Optimum Water Network Design for Multipurpose Batch Plants with an Electrodialysis Central Regeneration Unit*

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Abstract—This paper presents a mathematical formulation for the simultaneous optimization of the production schedule and utility consumption of a multipurpose batch plant. The amount of wastewater generated is minimized through the exploration of direct, indirect, and regeneration reuse opportunities within the plant. Water regeneration is achieved through partial purification of highly contaminated wastewater using electrodialysis (ED). A design model for the ED process is included in the formulation in order to minimize the amount energy consumed by the regenerator simultaneously with the amount of water used by batch operations. The resultant model was applied to a case study and proved to significantly decrease the freshwater usage by up to 41%, hence increasing the overall plant profit.

I. INTRODUCTION

Water is one of the most abundant natural resources in the world, and arguably the most important to life on earth. The demand of freshwater has drastically increased due to rapid industrial and population growth, and economic expansion in many regions worldwide. Consequently, there have been calls for the sustainable usage of water by different industries through the development of adequate water management methods. This can be achieved through process integration techniques such as direct, indirect, and regeneration reuse of water. Batch processes are very attractive due to their high level of flexibility and ability to produce high quality and low volume specialty chemicals.

Different methodologies have been developed by researchers to minimize freshwater use in batch processes. These techniques can be classified as insight based and mathematical modelling. Insight based techniques include graphical and algebraic techniques which give the engineer the ability to find possible reuse opportunities and design the resultant water network. Their main drawback is the inability to cater for multiple contaminants and optimize the schedule of batch processes. Mathematical modelling techniques on the other hand can handle complex problem since they are not limited in dimension.

Mathematical formulations developed for the optimization of water usage in batch processes usually consider a predefined production schedule (Almato et al., 1999; Lee et al., 2013). This approach finds its merit in simplifying the problem by reducing its complexity. However, the time dimension essential in batch processes is suppressed which leads to a suboptimal batch water network. Direct and indirect water reuse opportunities have been extensively explored in existing mathematical formulations for batch processes (Kim and Smith, 2004; Majozi, 2005; Majozi and Gouws, 2009), while regeneration reuse has received less attention. Wastewater regeneration not only increases reuse opportunities for water but also ensures that problems such as contaminant build-up are avoided in the plant. Authors that have considered regeneration reuse in batch processes used black box approaches to predict the regenerator performance (Zhou et al., 2009; Adekola and Majozi, 2011). These approaches generally result in an inaccurate cost of the regeneration units since a linear cost function and maximum liquid recovery are assumed without quantifying the amount of energy consumed.

Presented in this paper is a MINLP formulation for design and synthesis of a water network in multipurpose batch plants. It determines the maximum plant profit by simultaneously optimizing the production schedule and minimizing the usage of freshwater. Minimum freshwater consumption is achieved by exploring direct, indirect and regeneration reuse within the plant. Wastewater regeneration is achieved by partial purification using an electrodialysis (ED) regenerator and a design model is embedded in the overall formulation. This allows for the energy consumed by the regenerator to be accounted for in the total water network cost. Furthermore, storage tanks utilized in the water network are designed and optimized.

II. PROBLEM STATEMENT

The problem addressed in this paper can be stated as follows.

Given:

(i) The production recipe for each product, the available processing units and their capacities,
(ii) The task processing time and washing time in each unit,
(iii) The maximum storage capacity for each material,
(iv) The mass load and maximum concentrations of each contaminant,
(v) The available water storage tanks and their design capacity limits,
(vi) Membrane properties and design parameters of the electrodialysis (ED) regenerator, and

(vii) The time horizon of interest, determine the optimum schedule of a multipurpose batch plant that generates maximum profit, i.e. a plant design with minimum utility consumption (water and energy usage), optimum design of the ED regenerator and optimum sizes of storage tanks.

