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Optimal design and scheduling for batch water networks

[1,*1]Said M. ALY, Abeer M. SHOAIB, [1]Moustafa E. AWAD

[1]Department of Chemical and Refining Engineering, Faculty of Petroleum and Mining Engineering, Suez Canal University, Suez, EGYPT

ABSTRACT

Efficient scheduling model is developed for maximization of direct water recovery in batch processes. In the past, the task of optimizing the batch schedule and the batch water network design that satisfies the minimum freshwater requirements were performed individually. In this study, all these problems are incorporated in the same mathematical programming formulation. The resulting design specification includes the size of the required storage tank, the allocation of water flows, as well as the new production schedule. Two case studies are provided to show the potential benefits that could be achieved by integrating the scheduling and design model of a water reuse network.

KEYWORDS

Process integration; wastewater minimization; rescheduling;. Water; Storage; Batch; Optimization

INTRODUCTION

The growing interest on the part of the chemical industry in the production of high value added chemical and biochemical products in addition to the required high technology increased the importance of batch processing in recent years. In batch processes, not all streams coexist simultaneously; in order to match source and sink streams directly, they must coexist in the same time interval. Storage tanks are used to reduce the limitation of time constraints. However, the storage system is usually expensive. So there is a need to reduce such extra cost. This could be achieved through

* Corresponding author. Email said_1949@yahoo.com

rescheduling. Scheduling modifications can have important effects on direct water recovery in batch processes.

Rescheduling could be identified as the alteration of time period that each process could take place, without changing any concentration constraints. So that, the overall mass recovery, (water recovery) will not be affected by rescheduling. As a result, the direct water recovery relative to water recovery through storage will change. In other words, some water recovery that was carried out through storage should be carried out directly. So, it is a very important task to reschedule operations efficiently.

Rescheduling problem has been pointed out first by Kemp and Macdonald's (1988), but in energy integration process. However, no clear method had been introduced.

Obeng and Ashton (1988) used the time dependent chart which is a guide of how streams to be moved. Time dependent chart specify the time period in which waters are charged to or discharged from water using operations. However their method depends on trial-and-error analysis, which is not preferred and don't guarantee the optimality.

Kemp and Deakin (1989) illustrated that the cascade analysis could be applied to identify rescheduling opportunities systematically. Though, no suggestion for doing rescheduling in general is introduced. However, they have classified rescheduling opportunity into four generalized types listed below:

1- Rescheduling with no violation in duration and internal scheduling of each individual batch operation. This could be carried out by rescheduling the overall period of operation of two parallel batch processes relative to each other to permit more effective direct mass transfer between them.
2- Fixing the duration while altering the relative timing of two streams with an individual batch process cycle.
3- Altering the duration of a stream by changing its flowrate, retaining the previous start or finish time.
4- Altering both the timing and duration of a stream hence, it will occurs at a completely different point within the batch operation.

Kondili et al. (1993) handled the problem of multipurpose batch plants by introducing a general framework MILP, using the state task network (SNT) notion under discrete time representation. Shah et al (1993) have reformulated their work to improve the computational efficiency.

Pinto et al (1994) have addressed the cyclic scheduling of multistage multi product continuous plants by introducing a general model MINLP.

Most of mathematical programming techniques used to handle the problem of rescheduling, were restricted to one-to-one matches of streams or products, (Zhao et al 1998). One-to-one rule means that each stream could not be matched with two or more streams. This policy, obviously limits the direct water recovery chance. A more general way is needed. Zhao et al (1998) have introduced a systematic mathematical formulation for a general situation to reschedule heat recovery networks in repeated batch processes. However, their method was limited to small problems.

Papageorgiou et al (2004) have extended the work of Pinto et al (1994) to include units of performance decay. While Daniel Grooms et al (2005) introduced a MINLP that coordinating the synthesis of the interception and allocation networks as well as the operational scheduling of the system.

The objective of that work is to formulate and solve a general mathematical model that can handle the problem of operation schedule as well as stream matches that achieve the new schedule with the new cost target. Two case studies are solved to demonstrate our benefits.

PROBLEM STATEMENT

Rescheduling problem could be stated as follows:

Given:

1- A set of water sinks $\{SKj = 1, 2, \ldots, N_j\}$ that operate in batch process mode,
each sink SKj requires a water flow of F_{SKj}, and tolerates a limiting concentration (maximum inlet impurity concentration) of C_{SKj}.

