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Application of the water source diagram (WSD) procedure to water use minimization in a batch process

Ana Paula S. Immich[a], Marivone Gusatti[a], Josiane M. M. de Mello[a], Selene M. A. Guelli U. Souza[a], Fernando L. P. Pessoa[b], Antônio A. Ulson de Souza[a]

[a]*Department of Chemical Engineering and Food Engineering, Federal University of Santa Catarina - UFSC, Zip Code 88040-900 Florianópolis, SC, Brazil.*
Department of Chemical Engineering, Federal University of Rio de Janeiro - UFRJ, Zip Code 21949-900, Rio de Janeiro, RJ, Brazil

Abstract

This paper presents the water source diagram (WSD) procedure for the minimization of the quantity of water required in a batch process for a specific industrial case. The study of this case was carried out for four different scenarios with the following constraints: fixed outlet stream concentration without reusable water storage, fixed inlet water quantity of an operation without reusable water storage, fixed outlet stream concentration with reusable water storage, fixed inlet water quantity of an operation with reusable water storage. The WSD procedure is commonly applied to the minimization of water use in continuous processes. In order to apply this procedure to a batch process it was necessary to consider the constraints involving the stream concentrations and the time interval of each operation. The same case was also solved by a graphical technique, given in the literature, where stream concentration is taken as the primary constraint and the time dimension as a secondary constraint. Wastewater minimization was achieved through the exploitation of recycling and reuse opportunities, as well as the use of reusable water storage. The results obtained employing the two techniques were identical, showing that WSD can also satisfactorily solve batch process problems.

Keyword: minimization, batch process, storage tank, recycling, reuse

1 Introduction

The scarcity of some natural resources such as water, and the increasing concern for environmentally correct processes, make the rational use of this resource an urgent issue. To address this problem Faria (2004) proposed the reuse and/or recycling of water streams which are normally sent to effluent treatment plans.

According to Majozi (2005) most methodologies presented in the literature for wastewater minimization are for continuous processes. These methodologies include mathematical techniques (Alva-Argáez, Kokossis and Smith, 1998; Doyle and Smith, 1997; cited in Majozi, 2005) and graphical techniques (Wang & Smith, 1994; Hallale, 2002; cited in Majozi, 2005, Majozi et al., 2006).

Almató et al. (1997) cited in Faria (2004), carried out a study on water minimization for batch industrial processes which introduced storage tanks, giving greater opportunities for water reuse. An inherent characteristic of these processes is the necessity to consider the time variable for the optimization of the system. In these cases the storage tanks nullify the time constraint.

A technique which focuses strictly on batch processes was developed by Majozi (2005). This technique presented a mathematical formulation for wastewater and fresh water minimization in multipurpose batch plants (fresh water is used here to mean water entering the plant from an outside source such as the mains supply). This formulation is based on a superstructure which includes all the possibilities for the reuse and recycling of water, taking into account the time interval of each batch.

Gomes et al. (2005) developed a methodology to minimize the use of fresh water and the generation of effluent in continuous processes. The authors presented an algorithm procedure named the water source diagram (WSD) defining the aim of minimizing water consumption in industrial processes by reuse and recycling of water streams, for a single or multiple contaminants.

This study employs the water source diagram tool to identify the opportunities for reuse and recycling of water in a case study presented by Majozi (2005) for a batch process, which takes into account the variables of time and contaminant concentration.

2 Problem Statements

The problem defined in the article by Majozi (2005) can be stated as follows. Each water use operation is allocated a value for each of the following parameters:

(i) contaminant mass load;
(ii) water quantity required;
(iii) start and end times which achieve the desired effect, e.g. mass transfer, degree of cleanliness of the vessel, etc.;
(iv) maximum reusable water storage; and
(v) maximum inlet and outlet concentrations.

The minimum amount of wastewater that can be achieved through the exploitation of reuse and recycling opportunities is then determined. Reuse refers to the use of an outlet water stream from operation *j* in another operation *j'*. Recycling refers to the use of an outlet water stream from operation *j* in the same operation *j*. It should be noted that wastewater minimization is concomitant with a reduction in fresh water intake.

