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Synthesis of Zero Effluent Multipurpose Batch Processes Using Effective Scheduling

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Abstract

Wastewater minimization in batch processes has gained much attention in the very recent past. Mainly 2 reasons lie behind this heightened interest. Firstly, batch operations are inherently flexible, which renders them ideal for volatile conditions that characterize today's markets. Secondly, batch processes tend to produce highly toxic effluent streams, albeit in relatively small quantities in comparison to their continuous counterparts. The stringent environmental conditions militate against the latter characteristic of batch plants, hence the need to eliminate or minimize effluent.

In most published literature, wastewater minimization is achieved through water reuse, water recycle, water regeneration reuse and water regeneration recycle. These concepts generally exclude the possibility of water being used as a key ingredient in the water using operations. However, some pharmaceutical and agrochemical operations, which traditionally operate in a batch mode, offer a unique opportunity to use recycle or reuse water as the main constituent of the final product. In some of these operations water constitutes more than 90% of the final product makeup. The problem addressed in this paper bears this feature, which consequently allows the batch processes to operate in a near-zero effluent mode.

Moreover, the question of the number and size of the vessels used in a batch processing facility has always posed a problem. The incorrect approach to the synthesis of a batch plant can lead to the situation where processing vessels are over sized and even the possibility of idle processing vessels. This could pose a possible over capitalisation of an operation. In essence, an optimal design of a batch processing plant is determined by considering the scheduling of operations in the synthesis phase. The mathematically based method presented in this paper deals with the synthesis of a batch plant operating in the fashion mentioned above. The method determines the optimal size and number of processing vessels and wastewater storage vessels, while scheduling the operation in such a manner as to operate in a near-zero effluent fashion

Keywords: effluent, minimization, process, batch.

1. Introduction

Concern over the impact of industry on the environment is greater now than ever. Environmental legislation is becoming ever more stringent in an effort to reduce the negative impact industry has on the environment. Coupled with this is the fact that society is becoming ever more conscious of the state of the environment. Traditional end-of-pipe treatment methods are not always economically viable to meet stringent effluent targets. Therefore, process integration techniques are becoming ever more important in reducing the amount of effluent produced.

Wastewater minimisation in batch processes has slowly gained some attention in the past few years. Past wastewater methodologies can roughly be divided into two main categories, namely, graphical techniques [1,2,3] and mathematical techniques [4,5,6,7]. Graphical techniques have their roots in graphical techniques developed for continuous processes, while mathematical techniques have their roots in mathematical programming.

Past methodologies for wastewater minimisation in batch processes have been mainly focused on mass transfer based operations. In such operations water is consumed at the beginning of a unit operation and produced at the end. Reuse between different units is governed by availability of wastewater and the concentration of the contaminants present in the wastewater. Also, operations do exist where wastewater is produced as a result of a cleaning operation. If products produced from such operations require water as a raw material, it should be possible to reuse the wastewater as part of product formulation, since the wastewater is only contaminated with the residue in the previous batch of the same or another compatible product. The wastewater, when reused in this manner, is significantly reduced, hence the plant can operate in a near zero effluent fashion. Furthermore, the residue present in the wastewater is recovered, which could provide substantial economic benefits.

A mathematical formulation for the synthesis of plants operating in a near zero effluent mode of operation has been developed. The formulation determines the number and size of processing vessels and storage vessels, while ensuring wastewater is reused as part of product. Since product integrity is of paramount importance, wastewater containing different contaminants is not allowed to mix. Hence, there is a dedicated storage vessel for each type of wastewater. Furthermore, the methodology is derived to take into account operations where the contaminant mass in the wastewater is negligible and where it is not negligible.

2. Problem Statement

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

i) required production over a given time horizon,
ii) product recipe and production times,
iii) maximum number of processing vessels and storage vessels, and
iv) maximum and minimum capacity of processing vessels and storage vessels,

determine the plant design that will minimise cost, i.e. the design with the optimal number and size of processing vessels and storage vessels as well as minimum effluent generation.

3. Mathematical Formulation

The following sets, variables and parameters are used in the mathematical formulation

Sets

$S_{in,j} = \{s_{in,j} \mid s_{in,j} =$ input state into processing vessel $j\}$
$J = \{j \mid j =$ processing vessel$\}$
$U = \{u \mid u =$ storage vessel$\}$
$P = \{p \mid p =$ time point$\}$

Variables

$f_w(s_{in,j},p)$	mass of water used for a washout for state $s_{in,j}$ at time point p
$f_e(s_{in,j},p)$	effluent water from processing vessel j at time point p
$\mathrm{v}_{proc}(j)$	capacity of processing vessel j
$\mathrm{v}_{stor}(u)$	capacity of storage vessel u
$e_{proc}(j)$	existence binary variable for processing vessel j
$y(s_{in,j},p)$	binary variable showing usage of state $s_{in,j}$ at time point p

