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# Sequential Methodology for Simultaneous Batch Process Scheduling and Water Reuse Optimization

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This paper presents a new sequential methodology for incorporating water reuse optimization in batch process scheduling. First, the schedule is optimized to meet the economic objective such as makespan or profit. Next, alternate schedules are generated through a stochastic search-based integer cut procedure that adds further constraints to the scheduling formulation. Finally, source-sink allocation technique is applied to each of the resulting schedules to establish the minimum water costs. The method differs from other sequential approaches published in literature in that the water optimization problem is solved with the intent to retain the optimality of the scheduling solution.

## 1. Introduction

Due to its inherent flexibility, batch process has been favorable for the production of low-volume, seasonal and high-value-added chemicals. However, this flexibility leads to extra complexity in the design and operation of the plant. As the process is time-dependent, proper scheduling of tasks in equipment becomes exceedingly crucial for meeting the production demand in a timely and cost-effective manner. In the mean time, the multiple tasks that take place in equipment often give rise to high volume of wastewater. With growing concern for sustainable operation, much effort is expected from the batch process industry to reuse water as much as possible.

Several water reuse methodologies for wastewater minimization in batch processes have been proposed in literature. These include graphical pinch analysis and mathematical optimization. Overall, the mathematical optimization techniques can be differentiated into two groups, namely, sequential and simultaneous framework. The former requires determining the batch schedule a priori for synthesizing a water reuse network. One example is Almató et al. (1999) who addressed the problem of wastewater minimization through storage tank allocation. However the limitation of their method was that each water reuse from one operation to another need to pass through a storage tank thus leading to large and/or unnecessary storage tanks. 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. The main drawback with the sequential method is that since the scheduling and wastewater minimization are not considered simultaneously, they could lead to suboptimal water network. The simultaneous framework involves formulating an integrated mathematical model comprising of scheduling and water reuse network and solving them simultaneously. Majozi (2005) applied continuous-time scheduling framework to minimize the wastewater generation with and without the use of storage tank. Cheng and Chang (2007) proposed a MINLP model for simultaneous scheduling optimization, water reuse network and wastewater treatment network. While simultaneous approach can result in global optima, it is only applicable to single objective problem, e.g., profit maximization problem.

In this paper, we propose a novel sequential methodology that exploits alternate schedules in the batch scheduling solution to synthesize an optimal water reuse network. The methodology has been developed by extending our previous approach for heat integration in batch processes (Halim and Srinivasan, 2009). One important feature of this method is its ability to solve multi-objective problem involving scheduling and water network optimization.

## 2. Batch Scheduling Formulation

The mathematical model used in this work is based on the continuous-time synchronized-slot scheduling of Sundaramoorthy and Karimi (2005). The model involves splitting the batch horizon $H$ into $K$ ($k$ = 1, 2, …, $K$) number of slots. The slots are synchronized on all units ($j$ = 1, 2, …, $J$). A task starting at $T_{k-1}$ can finish before, at, or after time $T_k$ according to the following relation:

$$T_k = T_{k-1} + SL_k \tag{1}$$

All these where, $SL_k$ is the slot length. A balance on the status of a unit $j$ can be written as:

$$y_{ijk} = y_{ij(k-1)} + Y_{ij(k-1)} - YE_{ijk} \tag{2}$$

where, $Y_{ijk}$ , $y_{ijk}$ and $YE_{ijk}$ are binary variables described as follows: $Y_{ijk}$ = 1 if unit $j$ begins task $i$ at time $T_k$, $y_{ijk}$ = 1 if unit $j$ is continuing to perform task $i$ at time $T_k$ and $YE_{ijk}$ = 1 if unit $j$ ends task $i$ and releases its batch at time $T_k$. A time balance on task $i$ as it progresses from $T_k$ to $T_{k+1}$ on $j$ can be written as:

$$t_{j(k+1)} \geq t_{jk} + \sum_{i \in \boldsymbol{I}_j} (\alpha_{ij} Y_{ijk} + \beta_{ij} B_{ijk}) - SL_{(k+1)} \,, \;\; k < K \tag{3}$$

where $t_{jk}$ is defined as the time remaining at $T_k$ to complete the task that was in progress during slot $k$ on unit $j$, $B_{ijk}$ is the batch size of task $i$ that unit $j$ begins at $T_k$ , $\alpha_{ij}$ is the fixed processing time of task $i$ on $j$ and $\beta_{ij}$ is the variable processing time of task $i$ on $j$. A mass balance on unit $j$ can be defined using the following equation:

