Synthesis of Water Utilization System Using Concentration Interval Analysis Method (II) Discontinuous Process

LIU Yongjian(刘永健), YUAN Xigang(袁希钢)* and LUO Yiqing(罗祎青) State Key Laboratory of Chemical Engineering, Chemical Engineering Research Center, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

Abstract The first part of the series of this article proposed a systematic method for the synthesis of continuous water-using system involving both non-mass-transfer-based and mass-transfer-based operations. This article, by extending the method, proposes a time-dependent concentration interval analysis (CIA) method to solve the problems associated with the synthesis of discontinuous or batch water-using systems involving both non-mass-transfer-based and mass-transfer-based operation. This method can effectively identify the possibility of water reuse and the amount of water reused under time constraints for minimizing the consumption of freshwater in single or repeated batch/discontinuous water-using systems. Moreover, on the basis of the heuristic method adapted from concentration interval analysis method for the continuous process network design, the network design for the discontinuous or batch process can be obtained through the designs for every time interval. Case study illustrates that the method presented in this article can simultaneously minimize the freshwater consumption in single or repeated batch/discontinuous water system and can determine a preferable storage tank capacity for some problems. Keywords water network, target method, discontinuous process, concentration interval table

INTRODUCTION

Water-using system operations can generally be classified into continuous and discontinuous processes[1,2] according to the views of process systems engineering. Synthesis of continuous water utilization system, on the basis of mathematical optimization[3-9] and conceptual approaches[10-19], has been well established. In contrast, only few studies have been performed for the optimization of discontinuous or batch water networks processes. This can be attributed to the design complexity underlying water management with time constraints, that is, not only the concentration levels of individual operations but also the arrangement of operation time restrict the reuse of water in discontinuous water-using system. Therefore, the development of a systematic procedure is required for water minimization in discontinuous systems.

Wang and Smith[1] published their first study on water minimization for discontinuous systems on the basis of water pinch analysis technique. They developed a flow rate vs. time diagram and suggested a graphical method that combined the time constraints with concentration driving force constraints for the targeting and design of discontinuous water-using systems. However, the targeting and design may become complex and time-consuming in the case of large scale and complex situations because the integrations among concentration, flowrate, and time cannot be conceptually interpreted easily from the diagram. This method can be directly applied to mass transfer-based water using processes, whereas it can not be directly applied to non-mass transfer-based processes, which has several important applications such as in the construction of reactor, cooling tower, etc. Recently, Foo et al.[17,18]presented a two-stage procedure on the basis of water cascade analysis technique for the synthesis of discontinuous water-using system involving both mass transfer-based and non-mass-transfer-based water-using operations. However, these studies are applicable only in the case of batch/ discontinuous processes. The other studies on discontinuous water systems are mainly based on the mathematical optimization approach. Almato et al.[20-22] developed an optimization framework for water usage in batch processes. However, the result obtained by their proposed superstructure model may lead to the generation of water at different time, which is mixed in the same storage, this may reduce the driving force and the possibility for water reuse and it require large and/or unnecessary storage, and therefore fresh water consumption might not be minimized. In addition, the nonlinear program (NLP) model was optimized using simulated annealing (SA) and deterministic method, thus it requires significant computational effort and an initial feasible solution. Kim and Smith[2] introduced a novel optimization framework, in which the time constraints were considered to identify the feasible connections among water operation units. However, the optimization problem is a mixed integer nonlinear program (MINLP), which is very difficult to be solved. Recently, Majozi[23,24] presented a continuous-time mathematical formulation for water minimization in discontinuous water-using system.

In contrast to the afore-mentioned study on the repeated batch problem, this article proposes a time-dependent concentration interval analysis (CIA) technique, which is the extended form of the improved CIA technique for continuous process proposed in Part I[25], for targeting both the single and repeated batch/discontinuous water-using systems involving the two types of water-using operations. Some data have been obtained from the previous study on heat[26] and mass[17,18] integration for batch systems.

Received 2006-05-23, accepted 2006-11-27.

^{*} To whom correspondence should be addressed. E-mail: yuanxg@tju.edu.cn

2 PROBLEM STATEMENTS

The objective of this study is to minimize freshwater consumption and wastewater generation through maximizing the available water resources in designing the water network for discontinuous process. The water network design, according to Kim and Smith[2], depends not only on the contaminant levels of water, possibility of water reuse, operation constraints, and design limitations, but also on the time constraint, as the requirement and availability of water is time-dependent. To achieve these targets, a series of time interval, such as starting and ending time of every operation unit, must be established according to the time constraints, which is specifically given for every operation unit.

The reuse of water between operations within the same time interval, such as the operations between P1 and P3, P2, and P4 is a feasible design option as long as the concentration limits are satisfied, and it is illustrated in Fig.1[2]. To minimize the freshwater consumption, the water reuse should be maximized. However, for different time interval, water reuse must satisfy the time constraints. As shown in Fig.1, the water from operation P1 can be reused in the process 2 through storage tank if the concentrations of the effluents from P1 are within the maximum allowable limits of operation P2, but the water from operation P2 can not be reused in operation P1 because of the time constraints, even if the concentration is within the allowable limits.



Figure 1 Water reuse under time constraints

3 TIME-DEPENDENT CONCENTRATION INT-ERVAL ANALYSIS TECHNIQUE

The modified CIA technique presented in part I is an approach used to establish the targets for continuous processes, involving both mass transfer-based and non-mass-transfer-based water-using processes. In the present section, this technique is extended by introducing a time-dependent CIA for targeting discontinuous/batch water utilization systems through a case study.