Parameters

Ψ_{wash}	factor relating the size of a processing vessel to the amount of washout water
V^{min}	minimum capacity of a processing vessel
V^{max}	maximum capacity of a processing vessel
α_{proc}	cost of a processing vessel
β_{proc}	cost of a processing vessel based on size
α_{stor}	cost of a storage vessel
β_{stor}	cost of a storage vessel based on size
C_e	treatment cost of the effluent water

3.1. Mass balance constraints

The first part of the mathematical formulation constitutes the mass balance constraints. Mass balances are done over a processing unit and a storage vessel. The mass balances over a processing vessel can be divided into two main groups. The first group comprises of all the constraints related to product generation and the second group, all the constraints related to a washout. The mass balances related to product include a raw material balance and a mass balance over a processing unit. The raw material balance ensures that the correct ratio of water and other raw materials is used for a product. Apart from the two balances there are also capacity constraints. The washout mass balances comprise of an inlet water balance and an outlet water balance. The amount of water used for a washout is dependent on the size of the processing vessel, and is determined using Equation (1), which is the inlet water balance. Equation (1) contains a non-linear term that is linearised using a Glover transformation[8].

$$f_w\left(s_{in,j},p\right)=\Psi_{wash}\mathrm{v}_{proc}(j)\,y\left(s_{in,j},p\right),\ \forall\ j\in J, s_{in,j}\in S_{in,j} \tag{1}$$

Mass balances over a storage vessel include a water balance and if necessary a contaminant balance. The formulation is capable of dealing with both the scenario where the contaminant mass in the washout water is negligible and not.

3.2. Scheduling constraints

Since the processes dealt with are batch processes the inherent discontinuous nature has to be taken into account. Scheduling constraints are formulated to ensure that the processing of raw material occurs after a washout has taken place, i.e. once a vessel has been cleaned, and after a previous batch has finished processing. Further constraints ensure a washout begins directly after the product has been removed from a processing vessel. Duration constraints are formulated for the production and washouts.

Apart from the above constraints, the reuse of water in product also has to be scheduled. Constraints are formulated to ensure that water directly reused between two processing vessels occurs at the end of a wash from the source and the beginning of the processing of the sink. This is similar for indirect reuse, however, in this instance the timing of water moving to and from a storage vessel must coincide with the ending time of a washout and the beginning of product processing, respectively.

The formulation also caters for a maximum storage time of washout water in a storage vessel. Constraints are formulated to ensure the difference between the inlet time and outlet time of water from a storage vessel is less than the maximum allowable storage time.

3.3. Design constraints

The final constraints considered are the design constraints. The first of these are the existence constraints. An existence binary variable is defined for each processing vessel and each storage vessel. If a processing vessel processes material within the time horizon then the binary variable is set to one. This is similar for a storage vessel. The upper and lower bounds of a processing vessels size are defined using Equation (2) and similar constraint holds for a storage vessel.

$$e_{proc}(j)V^{\min} \le v_{proc}(j) \le e_{proc}(j)V^{\max} \quad \forall\ j \in J \tag{2}$$

3.4. Objective function

The objective function in the formulation is the minimisation of overall cost. In this instance the overall cost arises from the cost of the processing vessels, the cost of the storage vessels and the treatment costs of the effluent water. The objective function is given in Equation (3). The objective function is linear, as it was assumed that the cost of a processing vessel and storage vessel is a linear function of the size of the vessel.

$$\begin{aligned} \min \sum_{j} \alpha_{proc} e_{proc}(j) + \beta_{proc} \mathrm{v}_{proc}(j) + \sum_{u} \alpha_{stor} e_{stor}(u) + \beta_{stor} \mathrm{v}_{stor}(u) \\ + \sum_{s_{in,j} p} C_e f_e(s_{in.j}, p) \qquad \forall\ j \in J, u \in U, s_{in,j} \in S_{in,j}, p \in P \end{aligned} \tag{3}$$

4. Industrial Case Study

The methodology was applied to an industrial case study stemming from a pharmaceuticals mixing facility. The industrial case study involves the design of a small mixing operation that produces three different products. Each product has a fixed ratio between the amount of water used in the product and other raw materials. For product 1 the ratio of water to other raw material is 80:20, for product 2 the ratio of water to other raw material is 82.5:17.5 and for product 3 the ratio is 90:10. 4000kg, 6000kg and 5000kg are required for products 1, 2 and 3 over a 24 hour time horizon respectively. The number and size of batches required to fulfill the production requirements is not known. A maximum of 4 mixing vessels can be used with a minimum capacity of 1000kg and a maximum capacity of 4000kg. Maximum reuse opportunities are ensured through the inclusion of the possibility of wastewater storage. Three distinct types of wastewater will be produced from the cleaning operation, due to the three different products mixed. Each type of wastewater has the possibility of being stored in a distinct storage vessel. The minimum and maximum capacity of each storage vessel is 500kg and 1500kg, respectively.