3 Problem superstructure

Figures 1 and 2 show the structures of the problem. Figure 1 represents a situation where reusable water storage is not present. In this situation, water used in each operation *j* can be supplied from the fresh water header, the recycle/reuse water header or a combination of both headers. Water from each operation *j* can be recycled within the same operation, reused in downstream processes and/or dispensed with as effluent. On the other hand, Figure 2 represents a situation where reusable water storage exists. In this situation water from reusable water storage provides an additional source and water sent to reusable water storage provides an additional sink, for each operation *j*.

Each water-using operation shown in the structure belongs to a complete batch chemical process. The other unit processes are not shown, since the focus of the problem is the water-using operation.

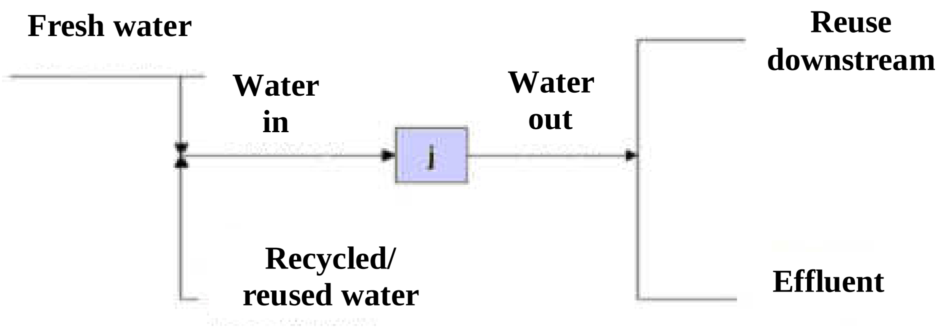

Figure 1: Batch process operation without a storage tank (MAJOZI, 2005)

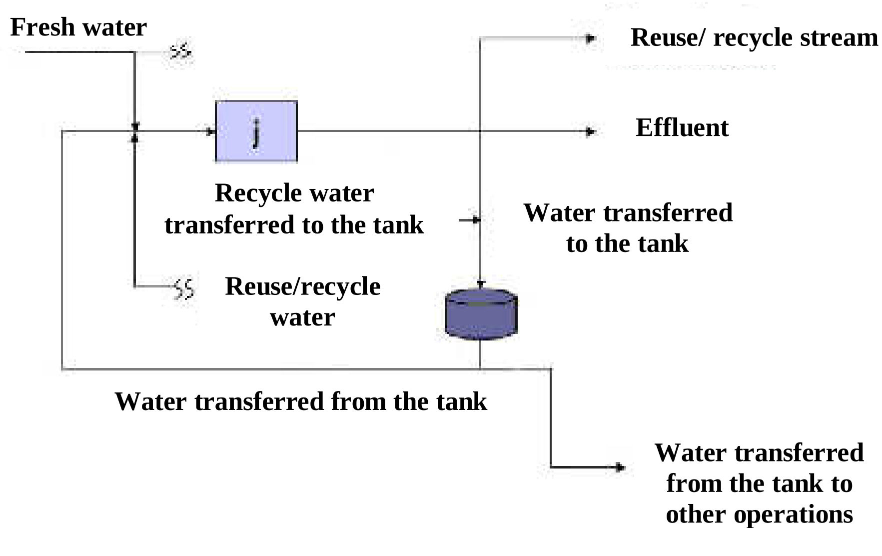

Figure 2: Batch process operation with a storage tank (MAJOZI, 2005)

4 Modules of the problem

The overall model is made up of two modules which are built within the same framework. One module focuses on the exploitation of water reuse/recycling opportunities and the other on proper sequencing to capture the time dimension.

4.1 Water reuse/recycling module

In exploring the recycling and reuse opportunities within a complete batch process, four scenarios are mathematically formulated in the following sections. The first scenario is based on a fixed outlet concentration for each water-using operation without the presence of reusable water storage. This situation allows for the quantity of water used in the operation to vary from the limiting water requirement. The second scenario is based on a fixed water requirement for each water-using operation without reusable water storage. The third and fourth scenarios consider the presence of reusable water storage and correspond to the first and second scenarios, respectively.