2– A set of water sources $\{SRi = 1, 2, \ldots, N_i\}$ that also operate in batch mode, each source SRi has a flow of F_{SRi}, and an impurity concentration of C_{SRi}. The water sources may be stored in tanks then recycled to the sinks provided they satisfy the flow and composition constraints of the sinks.

3- Initial time for each source ($T_{i(SRi)}$) and sink ($T_{i(Skj)}$)

4- Final time for each source ($T_{f(SRi)}$) and sink ($T_{f(Skj)}$)

Also available for service is a fresh (external) water source that may be purchased to supplement the water sink requirements.

It is required to reschedule these processes so that the freshwater requirements as well as wastewater discharge could be minimized. The number of storage tanks and capacity could be also reduced as a result of rescheduling and thus, the total capital cost. Rescheduling violation is preferred to be as low as possible.

OPTIMIZATION PROGRAM MODEL

The objective of this model is to reschedule batch processes (repeated) to achieve the minimum storage tank capacity that maintaining the required FW as the minimum (as that in continuous processes.

MinimizeST

1- Mass balance around sources:

$$F_{SRi} = \sum_{SKj} F_{SRi,SKj} \Delta t + F_{SRi,STk} + F_{WW,SRi} \qquad SR_i = 1,2,\ldots\ldots,N_i \quad (1)$$

This equation says that each source either supplied to sink SKj in the same time interval, stored for further use or discharged as wastewater.

2- Mass balance around sinks:

$$F_{SKj} = \sum_{SRi}^{i} F_{SRi,SKj} \Delta t + \sum_{STk} F_{STk,SKj} + F_{FW,SKj} \qquad ST_k = 1,2,\ldots\ldots,N_k \quad (2)$$

This equation says that each sink either supplied by source SRi in the same time interval, from water stored or supplied with freshwater to satisfy its property constraints.

3- Time constraints:

$$T_{i(SKj)} < T_{i(SKj+1)} \quad (3)$$

Where $T_{i(Skj)}$ is the starting or initial time of sink SK_j

$$T_{i(SRi)} < T_{i(SRi+1)} \quad (4)$$

Where $T_{i(SRj)}$ is the starting or initial time of source SR_i

The above two constraints satisfy the order of the processes. They demonstrate that if source SR_i (or sink SK_j) in the data is available in a time before source SR_{i+1} (sink SK_{j+1}), The violation in the new schedule will be the minimum. These constraints prohibit the impractical solutions.

This model has the flexibility of changing the start and/or finishing time and also changing the flowrate while fixing the flow, the order of processes and the total cycle time. Fixing the total cycle time is achieved by introducing the following two constraints:

$$T_{i(sk1)} = const.1;$$

$$T_{f(sn)} = const.2$$

Where constants 1,2 are given in the data and the difference between them is the cycle time.

4- Storage capacity

$$F_{STK} = \sum_{SRi} F_{SRi,STk} \qquad ST_k = 1,2,\ldots\ldots N_k \quad (5)$$

5- Concentration constraints

$$F_{STk} * C_{STk} = \sum_{SRi} F_{SRi,STk} * C_{SRi} \qquad ST_k = 1,2,\ldots\ldots N_k \quad (6)$$

$$\sum_{SRi} F_{SRi,SKj} * C_{SRi} + \sum_{STk} F_{STk,SKj} * C_{STk} <= F_{SKj} * C_{SKj} \qquad SKj = 1,2,....,N_j \quad (7)$$

The application of the above program generally is difficult but, it could be simplified by the aid of the time dependent chart given by Hung et al, 1994.

This could be more clarified and demonstrated by solving two alternative case studies;

Case study1:

Table 1 shows the limiting water data for a case study (adapted from Almat´o et al., 1999a,b; Li &Chang, 2005). This case study includes a combination of mass transfer and non-mass transfer based-water-using operations. (Foo et al., 2005; Manan et al., 2004). Annual operating time for batch processes is 8000h, while fresh water (zero content of the pollutant cost = $1/kg) may be used as needed.

Cost of storage tank is estimated based on Equation 8 (Kim and Smith, 2004).

Storage tank cost = r. ST + s (8)

Where *r* is referred to parameter of storage tank cost (slope of linear relationship); *s* is the parameter of storage tank cost (interception of linear relationship).

As presented in Kim and Smith (2004), the cost parameters *r* and *s* are given as 116.95 and 10142.16 respectively for carbon steel storage tank in mid 1980. In order to update the cost parameters, Marshal and Swift (M & S) cost index is in used. It is found that M & S for 1980 and 2007 are 813 and 1383.6 respectively.