$$b_{ijk} = b_{ij(k-1)} + B_{ij(k-1)} - BE_{ijk} \;\; , i > 0, \;\; k > 0 \tag{4}$$

where $b_{ijk}$ be the amount of material $m$ that resides in unit $j$ just before $T_k$ and $BE_{ijk}$ is the amount that task $i$ discharges at its completion at $T_k$ on unit $j$. Equation (4) states that whenever a unit $j$ is not performing a task $i$ at $T_k$ then $b_{ijk}$ is set as zero, and vice versa. An inventory balance of material $m$ can be described as follows:

$$I_{mk} = I_{m(k-1)} + \sum_{i \in OI_m, i \neq 0} \sum_{j \in J_i} \sigma_{mi} BE_{ijk} + \sum_{i \in II_m, i \neq 0} \sum_{j \in J_i} \sigma_{mi} B_{ijk} \tag{5}$$

where $I_{mk}$ is the inventory of material $m$ at $T_k$, $OI_m$ is the set of tasks that produce material $m$, $II_m$ is the set of tasks that consume material $m$, $J_i$ is a set of units that can perform task $i$ and $\sigma_{mi}$ is the stoichiometric yield coefficient of material $m$ in the mass balance of task $I$ ($\sigma_{mi}$ is set to be negative for the raw materials of task $i$ and positive for its products). The resulting mathematical formulation is a MILP model and can be solved for the objective function involving makespan or profit.

## 3. Source-Sink Allocation Method

The objective of source-sink allocation method is to create a water reuse network to minimize the flow of freshwater. Process sources represent the used wastewater streams that can be recycled to other operations. The later are called sinks. Maximizing the reuse of process sources to the sinks concomitantly reduces the amount of freshwater. The following defines the objective function for minimizing the flows of fresh resources ($F_r$) to process sinks:

$$\text{Min} \sum_{j=1}^{N_{\sin k}} f_{r,j} \tag{6}$$

Here, $r$ = 1, 2, … N$_{fresh}$ is the index of fresh resource streams, $j$ = 1, 2, … N$_{sink}$ is the index of process sinks, and $f_{r,j}$ is the stream flow from fresh resources to process sinks. A flow balance constraint over the process sources ($P_i$) that supplies the process sinks and contributes to the waste streams can be written as:

$$P_i = \sum_{i=1}^{N_{source}} p_{i,j} \times Y_{i,j} + p_{i,waste} \tag{7}$$

where $i$ = 1, 2, … N$_{source}$ is the index of process sources, $p_{i,j}$ is the flow from process sources to process sinks, $p_{i,waste}$ is the flow from process sources to waste streams, and $Y_{i,j}$ is the binary variable ($Y_{i,j}$ = 1 if the finishing time of source $i$ operation is less than or equal to the starting time of sink $j$ operation). The overall mass and concentration balances over the process sinks ($S_j$) are expressed as:

$$S_j = \sum_{i=1}^{N_{source}} p_{i,j} \times Y_{i,j} + \sum_{r=1}^{N_{fresh}} f_{r,j} \tag{8}$$

$$S_j \times c_j = \sum_{i=1}^{N_{source}} p_{i,j} \times b_i \times Y_{i,j} + \sum_{r=1}^{N_{fresh}} f_{r,j} \times a_r \tag{9}$$

where $a_r$ , $b_i$ , and $c_j$ are the contaminant concentration of the fresh resource stream, process source, and process sink, respectively.