4.1.1 Scenario 1: *formulation for fixed outlet concentration without reusable water storage*

For this case, some constraints are formulated.

Constraint 1: states that the inlet stream of any operation j comprises the reuse/recycle streams from all water-using operations j' as well as the fresh water stream.

Constraint 2: states that the outlet stream of any operation j can be reused in other processes j', recycled to the same process j and/or dispensed with as effluent.

Constraint 3: is the mass balance of unit j. It states that the contaminant mass-load difference between outlet and inlet streams for the same unit j is the contaminant mass-load picked up in unit j.

Constraint 4: is the definition of the inlet contaminant concentration of unit j. It is defined as the ratio of the overall mass-load of recycle/reuse streams to the total amount of the inlet stream.

Constraint 5: states that the outlet concentration of any unit j is fixed at a maximum predefined concentration corresponding to the same unit. It should be noted that streams are expressed in quantities instead of flow rates, as in any batch operation.

Constraint 6: states that the total quantity of water used at any point in time cannot exceed the limiting amount.

4.1.2 Scenario 2: *formulation for fixed water quantity without reusable water storage*

This case is applicable in a situation where the quantity of water is fixed and the outlet concentration is allowed to vary. In this situation, constraints 1–4 still hold, but constraints 5 and 6 have to be modified as follows:

Constraint 7: states that the outlet concentration from any operation j can be less than or equal to the maximum outlet contaminant concentration of an operation *j*.

Constraint 8: states that the water used is the maximum required.

4.1.3 Scenario 3: *formulation for fixed outlet concentration with reusable water storage*

The scenario presented in this section corresponds to the structure shown in Figure 2, in which central reusable water storage is taken into consideration. In this situation, constraints 3, 5 and 6 still hold, but constraints 1, 2 and 4 have to be modified as follows:

Constraint 9 states that the inlet stream of any operation *j* is made up of a recycle/reuse stream, a fresh water stream and a stream from reusable water storage.

Constraint 10: states that the outlet stream of operation *j* can be dispensed with as effluent, reused in other processes, recycled within the same operation and/or sent to reusable water storage.

Constraint 11: states that the inlet concentration of operation *j* is the ratio of the contaminant amount in the inlet stream and the quantity of the inlet stream.

The following specific storage constraints are also imperative for the completeness of the model for scenario 3:

Constraint 12: is the mass balance of the reusable water storage tank. It states that the amount of water stored at any time point *p* is determined by the amount stored at the previous time point $p-1$ plus the difference between the quantity transferred from and the quantity transferred to the water-using operations at time point *p*.

Constraint 13: ensures that the amount of water stored at any point in time does not exceed the capacity of reusable water storage.

Constraint 14: gives the inlet concentrations for the reusable water storage tank.

Constraint 15: gives the outlet concentrations for the reusable water storage tank.

4.1.4 Scenario 4*: formulation for fixed water quantity with reusable water storage*

Constraints 3 and 7-15 together constitute a complete water reuse/recycle model for a situation in which the quantity of water in each water-using operation is fixed.

4.2 Sequencing/scheduling module

In order to handle batch operations effectively, the time dimension cannot be ignored. This is due to the fact that almost all operations within the batch process environment are time dependent. In continuous operations, only the concentration constraint determines the feasibility of water reuse from one process to another. This implies that if the outlet water concentration of process A is less than the maximum allowed inlet water concentration of process B, then water from process A could be reused in process B. On the other hand, if water from process B is at a concentration higher than the maximum allowed in process A, the water reuse opportunity from process B to process A is nullified.

4.2.1 Sequencing in the absence of reusable water storage

The following constraints address the time dimension for water reuse/recycling in batch processes in the absence of central reusable water storage:

Constraint 16: states that if water from operation *j* is reused in operation *j'* at a given time point *p*, then operation *j'* should commence at time point *p*.

Constraint 17: ensures that the reuse of water from operation *j* in operation *j'* coincides with the completion of operation *j* at time point *p*.

Constraint 18: ensures that the reuse of water from operation *j* in operation *j'* coincides with the start of operation *j'* at time point *p*.