The time dependent chart is constructed to clarify the idea of the water streams distribution with time. It is a good guide that allows direct identification of some water reuse opportunities. Sources and sinks are represented in their corresponding time intervals as continuous lines as shown in Figure1. Discontinuous ones show the opportunities to shift the schedule of sources or sinks so as to maximize direct water recycle/reuse which leads to reducing storage tanks required to store water so as to construct a cost effective batch water network.

Table 1. Limiting water data for case study1

Water sink, SK_j	Flowrate (m^3/h)	Concentration, C_{SKj} (ppm)	Start time, t_i (h)	Endi time, t_f (h)	Flow, F_{SKj} (m^3)
SK_1	10	0	0.5	2.5	20
SK_2	10	6	5.0	7.0	20
SK_3	10	15	9.5	11.5	20
SK_4	8	5	17.0	19.0	16
SK_5	10	7	6.0	8.0	20
Water sources, SR_i	**Flowrate (m^3/h)**	**Concentration, C_{SRi} (ppm)**	**Starting time, t_i (h)**	**Ending time, t_f (h)**	**Flow, F_{SRi} (m^3)**
SR_1	10	5	2.5	4.5	20
SR_2	10	14	7.0	9.0	20
SR_3	10	20	11.5	13.5	20
SR_4	4	25	17.0	19.0	8
SR_5	4	10	10.5	14.5	16

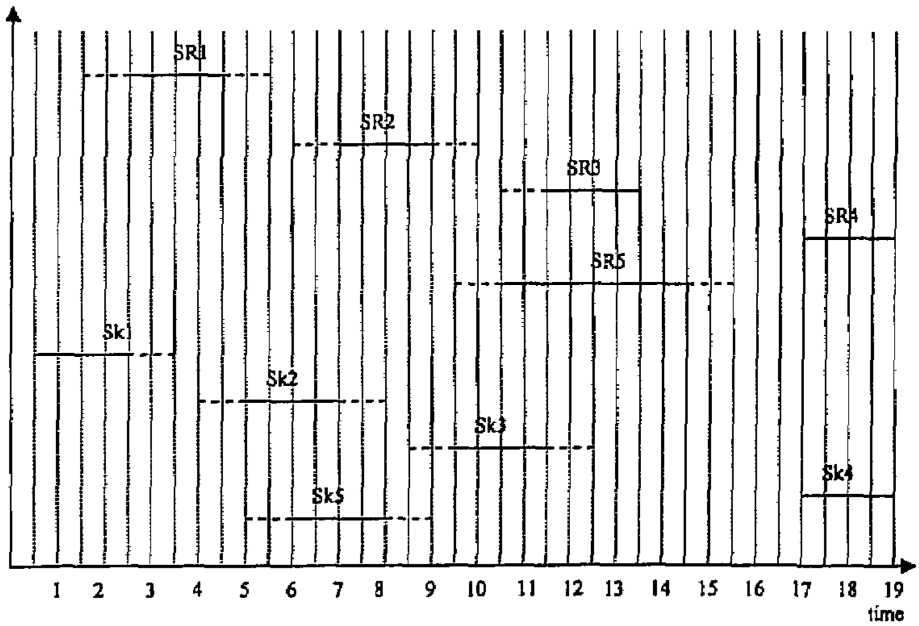

Figure 1: Time dependent chart for case study1

As shown in Figure1, the time interval of SK_4 (its duration) begins at time 17 h and ends at time 19 h, it has the same duration as source SR_4. It is obvious that rescheduling this process to overlap with another process to get direct reuse, requires a high schedule violation; which means that the alteration of start and end time of the process is high relative to the main schedule, which is not preferred in this work. High schedule violation could be permitted or acceptable if the real flowsheet of the processes is known and insured that it could be practical, otherwise, it may produce an impractical network, and so it should be ignored. Depending on that principle, rescheduling SK4 or SR4 is ignored. On the other hand, there could be direct recycle reuse between source SR1 and sinks SK2 and SK5 by shifting the duration of SR1 toward right and shifting the duration of sinks SK2 and SK5 toward left. These principles are applied for the rest of streams. All these shifts are just predicted and assumed to facilitate constructing our proposed model. These expected shifts could be taken as a limit to the predicted schedule violation. A non linear program (NLP) was run on Hyper LINGO version (API 3.00.386), from LINDO System using equations from equation1 to equation7. The solution resulted in a new schedule, shown in Figure2, is represented as hard lines, relative to the main schedule.