III. MATHEMATICAL FORMULATION

The mathematical formulation developed in this work integrates a scheduling model, a model for the water network design and synthesis and the ED design model. The design and synthesis of the water network is based on the superstructure depicted by Fig. 1. It shows all possible interconnections between batch processing units, storage tanks and the ED regenerator. Units $j$ and $j'$ represent two distinct units processing water-using operations which can possibly be integrated through direct reuse. This entails that effluents from unit $j$ can potentially be reused directly into unit $j'$ while unit $j'$ can also directly transfer its effluents into unit $j$. Direct reuse can only occur if the finishing time of the operation generating water and the starting time of the operation receiving water coincide. Indirect reuse on the other hand allows effluents from processing units to be temporarily stored for later reuse, thus relaxing the abovementioned timing constraint. In this formulation, indirect reuse is facilitated by the wastewater storage tank as shown in Fig. 1. Regeneration reuse is achieved by using both the wastewater and the diluate storage tanks where the former feeds wastewater to the regenerator and the latter receives treated water from the regenerator as shown in Fig. 1. The diluate tank can then be connected to any unit as a potential source of water. The regeneration of water increases the opportunities of wastewater reuse by reducing its contaminant level to meet the contaminant constraints of certain water-using operations. It is worth mentioning that the number of storage tanks as depicted by the superstructure is not subjected to change. This results from the fact that the regenerator is modelled to operate semi-continuously. Therefore, two storage tanks are required to ensure a smooth connection between the various units operating in a batch mode and the regeneration process.

A. Production scheduling model

The scheduling model ensures that the time dimension which is inherent in batch processes is captured. It determines the time at which a specific task happens, the size of the processed batch and the sequencing of tasks within a given time horizon. The scheduling model adopted in this formulation was developed by Seid and Majozi (2012). The model has proven to be robust in terms of handling shared resources, and requires less time points compared to other formulations. It consists of allocation constraints, material balance constraints, task duration constraints, sequencing constraints, storage constraints for processing materials, tightening and time horizon constraints.

B. Material balance for water network

The material balance constraints for water operations are formulated following the superstructure illustrated by Fig. 1. The water balance around unit $j$ is illustrated by Equations (1) and (2). Equation (1) states that the amount of water entering unit $j$ at time point $p$ is the summation of reuse streams from unit $j'$, freshwater stream as well as water streams coming from storage tanks $k$. Equation (2) defines the amount of water leaving unit $j$ as the sum of reuse water to other units operating
at time point \( p \), amount of water sent from unit \( j \) to storage tanks \( k \) and the effluent water stream.

\[
\text{mw}^{\text{in}}(s_j^\text{in},p) = \text{mw}^{f}(s_j^\text{in},p) + \sum_{s_j'} \text{mw}^{f}(s_j'^\text{in},s_j^\text{in},p) \\
+ \sum_k \text{ms}^{\text{out}}(s_j^\text{in},k,p) \\
\forall p \in P, s_j^\text{in}, s_j'^\text{in} \in S_j^\text{in}, k \in K \tag{1}
\]

\[
\text{mw}^{\text{out}}(s_j^\text{in},p) = \text{mw}^{f}(s_j^\text{in},p) + \sum_{s_j'} \text{mw}^{f}(s_j'^\text{in},s_j^\text{in},p) \\
+ \text{ms}^{\text{in}}(s_j^\text{in},p) \\
\forall p \in P, s_j^\text{in}, s_j'^\text{in} \in S_j^\text{in} \tag{2}
\]

Additional constraints include contaminant balance around processing units, water and contaminant balance around the storage vessels and the regenerator unit.

### B. Electrodialysis design model

The ED design model determines the dimensions of the regenerator required for a specific plant and the amount of energy it consumes. This allows for a more accurate cost of regeneration to be obtained and for a trade-off between the amount of freshwater intake and energy consumption to be made during optimization. The model followed the MINLP formulation developed by Lee et al. (2002). It consists of a set of constraints that determine design parameters such as the total membrane area required, the dimensions of the ED stack, and the required pumping and desalination energy. For instance, the total membrane area required for a desalination process was calculated using the following correlation.

\[
A = \left( \frac{\ln \left( \frac{C^f C^l}{C^d C^d \rho C^\Delta}}}{\delta} \right) zFQd C^{dl} \\
+ \left( \frac{C^{dl}}{C^c} + 1 + \frac{\rho C^\Delta}{\delta} \right)^{\frac{1}{\rho}} \beta \epsilon \right) \tag{3}
\]

### C. Sequencing constraints for the water network

In addition to the production scheduling constraints, the formulation included additional constraints which aimed to ensure that any reuse opportunity found within the plant follows the optimum schedule of batch operations. As an illustration, Equations (4) and (5) together ensure that the finishing time of the task discharging water and the starting time of the task receiving water coincide for direct reuse to occur between two units.