4.2.2 Sequencing in the presence of reusable water storage

In the presence of reusable water storage, the following additional sequence constraints are necessary:

Constraint 19: stipulates that when the water stream is transferred from operation *j* to reusable water storage, then the time of transfer should coincide with the completion of operation *j*.

Constraint 20: states that when the water stream is transferred from storage to any operation *j* for reuse, then the time of transfer must coincide with the start of operation *j*.

Constraint 21: ensures that whenever a water stream is transferred from storage to operation *j* at time point *p*, then operation *j* must commence at time point *p*. However, operation *j* can start at time point *p* even if there is no reusable water stream transferred from storage, since water could be received from recycle/reuse and fresh water streams.

5 Application of water source diagram (WSD) in batch processes

In order to solve the case study presented by Majozi (2005), regarding wastewater minimization using central reusable water storage in batch plants, the water source diagram

(WSD) was used. This diagram was developed with the aim of minimizing the use of fresh water in continuous processes and was proposed by Gomes et al. (2005).

6 Case study

The data for the case study taken from an agrochemical manufacturing facility are given in Table 1. The processes given in Table 1 were specifically selected on the basis of a common contaminant, since they all produce sodium chloride (NaCl) as a byproduct.

Operation j	Water (kg)	$C_{i,max}$ (kg salt/kg water)	$C_{f,max}$ (kg_salt/kg_water)	t_i (h)	t_f (h)	M (kg)
A	1000	0	0.1	0	3	100
B	280	0.25	0.51	0	4	72.8
C	400	0.1	0.1	4	5.5	0
D	280	0.25	0.51	2	6	72.8
E	400	0.1	0.1	6	7.5	0
Total	2360					245.6

Table 1: Data for the case study

This byproduct is removed from the organic phase using liquid–liquid extraction in which fresh water is introduced to form an aqueous phase. However, in the B and D operations water is also used as a solvent. In the C and E operations, water is used for polishing rather than extraction purposes, hence the zero contaminant loads. Each of the five operations belongs to a multi-stage batch process. Prior to the exploration of water reuse/recycle opportunities, these operations used 2360 kg of fresh water in a 7.5-h time period as shown in Table 1. The objective function in all the following four scenarios is the minimization of fresh water requirement.

6.1 Water reuse/recycle module

Since the formulation of the constraints was presented in detail in Section 4, only the new constraints will be presented in this section. The new constraints were necessitated by the presence of operations C and E. Water required in these operations is for polishing purposes, although this is not associated with any contaminant removal. The minimum amount of water required in these operations is 300 kg (constraint 22). This new constraint is valid for scenarios 1 and 3, fixed outlet concentration.

In scenarios 2 and 4, i.e. fixed water quantity and presence of reusable water storage, the following constraint is necessary to ensure that the capacity for reusable water storage is taken into account:

Constraint 23: the reusable water storage cannot amount to more than 800 kg of water.

In the following section the WSD will be used to solve the case study previously specified in Table 1.

In this case study the WSD will be applied to four different scenarios taking into account: fixed outlet concentration without reusable water storage, fixed water quantity without reusable water storage, fixed outlet concentration with reusable water storage, fixed water quantity with reusable water storage.

6.2 Application of the WSD to solve the case study

6.2.1 Scenario 1: outlet concentration without reusable water storage

It is possible to build the diagram shown in Figure 3 for scenario 1.