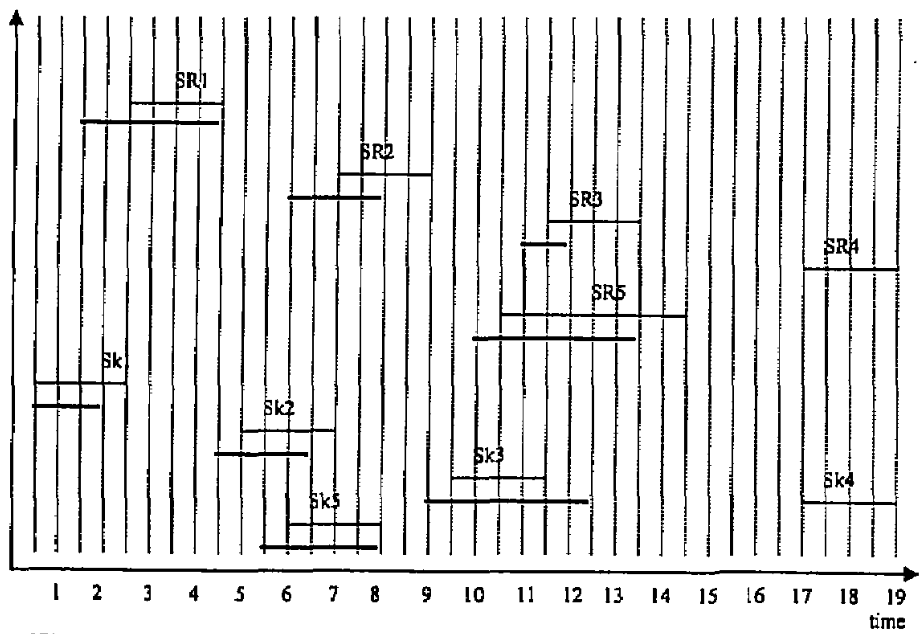

Figure 2: new schedule for case study1

The water allocation of water flows is represented in Figure 3.

Comparing this network with that proposed by Almato et al, 1999, which introduced a storage tank capacity of 100 and freshwater requirement of 38.7, it is found that there is a great saving in the storage capacity in addition to reduction in freshwater requirements. This case study has also solved by Shoaib et al. (2007), their proposal introduced a network that achieve the minimum freshwater requirement (35kg), however, this required the introduction of two storage tanks of capacities 25 and 36 respectively. Comparing these two designs from the cost view, it is found that the total cost required for the network of Shoaib et al. (2007) is $ 61396 while the cost for the resulted network after rescheduling in Figure 3 is $36175. There is more than 41% saving in cost due to the reduction in number and size of the required storage tanks. These results demonstrate the effectiveness of our proposed program.

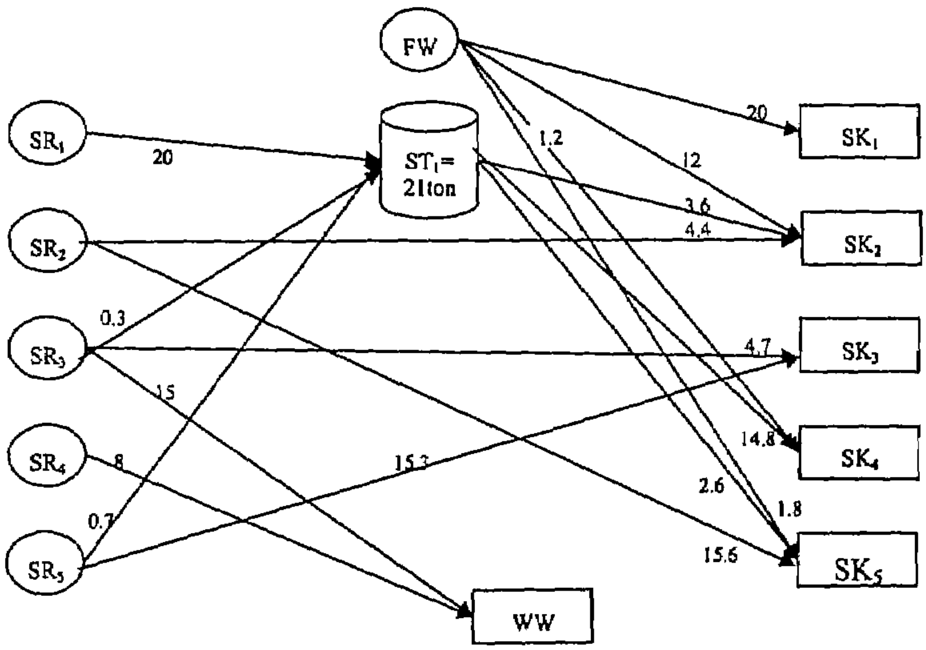

Figure 3: Batch water network for case study1 after rescheduling

CASE STUDY 2:

This study is taken from Majozi, 2005. Table2 represents the data for that case study.

Table 2. Limiting water data for case study2

process	Flow kg	Cin(j) (kg salt/kgwater)	Cout(j) (kg salt/kgwater)	Start time, t_i (h)	Endi time, t_f (h)
P1	1000	0.0	0.1	0	3
P2	280	0.25	0.51	0	4
P3	400	0.1	0.1	4	5.5
P4	280	0.25	0.51	2	6
P5	400	0.1	0.1	6	7.5

This case study differs from case study1 in that all processes are mass transfer based operations. Also, if processes are divided as sinks and sources, then it is an important constraint that must be taken into consideration in the program is to set that start and final time of each source and sink for the same process identical.

The time dependent chart for that case study is shown in Figure4.

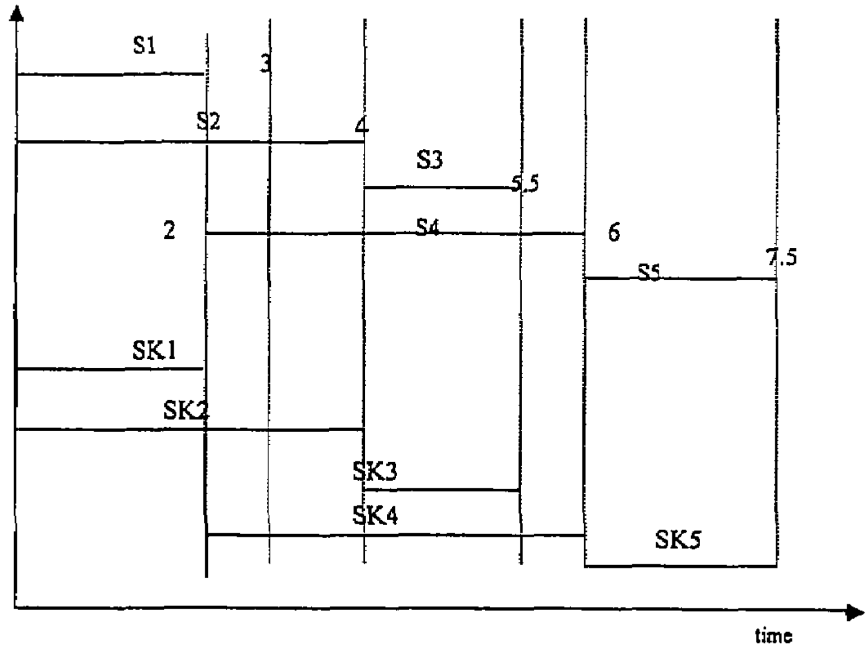

Figure 4: Time dependent chart for case study2

It is obvious from Figure2 that to minimize schedule violation, process1 is permitted to overlap with both processes 2 (P2) and 4 (P4). Process2 is permitted to overlap with both processes 3 and 4. While process4 is permitted to overlap with processes 2 and 3. Time dependent chart indicates that overlap between P1 with either P3 or P4 could result in an impractical operation. Thus, it is a good guide for ignoring such overlap. The same situation is applied to P2 with P5 and so on. Constructing the program that apply these ideas resulted in the new schedule represented in figure Figure5