## 4. Methodology for Combined Scheduling and Water Reuse

In this paper, a sequential framework for integrated scheduling and water reuse optimization is proposed. The sequence of steps employed in the framework can be described as follows. It starts with optimizing the schedule for maximum profit or minimum makespan as the objective function. The output from the optimization is a schedule which can be represented in the form of Gantt chart. This solution is not necessarily unique, however. In most cases, there exist alternative solutions to the scheduling formulation. Hence, such possibilities are explored next − this is done using an integer cut method that is invoked through stochastic search method. This is done by adding a set of constraints of size $L$ in the form of the starting time of various tasks on process units, i.e., the binary variables $Y_{ijk}$, which have not been previously specified in the original formulation. For instance, if the stochastic search specifies that Task 1 has to be performed in Unit 2 at time slot 3, the additional constraint takes the form of $Y_{123} = 1$. On the other hand, if it specifies that Task 1 not to be performed in Unit 2 at time slot 3, the additional constraint is then $Y_{123} = 0$. If a new solution is obtained, it is then an alternate schedule – such a schedule is termed an alternate optima if it achieves the same optimal value of the objective function. This procedure is iterated over $N$ different sets of cuts to generate as many feasible alternatives as possible. The subsequent step of the procedure involves water reuse synthesis to each of these proposed schedules. For this, the entire schedule horizon is split into time intervals by associating the boundaries of these intervals with the water flows requirement of tasks. The freshwater consumption within each time interval is minimized using a source-sink allocation method that allows optimal design of water reuse network structure. The combined outputs from scheduling and water reuse optimization then yield the complete economic measures for the process.

## 5. Application to Case Study

To illustrate the methodology, we have used the following case study that is adapted from Cheng and Chang (2007). In this process, two products Prod1 and Prod2 are to be produced from three materials FeedA, FeedB and FeedC. Figure 1 shows the state-task-network (STN) of the process. Table 1 shows information on the processing times of the tasks, units and storage capacity, inventory of materials while Table 2 describes the water requirement for each of the tasks. The freshwater and wastewater costs are assumed to be \$0.1 and \$ 0.05 per kg, respectively. The production demand is 200 kg for both Prod1 and Prod2. The objective here is optimization of the schedule with respect to makespan and total water cost (freshwater and wastewater).

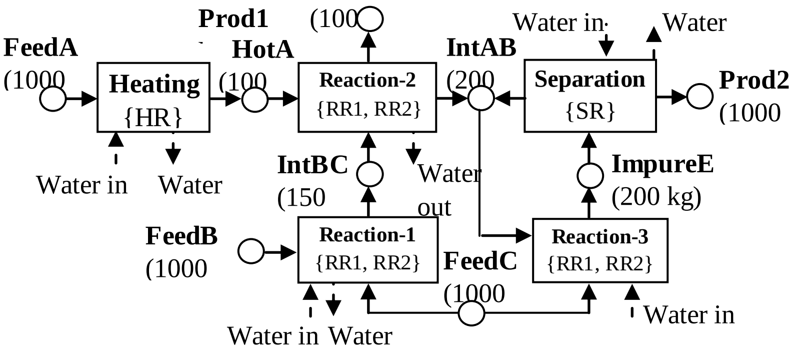


*Figure 1: STN of a process. The numbers in brackets are the maximum storage size.*

This case study has been successfully solved using the proposed sequential optimization methodology. We divided the horizon into 8 time slots. We set the number of cut variables to 6, that is, in each iteration, six tasks were pre-assigned to different units at different slots. Figure 2 shows the optimal schedule with makespan of 19.96 h – this is the global optimal value. The total water cost for this schedule is \$81.44 which corresponds to 414.29 kg of freshwater use and 800.11 kg of wastewater generation. To illustrate the procedure for calculating the water cost, consider Figure 3 which shows the water source and sink within the time interval 2.694 – 4.036 h. Using the source-sink allocation method, the minimum freshwater demand and wastewater generation at this interval can be calculated as 10 and 25 kg/h, respectively. This procedure is thus repeated for all other time intervals to obtain the total water cost of the schedule. Figure 4 shows an alternate schedule from the scheduling model. This alternate schedule has all tasks differing in size and timing compared to the optimal schedule in Figure 2.

*Table 1: Task, unit and stream information of batch case study*

| Task | Max inlet pollutant concentration (ppm) | Max outlet pollutant concentration (ppm) | Unit | Max batch size (kg) | $\alpha_{ij}$ (h) | $\beta_{ij}$ (h) |
|---|---|---|---|---|---|---|
| H | 0 | 5 | HR | 100 | 0.667 | 0.007 |
| R1 | 6 | 14 | RR1 | 50 | 1.334 | 0.027 |
| | | | RR2 | 80 | 1.334 | 0.017 |
| R2 | - | 10 | RR1 | 50 | 1.334 | 0.027 |
| | | | RR2 | 80 | 1.334 | 0.017 |
| R3 | 7 | - | RR1 | 50 | 0.667 | 0.013 |
| | | | RR2 | 80 | 0.667 | 0.008 |
| S | 10 | 15 | SR | 200 | 1.334 | 0.007 |

