Wastewater Minimisation Using Inherent Storage Capacity in Multipurpose Batch Plants: An Unexplored Dimension

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Wastewater minimisation in batch processes is becoming evermore important as environmental legislation becomes more stringent and fresh water sources are becoming scarce. Added to this, is the need for batch plants to occupy the least amount of space. Therefore, one would like to minimise any storage in a batch process, since storage takes up a large amount of space with relatively low economic return.

Generally, in any batch process there are processing vessels that are idle at some point during a given time horizon. In essence, any processing vessel standing idle can be used as a storage vessel. Under correct conditions, the idle processing vessels can be used as storage for wastewater. This would mean that the size of dedicated wastewater storage is reduced and in some cases not even required. Furthermore, the capital utilisation of the installed processing vessels is greatly increased.

Past wastewater minimisation methodologies in batch processes (Wang & Smith, 1995, Kim & Smith, 2004, Foo et al., 2005; Majozi, 2005) have generally accepted that there will always be storage vessels dedicated to the storage of wastewater. The usage of wastewater storage allows for greater reuse opportunities since it enables the inherent time constraint of batch processes to be bypassed to a certain extent. Therefore, the usage of wastewater storage will enable a lower overall wastewater target. Majozi et al. (2006) explored the idea of inherent wastewater storage in idle processing vessels in their graphical method for wastewater minimisation. The authors make use of an inherent storage diagram to determine possible storage opportunities. Since this is a graphical technique, it suffers in that the schedule has to be determined a priori. This is an intrinsic limitation of all graphical techniques.

The usage of the inherent storage within a plant for wastewater storage has been included into a mathematical wastewater minimisation technique in batch processes. The technique has its roots in the scheduling technique for batch processes proposed by Majozi and Zhu (2001), which is based on the uneven discretisation of the time horizon. The technique determines the minimum amount of wastewater generation through the exploitation of the inherent storage in idle processing vessels.

An illustrative example is presented and solved considering two different types of wastewater storage. In the first case, a central storage vessel for wastewater is considered without any inherent storage. In the second case no central storage is considered, but inherent storage is considered. In both cases the objective is to minimise the amount of wastewater through the exploitation of direct and indirect reuse opportunities. The solutions attained for each case achieved the same wastewater target, providing evidence that the usage of inherent storage can reduce the required size of the central storage vessel.

1. Introduction

Wastewater minimisation in batch processes is gaining importance as need for "clean" industrial operations increases. Furthermore, storage for wastewater in batch processing facilities often accounts for sizeable capital investment in the processing plant. The wastewater storage vessels are often underutilized and, therefore, the return on investment is not always favourable. One would like to minimise the storage required for wastewater in a processing facility, while not impacting negatively on the opportunities to reduce effluents. However, the focus in the past has been mainly on wastewater minimisation and not on different storage possibilities within a batch plant.

Methodologies developed in the past that deal with wastewater minimisation in batch plants can roughly be divided into graphical techniques and mathematical techniques. The graphical techniques (Wang & Smith, 1995; Foo et al., 2005; Majozi et al., 2006) have their roots in pinch analysis and in most cases are a direct extension of a graphical based technique for wastewater minimisation in continuous processes. Graphical techniques have the advantage of giving the designer insight into some interactions between the various units and any wastewater reuse bottlenecks are easily identifiable. However, graphical techniques are more suited to single contaminant problems and wastewater minimisation can only be done within a given schedule. Mathematical based techniques (Almató et al., 1997; Kim & Smith, 2004; Majozi, 2005; Gouws & Majozi, 2008) have their roots in mathematical programming and optimisation. Mathematical techniques have the advantage of being able to deal with multiple contaminants and do not require any presupposition of an optimal schedule. The disadvantage of such techniques is that the involvement of the designer ends in problem formulation, with no influence in the solution procedure leading to the final result. Consequently, these techniques have been referred to as "black box" approaches in literature.

All the methodologies mentioned previously are based on the utilisation of intermediate wastewater storage to allow for bypassing of the inherent time constraints of wastewater reuse. However, in most batch processing facilities there are idle processing vessels at some stage in the time horizon. These processing vessels can be used as water storage vessels, since any vessel standing idle can also act as a storage vessel. This concept was explored in the methodology derived by Majozi *et al.* (2006), where an inherent storage graph is drawn to show possible wastewater storage opportunities in idle processing vessels. The method proposed by Majozi *et al.* (2006), however, is based on the schedule being known a priori.