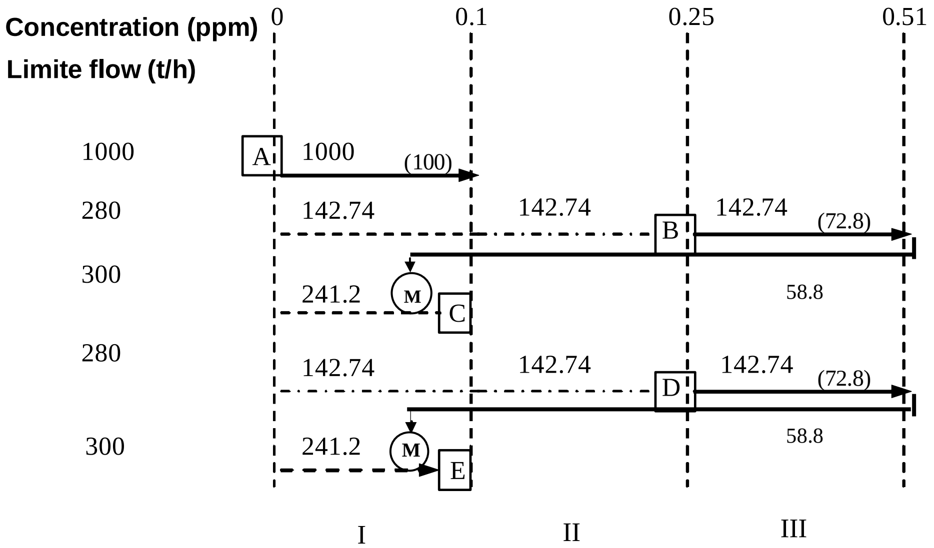

Figure 3: Water source diagram for scenario 1

Operations C and E do not involve contaminant removal, and the water required is for polishing purposes. However, there are constraints for the concentration of the inlet water stream which must be 0.1 Kg *salt*/Kg *water*. As operations C and E start at the same instant at which operations B and D finish, it is possible to reuse the outlet stream from operations B and D for operations C and E, respectively. With the time constraint satisfied, it is necessary to satisfy the concentration constraints. Since the outlet streams of operations B and D have concentrations of 0.51 Kg *salt*/Kg *water* (over the maximum concentration for the inlet streams of operations C and E) it is necessary to dilute these streams with fresh water. Thus, the inlet stream for operation C will be made up of 58.8 Kg of water from the operation B outlet stream (0.51 Kg *salt*/Kg *water*) plus 241.2 Kg of fresh water. The same occurs for the operation E inlet stream, made up of 58.8 Kg of water from the operation D outlet stream plus 241.2 Kg of fresh water. Based on the water source diagram shown in Figure 3, it is possible to build the water minimization flowchart for scenario 1 shown in Figure 4.

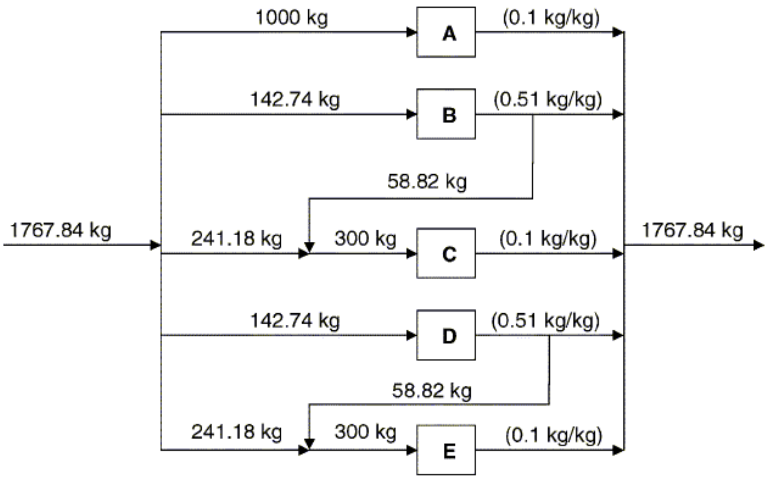

Figure 4: Water minimization flowchart for scenario 1

Figure 4 shows that 1767.84 Kg of fresh water are required. This corresponds to a 25% reduction in fresh water requirement compared to the situation without water recycling/reuse. Although water from process A has a relatively lower concentration of 0.1 kg *salt*/kg *water*, the time constraint in the absence of reusable water storage forbids any possibility for recycling/reuse. According to Table 1, none of the other operations commences when operation A finishes at 3 h. Consequently, all the wastewater from operation A is dispensed with as effluent. However, the time constraint allows the reuse of water from operations B and D in operations C and E, respectively.

6.2.2 Scenario 2: fixed water quantity without reusable water storage

It is possible to build the diagram shown in Figure 5 for scenario 2.