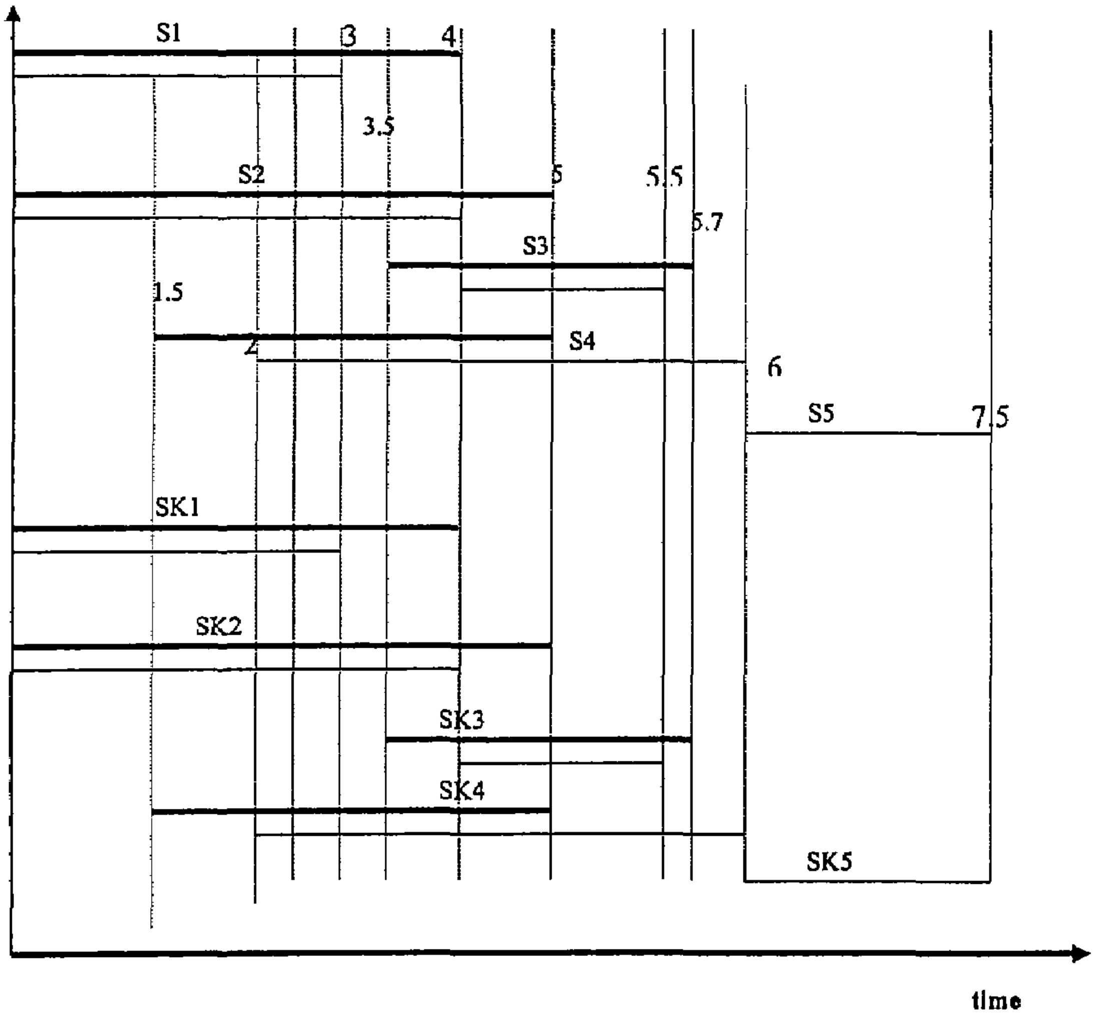

Figure 5: new schedule for case study2

Majozi, (2005) introduced four solutions through four different scenarios. It introduced two networks without the use of storage tanks which required 1767 and 2052 kg freshwater respectively. While the two other proposed networks introduced storage tanks of capacity 800kg, which reduced the required freshwater to 1560 and 1285 kg in two alternatives respectively.

Our proposed schedule procedure has resulted in a storage tank capacity of 800 while freshwater required has been reduced to 1000kg (the minimum).