The method presented below utilises inherent storage in idle processing vessels within a wastewater minimisation framework to allow for the minimisation of wastewater. The methodology can be utilised to either minimise the size of the central storage vessel or provide alternative storage opportunities for wastewater.

2. Problem Statement

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

Given the following,

- i) the maximum inlet and outlet water concentration for each process in the plant,
- ii) the contaminant mass load in each operation,
- iii) the average task duration in each operation,
- iv) the number and the capacity of each processing vessel, and
- v) the time horizon of interest,

determine the process schedule that will result in minimum wastewater generation through the exploitation of inherent storage opportunities in idle processing units, direct reuse opportunities and central storage opportunities.

3. Mathematical Formulation

The proposed mathematical formulation involves the following sets, variables and parameters.

Sets

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P = \{p \mid p = \text{time point}\}
J = \{j \mid j = \text{unit}\}
S_{in} = \{s_{in} \mid s_{in} = \text{input state into any unit}\}
S_{out} = \{s_{out} \mid s_{out} = \text{output state from any unit}\}
S_{in,j} = \{s_{in,j} \mid s_{in,j} = \text{input state into unit j}\} \subseteq S_{in}
S_{out,j} = \{s_{out,j} \mid s_{out,j} = \text{output state from unit j}\} \subseteq S_{out}
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Variables

$m_f(s_{in,j},p)$ mass of fresh water into unit j at time point p mass of water recycled to unit j' from j at time point p mass of water to the central storage vessel from unit j at time point p mass of water from the central storage vessel to unit j at time point p mass of water from unit j' to unit j , operating in inherent storage mode, at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p time at which unit j finishes operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p	$m_u(s_{in,j},p)$	mass of water into unit j at time point p
$m_r(j,j',p)$ mass of water recycled to unit j' from j at time point p mass of water to the central storage vessel from unit j at time point p mass of water from the central storage vessel to unit j at time point p mass of water from unit j' to unit j , operating in inherent storage mode, at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p binary variable showing water into unit j , operating in inherent storage	$m_p(s_{out,j},p)$	mass water produced at time point p from unit j
$ms_{in}(j,p)$ mass of water to the central storage vessel from unit j at time point p mass of water from the central storage vessel to unit j at time point p mass of water from unit j' to unit j , operating in inherent storage mode, at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p binary variable showing water into unit j , operating in inherent storage	$m_f(s_{in,j},p)$	mass of fresh water into unit j at time point p
$ms_{out}(j,p)$ mass of water from the central storage vessel to unit j at time point p mass of water from unit j' to unit j , operating in inherent storage mode, at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p to time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p binary variable showing water into unit j , operating in inherent storage	$m_r(j,j',p)$	mass of water recycled to unit j' from j at time point p
$mstu_{in}(j,j,p)$ mass of water from unit j' to unit j , operating in inherent storage mode, at time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p $t_p(s_{out,j},p)$ time at which unit j finishes operating at time point p $tstu_{in}(j,j,p)$ time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p $tstu_{in}(j,j,p)$ binary variable showing water into unit j , operating in inherent storage	$ms_{in}(j,p)$	mass of water to the central storage vessel from unit j at time point p
time point p mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p $t_p(s_{out,j},p)$ time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p y y t	$ms_{out}(j,p)$	mass of water from the central storage vessel to unit j at time point p
$mstu_{out}(j',j,p)$ mass of water from unit j' , operating in inherent storage mode, to unit j at time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p $ystu_{in}(j',j,p)$ binary variable showing water into unit j , operating in inherent storage	$mstu_{in}(j,'j,p)$	mass of water from unit j' to unit j , operating in inherent storage mode, at
time point p inlet concentration into unit j at time point p outlet concentration from unit j at time point p time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p $y(s_{in,j}, p)$ binary variable showing water into unit j , operating in inherent storage		time point p
$c_{in}(s_{in,j}, p)$ inlet concentration into unit j at time point p $c_{out}(s_{out,j}, p)$ outlet concentration from unit j at time point p $t_p(s_{out,j}, p)$ time at which unit j finishes operating at time point p $tstu_{in}(j, j, p)$ time at which water goes to unit j , operating in inherent storage mode, from unit j ' at time point p $y(s_{in,j}, p)$ binary variable showing usage of unit j at time point p $ystu_{in}(j', j, p)$ binary variable showing water into unit j , operating in inherent storage	$mstu_{out}(j', j, p)$	mass of water from unit j' , operating in inherent storage mode, to unit j at
$c_{out}(s_{out,j}, p)$ outlet concentration from unit j at time point p $t_p(s_{out,j}, p)$ time at which unit j finishes operating at time point p $tstu_{in}(j, j, p)$ time at which water goes to unit j , operating in inherent storage mode, from unit j at time point p $y(s_{in,j}, p)$ binary variable showing usage of unit j at time point p $ystu_{in}(j', j, p)$ binary variable showing water into unit j , operating in inherent storage	,	time point p
$t_p(s_{out,j}, p)$ time at which unit j finishes operating at time point p time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p $y(s_{in,j}, p)$ binary variable showing water into unit j , operating in inherent storage	$c_{in}(s_{in,j},p)$	inlet concentration into unit j at time point p
$tstu_{in}(j,'j,p)$ time at which water goes to unit j , operating in inherent storage mode, from unit j' at time point p binary variable showing usage of unit j at time point p $ystu_{in}(j',j,p)$ binary variable showing water into unit j , operating in inherent storage	$c_{out}(s_{out,j},p)$	outlet concentration from unit j at time point p
unit j' at time point p $y(s_{in,j}, p)$ binary variable showing usage of unit j at time point p $ystu_{in}(j', j, p)$ binary variable showing water into unit j , operating in inherent storage	$t_p(s_{out,j},p)$	time at which unit j finishes operating at time point p
$y(s_{in,j}, p)$ binary variable showing usage of unit j at time point p $ystu_{in}(j', j, p)$ binary variable showing water into unit j , operating in inherent storage	$tstu_{in}(j,'j,p)$	time at which water goes to unit j , operating in inherent storage mode, from
$ystu_{in}(j',j,p)$ binary variable showing water into unit j , operating in inherent storage		unit j' at time point p
	$y(s_{in,j},p)$	binary variable showing usage of unit <i>j</i> at time point <i>p</i>
mode, from unit j' at time point p	$ystu_{in}(j',j,p)$	binary variable showing water into unit j, operating in inherent storage