The amount of water used for a washout was dependent on the size of the processing vessel. For every 1000kg increase in the mixers size the amount of water used for a washout would increase by 200kg. Therefore, Ψ_{wash} has the value of 0.2.

The constants used for the objective function are given in Table 1.

Table 1. Cost data used in industrial case study

Constant	Value
α_{proc}	400 (c.u./mixer)
β_{proc}	0.8
α_{stor}	100 (c.u./storage vessel)
β_{stor}	0.5
C_e	5 (c.u./kg wastewater)

The problem was formulated in GAMS and subsequently solved using CPLEX. The final design required 4 mixing vessels and no storage vessels for the wastewater. Mixing vessels 2, 3 and 4 each had a capacity of 1000kg and mixer 1 had a capacity of 3000kg. The total amount of effluent generated from the process was 600kg and the objective function had an optimal value of 9400 c.u. Effluent is generated, since there is no opportunity for further reuse of the wastewater at the end of the time horizon. The solution time was 7665 CPU seconds using a Pentium 4, 3.2 GHz processor. The problem had 423 binary variables and 2855 continuous variables. The Gannt chart showing the production schedule is given in Figure 1. The black striped boxes represent a production and the grey boxes represent a mixer being washed. The “P” in the striped boxes represents product and the number after the “P” represents the respective product number. The bold numbers represent the amount of water reused in product.

From Figure 1 one can see that mixer 2 is dedicated to the production of product 2. This is similar for mixer 3, which is dedicated to the production of product 3. Mixers 1 and 4, however, produce batches of all three products. The size of the batches produced from each mixer is determined by the optimal size of the mixer, hence the size of the batches from mixers 2, 3 and 4 are 1000kg and from mixer 1 is 3000kg. Interesting to note is that mixer 3 does not produce any effluents throughout the time horizon.

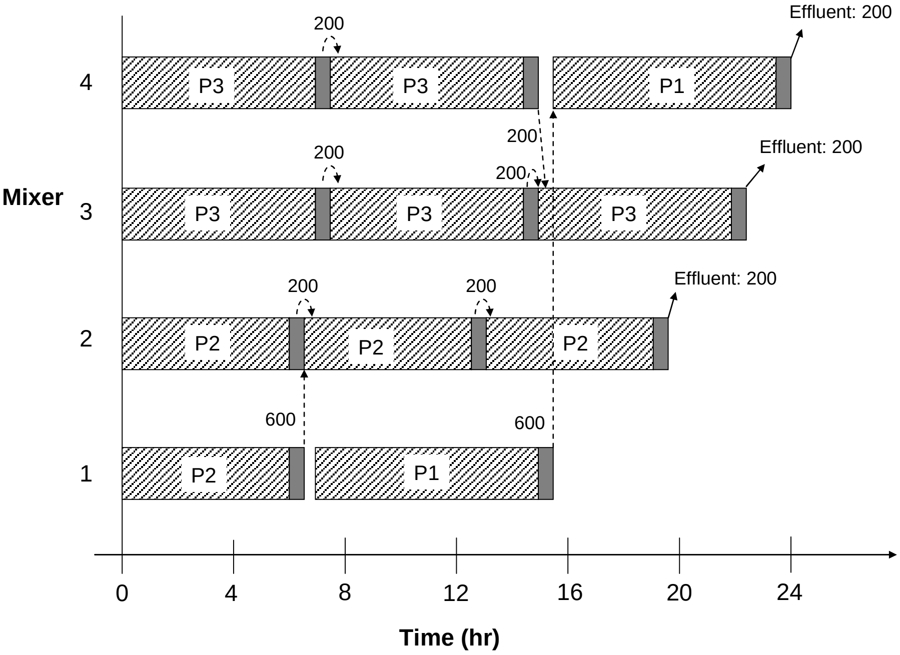

Figure 1. Gannt chart representing the production schedule

5. Conclusions

A methodology for the synthesis of batch plants incorporating the zero effluent mode of operation has been presented. In the zero effluent mode of operation, the wastewater generated in the operation is reused as a constituent in a batch of subsequent compatible product. The methodology determines the optimal size and number of processing vessels and wastewater storage vessels.

The methodology has been applied to an industrial case study. The industrial case study involved the design of a pharmaceuticals mixing operation that produces three products. The resulting design for the industrial case study had 4 mixing vessels and no wastewater storage vessels. Three of the mixing vessels had a capacity of 1000kg and the remaining mixing vessel had a capacity of 3000kg.

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