Figure 6 indicates our proposed network

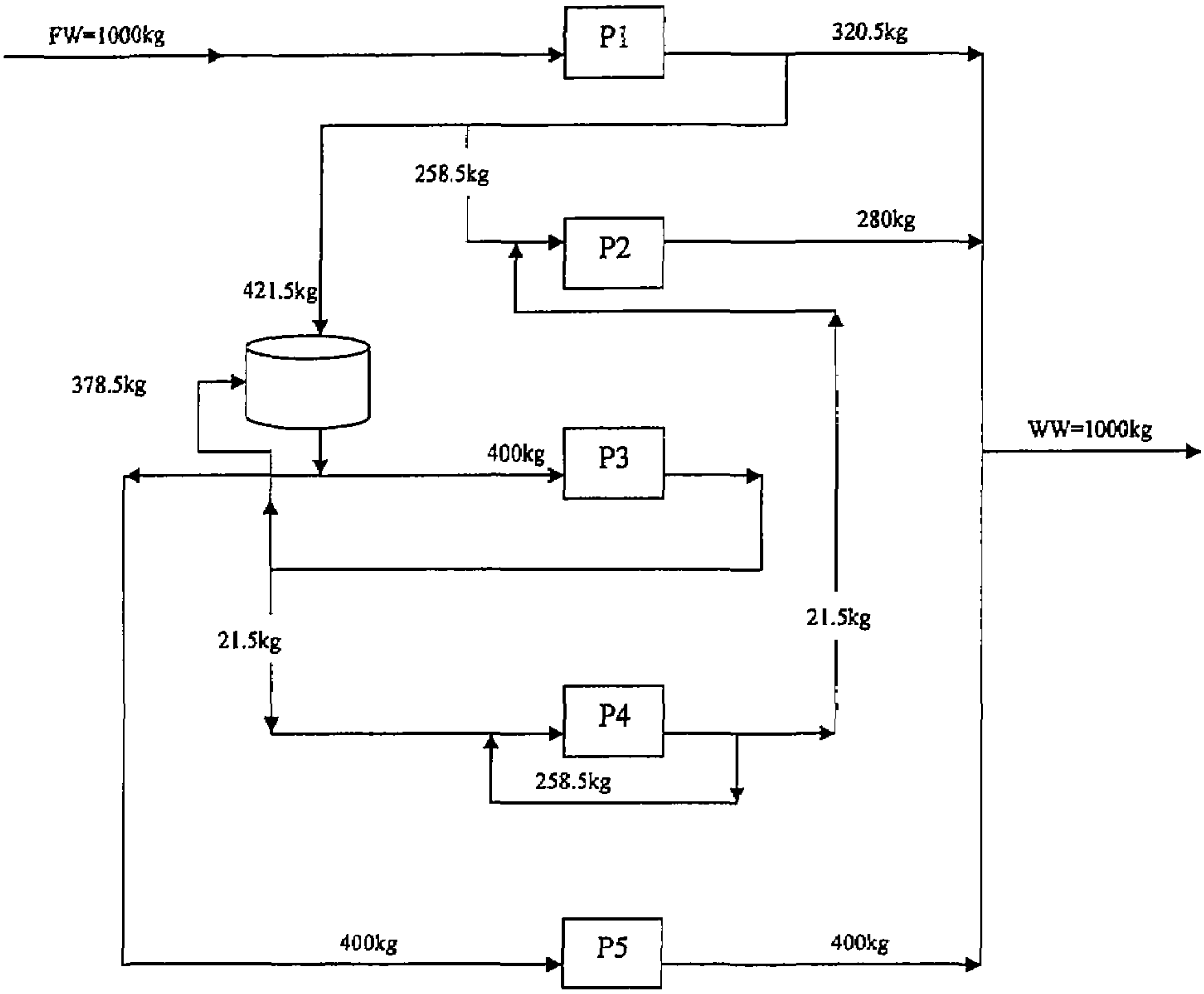

Figure 6: Batch water network for case study2 after rescheduling

CONCLUSION

This work presents a novel non linear programming (NLP) optimization approach that synthesizes and reschedules the batch water network simultaneously. It is an improvement to the previous published trials-and-error techniques which relies on the time dependent chart. An observable reduction in number and capacity of storage tank is highlighted through solving two different case studies.

The effectiveness of our program is not to put only a new schedule, but it also introduce the water reuse network depending on that new schedule in the same stage.

List of symbols:

SKj	set of water sinks
SRi	set of water sources
F_{SRi}	flow of water from source i
F_{SKj}	flow of water required by sink j
$F_{SRi,SKj}$	flow of water from source i to sink j
$F_{STk,SKj}$	flow of water from storage tank k to sink j
$F_{SRi,SKj}$	flow of water from source i to sink j
$F_{FW,SKj}$	flow of freshwater supplied to sink j
$F_{WW,SRi}$	flow of wastewater discharged from source i
F_{STk}	size of storage tank k
$F_{SRi,STk}$	flow of water from source i to storage tank k
C_{SRi}	concentration of source i
C_{SKj}	maximum allowable concentration to sink j
C_{STk}	concentration of water stored in storage tank k
$Ti_{(SKj)}$	start time of sink j
$Tf_{(SKj)}$	start time of sink j

REFERENCES

1- Almató, M., Espuña, A. and Puigjaner, L. (1999a). Optimisation of water use in batch process industries. *Computers and Chemical Engineering*. 23: 1427-1437.