Parameters

$M(s_{in,j})$	mass load added from unit j to the water stream
H	time horizon of interest

3.1 Mass Balance Constraints

The mass balance constraints that comprise the model can be divided into three sections, namely, unit mass balances, inherent storage mass balances and central storage mass balances.

Unit mass balances

The unit mass balances comprise of water and contaminant balances around a unit. An inlet water balance is given in constraint (1). The mass of water entering a unit for processing purposes is a combination of freshwater, directly reused water, water from the central storage vessel and water from inherent storage. A similar constraint holds for water leaving a processing unit.

$$m_{u}(s_{in,j},p) = m_{f}(s_{in,j},p) + \sum_{j' \in J} m_{r}(j',j,p) + ms_{out}(j,p) + \sum_{j' \in J} mstu_{out}(j',j,p),$$

$$\forall j \in J, s_{in,j} \in S_{in,j}, p \in P$$

$$(1)$$

Apart from the water balances, contaminant balances also have to be performed over a unit. These balances comprise of an inlet contaminant balance, which defines the inlet concentration, and a balance over the unit itself, given in constraint (2).

$$m_{p}(s_{out,j}, p)c_{out}(s_{out,j}, p) = m_{u}(s_{in,j}, p-1)c_{in}(s_{in,j}, p-1) + M(s_{in})y(s_{in,j}, p-1),$$

$$\forall j \in J, s_{in,j} \in S_{in,j}, s_{out,j} \in S_{out,j}, p \in P, p > p_{1}$$
(2)

Constraints are also derived to ensure that the maximum inlet and outlet concentration of a unit are not exceeded and the amount of water entering a unit does not exceed the maximum allowable.

Mass balances around central storage vessel

The mass balances around the central storage vessel comprise of a water balance around the vessel and a contaminant balance around the vessel. Constraints also ensure that the amount of water present in the vessel does not exceed the capacity of the vessel and the amount of water entering the vessel is less than the capacity of the vessel. These constraints are similar to those presented by Majozi (2005).