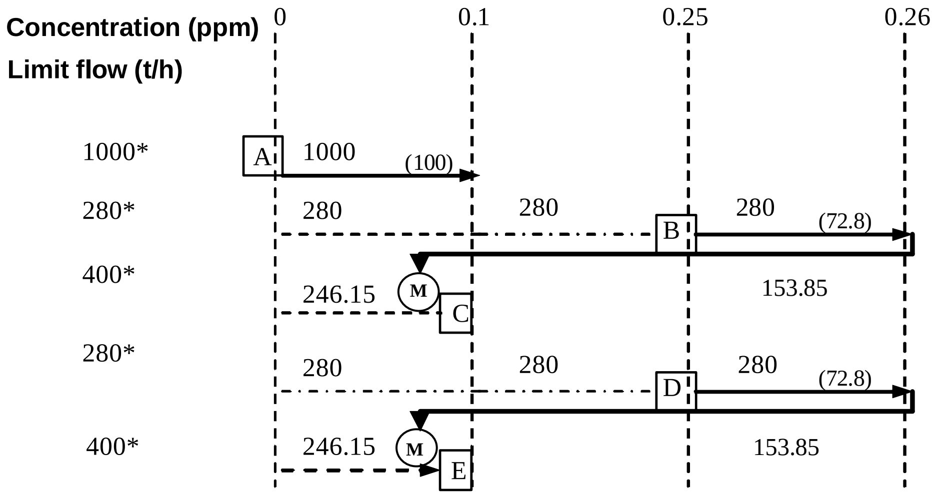

Figure 5: Water source diagram for scenario 2

Based on the water source diagram shown in Figure 5, it is possible to build the water minimization flowchart for scenario 2 shown in Figure 6.

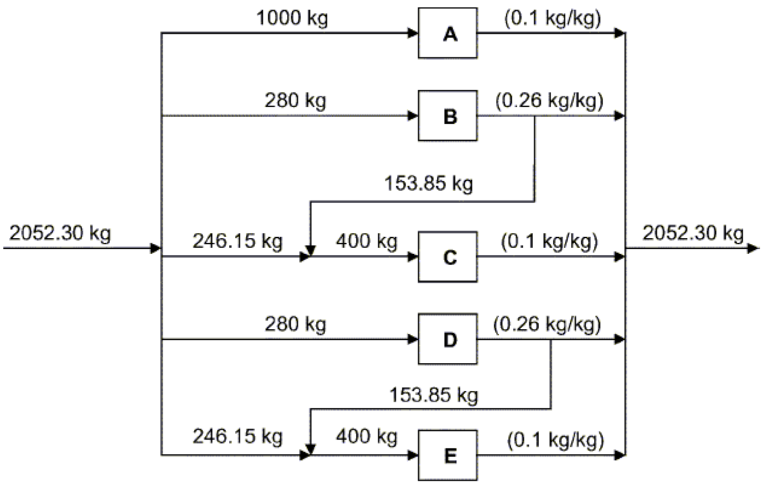

Figure 6: Water reuse flowchart for scenario 2

Figure 6 shows that 2052.30 Kg of fresh water are required. This corresponds to a 13% reduction in fresh water requirement.

6.2.3 Scenario 3: fixed outlet concentration with reusable water storage

It is possible to build the diagram shown in Figure 7 for scenario 3. Based on this diagram, the flowchart for water reuse for scenario 3 can be built, as is shown in Figure 8.