\[
tw^p(s_j^\text{in},p) \geq tw^d(s_j^\text{in},p) - H(1 - y^r(s_j^\text{in},s_j^\text{in},p)) \\
\forall p \in P, s_j^\text{in}, s_j'^\text{in} \in S_j^\text{in} \tag{4}
\]

\[
tw^p(s_j^\text{in},p) \leq tw^d(s_j^\text{in},p) + H(1 - y^r(s_j^\text{in},s_j^\text{in},p)) \\
\forall p \in P, s_j^\text{in}, s_j'^\text{in} \in S_j^\text{in} \tag{5}
\]

### D. Objective function

The objective function of this work consists of maximizing the annualized profit of the plant as shown by Equation (6). It takes into account the production revenue, the costs of freshwater and wastewater treatment, the capital and operating costs of ED unit, as well as the costs of storage tanks used.
TABLE I. LIMITING DATA FOR WATER INTEGRATION

<table>
<thead>
<tr>
<th>Units</th>
<th>Task</th>
<th>Max inlet concentration (ppm)</th>
<th>Max outlet concentration (ppm)</th>
<th>Contaminant loading (g MgCl₂/kg batch)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heater</td>
<td>Heating</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Reactor 1</td>
<td>Reaction 1</td>
<td>500</td>
<td>1,000</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Reaction 2</td>
<td>10</td>
<td>200</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Reaction 3</td>
<td>150</td>
<td>300</td>
<td>0.2</td>
</tr>
<tr>
<td>Reactor 2</td>
<td>Reaction 1</td>
<td>50</td>
<td>100</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Reaction 2</td>
<td>30</td>
<td>75</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Reaction 3</td>
<td>300</td>
<td>2,000</td>
<td>0.2</td>
</tr>
<tr>
<td>Still</td>
<td>Separation</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

where no process integration was employed. For this case study, the proposed formulation was able to reduce freshwater intake by 41.1% while maintaining the same production revenue. It is worth mentioning that the base case, i.e. the formulation with no integration, does not cater for addition costs of the water network such as regeneration and storage costs. Hence, no comparison is performed between the two cases in terms of the annualized plant profit as shown in Table II. Table II also gives the model statistics for both cases and as it can be seen, the proposed formulation yielded a higher CPU time. This is explained by the higher number of constraints, variables and nonlinear terms that the resultant formulation entailed. Although the number of constraints and variables is roughly doubled when compared to the base case, the drastic increase in computational time is mainly due the high nonlinearity of the proposed formulation. Complex nonlinear terms are found in the design constraints of the ED regenerator and constraints involved in the synthesis of the water network yield a large number of bilinear terms.

The Gantt chart obtained as a result of the implementation of the proposed formulation for this case study is shown in Fig. 3. It gives the sequence of tasks and network configuration the plant has to follow in order to achieve the optimum plant

IV. ILLUSTRATIVE EXAMPLE

The developed formulation was applied to a literature example of a multipurpose batch plant. The process aims to manufacture two products using three different raw materials. The recipe of production involves a heating task, three reactions occurring in two reactors and a separation process as shown in Fig. 2. The scheduling data were obtained from Kondili et al. (1993), the data pertaining to water integration were taken from Halim and Srinivasan (2011) and the design parameters of the ED process were adapted from Tsiakis and Papageorgiou (2005). Table I gives a set of parameters pertaining to washing operations for units with cleaning requirements for the removal of magnesium chloride (MgCl₂). From Table I, it can be seen that washing operations are only required for the two reactors to avoid contamination between the three different reactions occurring in these units. The formulation considered a 12h time horizon and the regenerator was modeled with a fixed removal ratio of 0.95

A. Computational results and discussion

Table II gives the computational results for case study II while comparing them with results obtained from the case
The model yielded a water network with freshwater use, indirect and regeneration reuse opportunities whilst no direct reuse opportunities were found. The regenerator operated for 2.6h with the process starting at time 5.9h within the time horizon. The delay in the starting time of the regeneration process is explained by the fact that the wastewater storage tank needed to have a considerable amount of water to allow the ED regenerator to operate continuously. The short operation time of the process is due to the fact that this formulation forces both the diluate and wastewater storages to be empty at the end of the time horizon of interest. In a cyclic scheduling problem, this constraint could be relaxed to allow for reuse between different productions cycles within the facility. The design specifications of the ED regenerator required for this plant are given in Table III. The regeneration process requires an ED stack of 0.7 m length which contains 10 cell pairs and requires a total membrane area of 5.9 m². The energy requirements, flow velocity and process efficiency of the electrodialysis regenerator are also included in Table III.