Mass balances around a unit operating in inherent storage mode

The mass balances considered for inherent storage are similar to those for a central storage vessel, except that the balances hold for each unit that can operate in inherent storage mode. A water balance and contaminant balance is performed over the unit. The water balance is given in constraint (3). Constraints also ensure the amount of water stored in a unit is within the capacity of the unit, as is the amount of water entering a unit.

$$qu(j,p) = qu(j,p-1) + \sum_{j'} mstu_{in}(j,'j,p) - \sum_{j} mstu_{out}(j,j',p),$$

$$\forall j \in J, p \in P, p > p_1$$

$$(3)$$

3.2 Scheduling constraints

The scheduling constraints are divided into five groups. The first group comprises of those constraints pertinent to task scheduling, the second group comprises of scheduling constraints necessary for proper scheduling of direct reuse. The third and fourth group deal with the scheduling aspects of the central storage vessel and inherent storage respectively. The final group comprises of feasibility constraints and time horizon constraints.

Task scheduling constraints

The task scheduling constraints deal with the correct scheduling of the tasks within the processing units. The task scheduling constraints ensure that a unit finishes processing a batch before the next batch begins and if a unit starts or ends its operation at a later time point, the time at which this happens corresponds to a later absolute time in the time horizon of interest. A duration constraint captures the time over which the unit is active whilst processing a task.

Direct reuse sequencing constraints

The direct reuse scheduling constraints ensure that direct reuse of wastewater occurs at the correct times within the time horizon. These constraints make sure that the time at which wastewater is produced correspond to the same time at which wastewater is reused in another unit. These constraints also ensure that the receiving unit is indeed operating at the time of the receiving water.

Scheduling constraints associated with central storage

The scheduling constraints used for the central storage vessel are centred on the timing of streams entering and exiting a unit. They ensure that the time at which wastewater is sent to a storage vessel and the time at which wastewater is produced corresponds to the same absolute time. Similar constraints ensure that the time at which water is sent to a unit and the starting time of the task in the unit corresponds to the same time.

Further constraints ensure that two or more streams entering the central storage vessel at a time point do so at the same time. The same condition holds for two or more streams leaving the central storage vessel at the same time point and two or more streams exiting and entering the storage vessel at the same time point. Finally these constraints ensure that streams entering or exiting the central storage vessel at later time points do so at later actual time.

Inherent storage scheduling

The scheduling constraints required for inherent storage comprise of a number of binary variable constraints and a number of timing constraints. The binary variable constraints ensure that if wastewater is sent to a unit for storage, the unit producing water has indeed operated, and if wastewater is sent from storage the receiving unit is operating at that time

point. A final binary constraint ensures that at a time point a unit operating in inherent storage mode is not sending and receiving material.

The timing constraints for inherent storage ensure that the time at which wastewater is sent for storage in a unit is the same time as that at which wastewater is produced. Also, the time at which wastewater leaves storage coincides with the time at which the receiving unit starts operating.

The timing constraint given in constraint (4) ensures that wastewater can only be sent to a unit for storage once the unit has finished processing a batch. Similar constraints ensure that wastewater entering a unit for storage does so before the unit processes the next batch and wastewater stored in a processing unit leaves the unit before the unit starts processing the next batch.

$$tstu_{in}(j',j,p') \ge t_p(s_{out,j},p) - H\left(2 - ystu_{in}(j',j,p') - y(s_{in,j},p)\right),$$

$$\forall j,j' \in J, p \in P, p' \ge p$$

$$(4)$$

The final timing constraints that comprise the inherent storage sequencing are similar to those for the central storage vessel and ensure the correct timing of multiple streams entering and exiting a unit.

Feasibility and time horizon constraints

Constraints in this section ensure that only one task can occur in a unit at any given time and that each event that occurs within the operation does so within the time horizon of interest.

3.3 Objective

The objective used is dependent on the information given. If the production is fixed, the objective is the minimisation of effluent. Otherwise, the objective is based on the maximisation of profit.

4. Illustrative example

The operation considered in the illustrative example involves four water using operations. Operation 1 operates twice and operations 2, 3 and 4 operate once in the 12 hour time horizon. It is required that unit 2 starts its operation at the beginning of the time horizon, and the operation of unit 3 must always precede the operation of unit 4. The starting time of unit 4 need not coincide with that of unit 3. The example was solved first considering no inherent storage and only a central storage vessel. The example was then solved without the central storage and only considering inherent storage. In both cases the possibility of direct reuse was included.