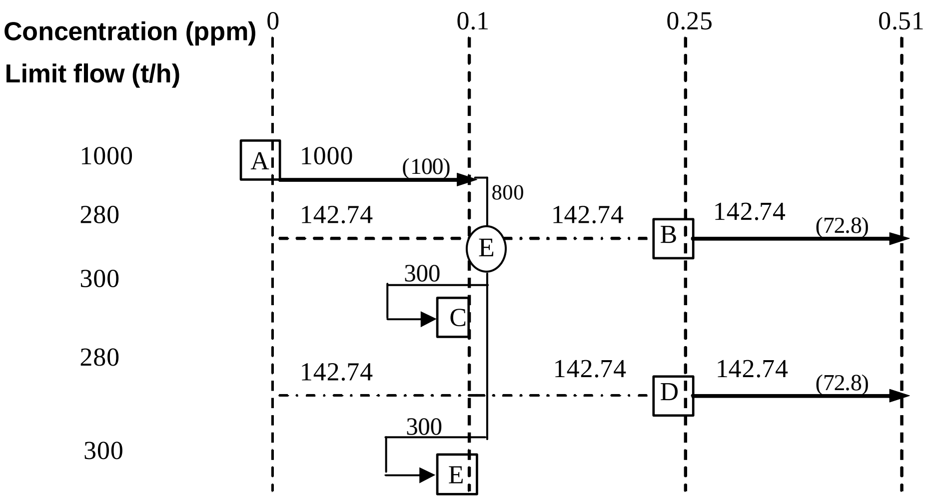

Figure 7: Water source diagram for scenario 3

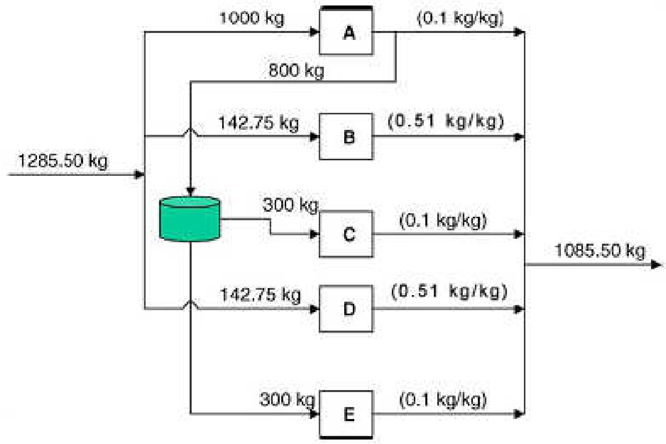

Figure 8: Water reuse flowchart for scenario 3

It is evident from Figure 8 that the presence of central reusable water storage allows the time constraint to be overridden, thereby providing an opportunity for reuse of effluent from operation A in operations C and E. Figure 8 shows that 1285.5 Kg of water are required for scenario 3. This corresponds to a 45.53% reduction in the fresh water requirement. The main reason for this reduction is the presence of a reusable water storage tank. Scenario 1, which is similar to scenario 3, but there is no reusable water storage, resulted in a 25% fresh water reduction. It is worth noting that there is also a reduction in the amount of wastewater generated, 1085.50 kg. This is due to the fact that some reusable water remains in the reusable water storage tank. According to constraint 23, the tank has the capacity to store 800 Kg of water.

6.2.4 Scenario 4: fixed water quantity with reusable water storage.

It is possible to build the diagram shown in Figure 9 for this scenario. Based on this figure, the flowchart for water reuse can be built, as shown in Figure 10.

Figure 10 shows that 1560 Kg of fresh water are required for scenario 4. This corresponds to a 33.89% reduction in the fresh water requirement. Scenario 2, similar to scenario 4, but without the storage tank, resulted in a 13% reduction in the fresh water requirement.

