended time point pp
$tpp(s_{inj}, p, pp)$	finishing time of a heat flow for a task active at time point p and extended time point pp
$T^{in}(s_{inj}, p, pp)$	inlet temperature of a task active at time point p and extended time point pp
$T^{out}(s_{inj}, p, pp)$	outlet temperature of a task active at time point p and extended time point pp
$qe(s_{inj_c}, s_{inj_h}, p, pp)$	amount of heat load exchanged by the hot and cold unit active at time point p and extended time point pp
$cw(s_{inj_h}, p)$	external cooling water used by the hot task
$st(s_{inj_c}, p)$	external heating used by the cold task
$mwin(s_{inj}, p)$	mass of water entering to wash a unit after a task is performed
$mwout(s_{inj}, p)$	mass of water leaving after washing
$mfw(s_{inj}, p)$	mass of freshwater entering to a unit
$mrw(s_{inj}, s'_{inj}, p)$	mass of water recycled from unit j to another unit j
$mew(s_{inj}, p)$	mass of water entering to effluent treatment produced from washing
$cin(s_{inj}, c, p)$	inlet contaminant concentration at time point p
$cout(s_{inj}, c, p)$	outlet contaminant concentration at time point p
$tuw(s_{inj}, p)$	starting time of washing operation for unit j
$tpw(s_{inj}, p)$	finishing time of washing operation for unit j

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