The maximum inlet and outlet concentrations are given in Table 1, together with the mass load in each unit, the maximum water and the process duration. The central storage vessel has a capacity of 1000 kg and each processing vessel has a capacity of 2000 kg which can be used for either processing or storage.

Table 1. Data for the second illustrative example

Unit	Max. inlet concentration (g/ kg water)	Max. outlet concentration (g/ kg water)	Mass load (g)	Mass Water (kg)	Duration (h)
1	0.10	0.15	10	200	4.5
2	0	0.10	10	100	2
3	0.20	0.50	15	50	3.75
4	0.05	0.65	75	125	5.5

Solution with central storage without inherent storage

The resulting model was solved using the solution algorithm proposed by Gouws *et al.* (2008). The model was solved using GAMS/DICOPT, with CPLEX as the MIP solver and CONOPT for the NLP solver.

The solution to the model was found in 0.94 CPU seconds using an Intel Core 2 Duo processor 1.66GHz. The solution required only 4 time points resulting in 112 binary variables. The final value of the objective function was 313.3 kg. Without reuse of wastewater the amount of effluent would have been 378.7 kg. The effluent was thus reduced by 17.2%. The resulting schedule that achieves the wastewater target is given in Figure 1. One would notice from the figure that 100kg of wastewater was reused through the central storage vessel.

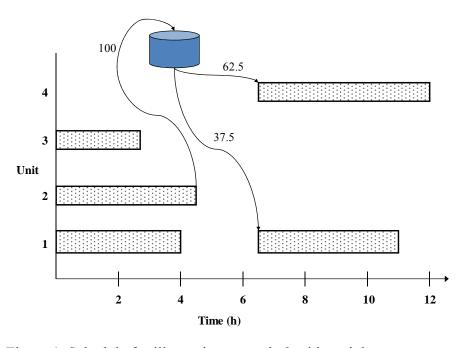


Figure 1. Schedule for illustrative example 2 without inherent storage

Solution using inherent storage without central storage

The resulting model for this case was once again solved using the solution procedure proposed by Gouws et al. (2008). The resulting mathematical model was formulated in

GAMS/DICOPT with CLPEX as the MIP solver and CONOPT as the NLP solver. The total solution time was 54.5 CPU seconds using the same processor as in the previous case. In this case the required number of time points was 6 for an optimal solution, with 312 binary variables in the resulting formulation. The final objective function had a value of 313.3 kg of effluent, exactly the same as the previous example. The wastewater reduction was thus 17.2%, as in the previous example.

The resulting schedule is shown in Figure 2. One would notice from Figure 2 that unit 2 has 37.5kg of water stored in it, which is reused to unit 1 at a later stage.

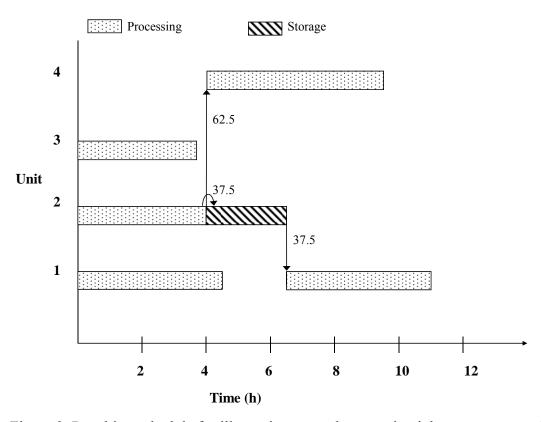


Figure 2. Resulting schedule for illustrative example two using inherent storage only

5. Conclusions

A methodology that explores the inherent storage possibilities for wastewater in idle processing units has been presented. The methodology determines the minimum wastewater target while determining the optimal process schedule that will achieve the minimum wastewater target.

The methodology was applied to an example problem. The example problem was first solved without inherent storage and only central storage for wastewater. The solution in this case achieved a 17.2% decrease in the amount of effluent generated. The same example was solved with inherent storage and no central storage. The same wastewater target was identified, i.e., a 17.2% reduction in effluent. The example demonstrates that the usage of inherent storage can negate the need for a central storage vessel.

6. References

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