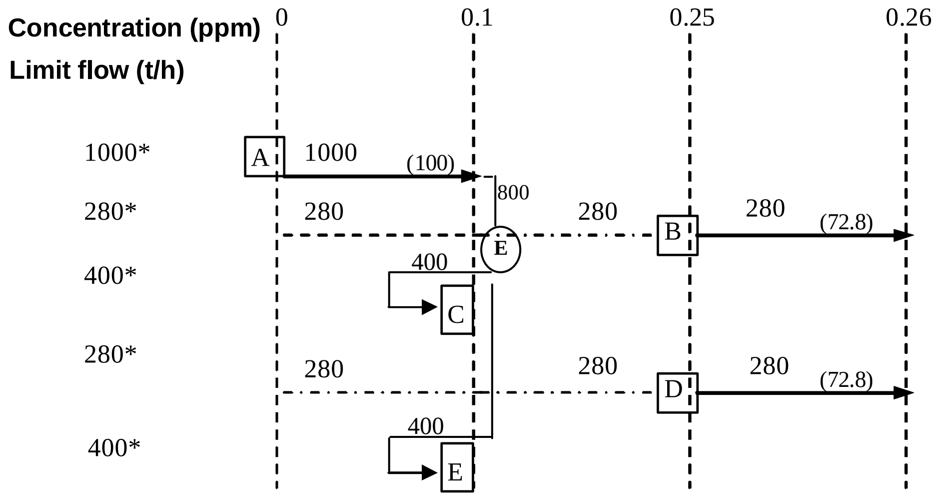

Figure 9: Water source diagram for scenario 4

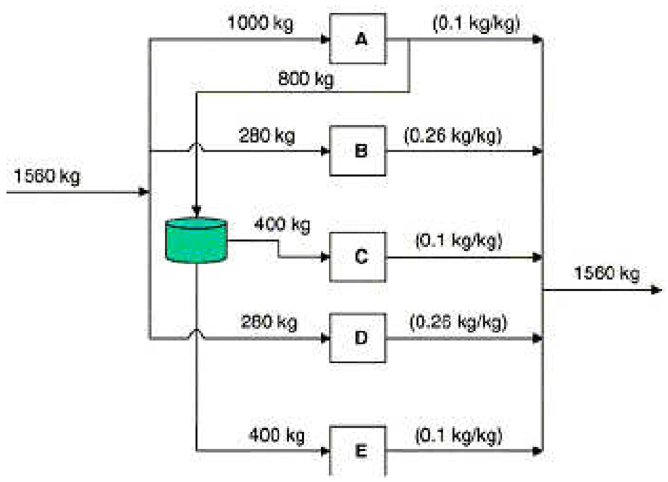

Figure 10: Water reuse flowchart for scenario 4

Table 2 presents a summary of the results obtained for the minimization of fresh water required in batch process operations.

	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Fresh water required (kg)	1767.84	2052.30	1285.50	1560
Effluent generated (Kg)	1767.84	2052.30	1085.50	1560

Table 2: Results for the minimization of water required in a batch process

Scenario 3 presented the best results for the minimization of fresh water required, as well as for the generation of aqueous effluent. This was due to the presence of a reusable water storage tank which allowed the storage of water previously used in other operations, when the finishing time does not coincide with the start of other operations, and immediate reuse is not possible.

7 Application of the graphical technique to solve the case study

The graphical technique proposed by Majozi et al. (2006) for wastewater minimization was applied in the four scenarios described in Section 4 and the results obtained were identical to those given in Section 6, and can be seen in Figures 4, 6, 8 and 10.

The graphical technique proposed by Majozi et al. (2006) to solve the case study is recommended for problems with less time intervals. The disadvantage of this technique is its restricted application to processes with a common contaminant.

8 Application of the computational method to solve the case study

Majozi (2005) proposed a mathematical model to solve the case study presented in Table 1 for the four different scenarios described in Section 4. The results obtained by the author, through the computational program GAMS, are identical to the results obtained in Section 6 in this article, which are shown in Figures 4, 6, 8 and 10.

9 Conclusions

The purpose of this article is the application of the WSD technique for water minimization in batch processes. For this it was necessary to consider the water stream concentration constraints and each operation time interval constraint. The batch processes allow, besides water reuse/recycling, the use of a reusable water storage tank, which can store water to be reused in future operations at a later time or in other batch cycles. The presence of this tank improves enormously the opportunities for water minimization, as was verified particularly in the flowchart of scenario 3 (Figure 8) with a reduction in the water consumption of 45.53%. For this batch process the WSD was shown to be easily applicable, as has been previously reported for several cases of continuous processes.

The graphical technique proposed by Majozi et al. (2006) to solve this case study was shown to be simple, although very laborious. This technique is recommended for problems with less time intervals. The disadvantage of this technique is that its application is restricted to processes with a common contaminant.

According to Majozi (2005), the advantage of the computational method application is the possibility to obtain trustworthy and exact results. The disadvantage of this method is that it can be applied only in cases where there is a common contaminant.

All of the methods applied gave the same results. However, the simplicity of the application of the WSD method makes it an important candidate for solving one of the greatest industrial problems relating to the use of natural resources, since the increasing concern for environmentally correct processes makes the rational use of these resources an urgent issue.

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