*Table 2: Type of water-using operation for each task*

| Task | Water requirement | Ratio of water flow to batch size |
|---|---|---|
| H | Inlet-outlet simultaneous | 1 |
| R1 | Inlet-outlet sequential | 0.5 |
| R2 | Outlet only | 0.5 |
| R3 | Inlet only | 1 |
| S | Inlet-outlet sequential | 0.5 |

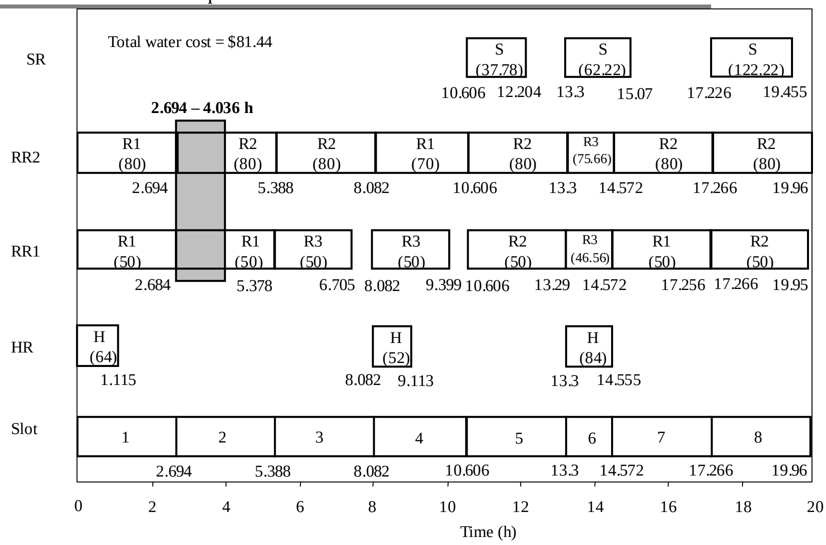


*Figure 2: Optimal schedule with minimum makespan.*

In this case, the makespan of the alternate schedule is 20.02 h − this is the local optima of the scheduling optimization problem. However, the total water cost for this schedule is lower. In this case, the total water cost is $78.05 which corresponds to 391.7 kg freshwater and 777.6 kg wastewater. This highlights a trade-off between makespan and the water cost.

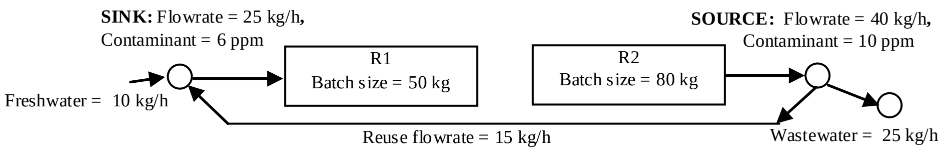


*Figure 3: Water reuse network for interval 2.694 − 4.036 h.*

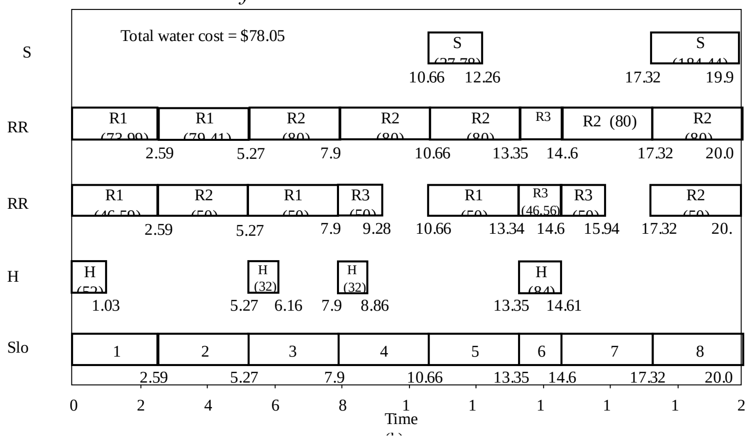


*Figure 4: Alternate schedule with longer makespan but lower total water cost*

## 6. Conclusions

We propose a novel sequential methodology for incorporating water reuse optimization in batch process scheduling. The method proposed here differs from other sequential methods published in literature in that the water reuse synthesis problem is solved with the intent to retain the optimality of the scheduling solution. The method has been tested successfully using a literature case study.

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