2- Almató, M., Sanmatí, E., Espuña, A. and Puigjaner, L. (1999b). Economic optimization of the water reuse network in batch process industries. *Computers and Chemical Engineering*. 23: S153-S156.

3- Alle, A., Papageorgiou, L. G., & Pinto, J. M. (2004). A mathematical programming approach for cyclic production and cleaning scheduling of multistage continuous plants. *Computers and Chemical Engineering*, *28*, 3–15.

4- Chang, C., and Li, B. H. (2006). A mathematical programming model for discontinuous water-reuse system design. *Industrial & Engineering Chemistry* 575 *Research*, 45, 5027–5036.

5- Foo, D. C. Y., Manan, Z. A., Yunus, R. M. and Aziz, R. A., (2002). Synthesis of Mass Exchange Network for Batch Process Systems. Part 1: Calculation of Utility

Targets, *paper presented in Regional Symposium on Chemical Engineering (RSCE 2002), Kuala Lumpur*

6- Foo, D. C. Y., Manan, Z. A. and Tan, Y. L. Synthesis of Maximum Water Recovery Network for Batch Process Systems, *Journal of Cleaner Production.* 2005. 13(15): 1381-1394.

7- Grooms, D., Kazantzi, V. and El-Halwagi, M. M., (2005). Optimal synthesis of hybrid/steady-state property integration networks. *Computers and Chemical Engineering, 29*, 2318–2325.

8- Kim, J.-K. and Smith, R. (2004). Automated design of discontinuous water systems. *Transactions of the Institute of Chemical Engineers, Part B.* 82(B3): 238-248.

9- Kemp, I.C., Deakin, A.W., 1989, The Cascase analysis for energy and process integration of batch processes, Part 1. *Chem Eng Res Des.* 67, 495–509

10- Kemp, I. C. and Macdonalds, E. K., (1988)*.IChemE Symposium Series.* 109, 239-257

11- Kondili, E., Pantelides, C. C., & Sargent, R. W. H. (1993). A general algorithm for short-term scheduling of batch operations. I. MILP formulation. *Computers and Chemical Engineering, 17*, 211–227

12- Majozi, T. (2005a). Wastewater minimisation using central reusable water storage in batch plants. *Computers and Chemical Engineering.* 29: 1631–1646.

13- Majozi, T. (2005b). An effective technique for wastewater minimisation in batch processes, *Journal of Cleaner Production.* 13(15): 1374-1380.

14- Manan, Z. A., Tan, Y. L. and Foo, D. C. Y. (2004). Targeting the minimum water flowrate using water cascade analysis technique. *AIChE Journal.* 50(12): 3169-3183.

15- Obeng, E.D.A., Ashton, G.J., (1988). On pinch technology based procedures for the design of batch processes. *Chem. Eng. Res. Des.* 66, 255–259.

16- Pinto, J. M., & Grossmann, I. E. (1994). Optimal cyclic scheduling of multistage continuous multiproduct plants. *Computers and Chemical Engineering, 18*(9), 797–816

17- Polley, G. T. and Polley, H. L. (2000). Design better water networks. *Chemical Engineering Progress.* 96(2): 47-52.

18- Puigjaner, L., Espuña, A. and Almató, M. (2000). A software tool for helping in decision-making about water management in batch process industries, *Waste Management*. 20: 645-649.

19- Shah, N., Pantelides, C. C., & Sargent, R. W. H. (1993). A general algorithm for short-term scheduling of batch operations. II. Computational issues. *Computers and chemical Engineering*, *17*, 229–244.

20- Shelley, M. D., & El-Halwagi, M. M. (2000). Componentless design of recovery and allocation systems: a functionality-based clustering approach. *Computers and Chemical Engineering*, *24*, 2081–2091.

21- Shoaib, A. M., Aly, S. M., Awad, M. E., Foo, D. C. Y. and El-Halwagi, M. M. (2007) A Hierarchical Approach for the Synthesis of Batch Water Network, *Computers & Chemical Engineering* (in press).

22- Zhao, X. G., O"Neill, B. K., Roach, J. R. and Wood, R. M. (1998). Heat integration for batch processes, Part I: Process scheduling based on cascade analysis. *Institution of chemical engineers, Trans IChemE.* 46, 685-699.