V. CONCLUSION

The presented formulation has proved to be effective to achieve minimum water usage in batch processes by achieving 41 % reduction in freshwater consumption when applied to a literature example. Although the current work focuses on the usage of water as a mass separating agent (MSA), it can be readily adjusted to cater for both mass transfer and non-mass transfer based operations. However, the presented technique is limited to single contaminant cases which are very seldom in the process industry. The model also obtains solutions in a considerably high CPU time. Future work will therefore extend and modify this formulation to account for multiple contaminants and medium to long scheduling which involves cyclic production. Substantial effort will also be directed towards reducing the CPU time by adopting preprocessing techniques or relaxation techniques that can reduce the degree of non-linearity that the model exhibits.

NOMENCLATURE

Sets

\[ P \quad \{ p \mid p \text{ represents a time point} \} \]

\[ J \quad \{ j \mid j \text{ denotes a unit} \} \]
$S^m_j \{s^m_j \mid s^m_j \text{ is an effective state representing a task performed in unit } j \}$

$K \{k \mid k \text{ is a storage tank}\}$

$s_p \{s_p \mid s_p \text{ is state representing a product}\}$

**Parameters**

$SP(s_p)$ selling price of product

$C^{fw}$ freshwater cost in c.u/kg

$C^{cw}$ cost of wastewater treatment in c.u/kg

$C^{el}$ electric power cost

$C^{mb}$ membrane capital cost

$C^{ist}$ installation cost of storage tanks

$C^{vst}$ purchased cost of storage tanks

$n$ cost coefficient of storage tanks

$i^{max}$ estimated maximum membrane equipment life

$t^d$ total operating time per year

$z$ electrochemical valence

$\beta$ effective area of cell factor (spacer shadow)

$\delta$ thickness of an electrodialysis cell

$F$ faraday constant

$\varepsilon$ current utilization

$\rho$ total resistance of anionic and cationic exchange membrane

$\psi^{eq}$ equivalent conductance of water

$H$ time horizon of interest

**Variables**

$mw^{in}(s^m_j,k) \text{ amount of material processed by a task at time slot } p$

$mw^{out}(s^m_j,k) \text{ amount of water entering a unit at time slot } p$

$mw(s^m_j,s^m_{j'},k) \text{ amount of water reused from unit } j \text{ to } j' \text{ at time slot } p$

$mw^f(s^m_j,k) \text{ amount of water sent from unit } j \text{ to effluent at time slot } p$

$mw^f(s^m_j,k) \text{ amount of freshwater used in unit } j \text{ at time slot } p$

$ms^{in}(s^m_j,k) \text{ amount of water transferred from unit } j \text{ to storage at time slot } p$

$ms^{out}(s^m_j,k) \text{ amount of water transferred from storage } k \text{ to unit } j \text{ at time slot } p$

$t^w(s^m_j,k) \text{ starting time of a task at time slot } p$

$t^p(s^m_j,k) \text{ finishing time of a task at time slot } p$

$tw^{in}(s^m_j,k) \text{ starting time of washing task at time slot } p$

$tw^f(s^m_j,k) \text{ finishing time of washing task at time slot } p$

$y^r(s^m_j,s^m_{j'},k) \text{ binary variable associated with the existence of a direct reuse stream from } j \text{ to } j' \text{ at time slot } p$

$y^s(k) \text{ design capacity of storage tank } k$

$A \text{ total membrane area required for desalination}$

$Q^d \text{ dilute stream flowrate}$

$Q^{dil} \text{ dilute product flowrate}$

$C^{dil} \text{ outlet concentration of dilute stream}$

$C^{des} \text{ concentration of concentrate stream}$

$C^{comp} \text{ concentration of outlet concentrate compartment stream}$

$C^f \text{ concentration of inlet feed stream to the regenerator}$

$L^{des} \text{ specific desalination energy required by regenerator}$

$E^{pu} \text{ pumping energy required by regenerator}$

$i^{prac} \text{ practical limiting current density}$

**REFERENCES**