3.1 The statement of example problem

The example problem used for the case study is from the studies of Wang and Smith (1995). Table 1 shows the limiting water data as well as the time duration for this problem. It consists of three water-using processes operating in different time intervals with a

Table 1 Limiting water data for the example

Process	Demand	Concentrati	Time, h		
number	flowrate, t·h ⁻¹	$C_{i,\mathrm{in}}^{\mathrm{max}}$	$C_{i,\mathrm{out}}^{\mathrm{max}}$	ts	t _e
1	100	100	400	0.5	1.5
2	80	0	200	0	0.5
3	50	100	200	0.5	1

single contaminant. The starting time and ending time for the process operation are represented by t_s and t_{e} , respectively.

3.2 Synthesis method using time-dependent CIA

The target procedure using time-dependent CIA for batch/discontinuous water network is successively presented in the following subsections:

3.2.1 *Targeting the amount of minimum freshwater consumption for every time interval*

To establish the time-dependent concentration interval table (CIT), the time intervals should be first determined. The time intervals are defined as the time durations between the starting time and the ending time of the operations, which is analogous to the concentration intervals[14,25] and the number of time intervals can be calculated using the analogous expression,

$$N_{\rm in,t} = 2N_{\rm o} - N_{\rm du,t} - 1 \tag{1}$$

where $N_{in,t}$ is the number of time interval, N_0 is the number of operation unit, $N_{du,t}$ is the duplicate number of the starting and ending time of operation.

Any process operation that involves more than one time interval is considered as a series of operations operating in each time intervals with the same limiting data. In this example, considering the time intervals, process P1 is divided into two operations: P1 and P1'. Correspondingly, the modified limiting water data consider the artificial partition of the operation for the example problem, and it is shown in Table 2.

 Table 2
 The modified limited water data for example

Process	Demand	Concentrati	Time, h		
number	flowrate, t·h ⁻¹	$C_{i,\mathrm{in}}^{\mathrm{max}}$	$C_{i,\mathrm{out}}^{\mathrm{max}}$	ts	t _e
1	100	100	400	0.5	1.5
2	80	0	200	0	0.5
3	50	100	200	0.5	1
1'	100	100	400	1.0	1.5

Within each time interval, the water-using system can be considered as a continuous process, and CIT can be established using the approach described in part I of the series of this article. The time-dependent CIT can be constructed by cascading the CIT for all the time intervals for the example problem, as shown in Table 3. The nomenclatures in Table 1 is the same as in Part I.

Comparison C							Г	Time, h						_
Concentration C_j , interval ma I^{-1}	0-0.5				0.5-1.0			1.0—1.5				$f_{\rm w}$		
intervar	IIIg L	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\rm w}$	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\rm w}$	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\rm w}$	
					40				43.75				37.5	121.25
	400							17.5	43.75			15	37.5	
3						50	10			50	10			
	200			8	40			7.5	37.5			5	25	
2		40	4			75	7.5			50	5			
	100			4	40									
1		40	4											
	0													

 Table 3
 The CIT without considering the reuse between different time interval

On the basis of the as-defined time intervals, the water using process within each time intervals can be considered as a continuous process. The time-dependent CIT for the whole discontinuous water-using process can be constructed by cascading the CIT for all the time intervals[14,25], as shown in Table 3 for the example problem. From Table 3, it is evident that targeting can be carried out within each time intervals using the CIA technology given in Part I. After finishing targeting for all the time intervals, the accumulated result, which is obtained as 121.25t for the example problem in Table 3, is known as the minimum freshwater targeted for the discontinuous water system without considering the water reuse between different time intervals. This in fact, sets an upper bound for the targets with any considerations of water reuse among different time intervals. Furthermore, the pinch point within every time interval can be identified as the concentration interval that leads to the maximum flowrate of fresh water [1,3,4].

3.2.2 *Targeting the minimum amount of freshwater consumption for single batch*

According to the pinch principles for continuous process[10,11], above the pinch, only freshwater is used to remove the corresponding load; and below the pinch, wastewater is sufficient for removing the corresponding load. Therefore, for the water reuse between different time interval, as shown in Fig.2, if concentration interval j+1 is above the pinch point in a time interval, freshwater is required to remove the corresponding load, and if in a previous time interval, the *j*th or an upper concentration interval is below the pinch point of that time interval, it releases wastewater, and thereby the water reuse between these two time intervals can be realized. It should be noted that, for water reuse between time intervals, storage tank must be introduced to keep the released wastewater from



Figure 2 Water reuse between different time intervals

the time interval to be used in another time interval. The concentration constraints must be considered to ensure the feasibility of the driving force that results in mass transfer in the water-using operation.

For example, in the second time interval of 0.5— 1.0h in Table 3, the fresh water f_w up to concentration interval 3 is 43.75t, whereas it is 37.5t up to the concentration interval 2, thus, more water is required to remove the mass load of the concentration interval 3. At the same time, in the first time interval 0—0.5h, there is 40t water to be discharged at the end of concentration interval 2. Therefore, water can be reused between the two time intervals by the use of storage tank. Similarly, water can be reused between the time intervals 0—0.5 and 1.0—1.5h.

After the water reuse opportunity are identified, the amount of water that can be reused through the storage tank should be calculated using the following expression

$$f_{\mathrm{r},j} = \frac{\left(f_{\mathrm{w},j+1} - f_{\mathrm{w},j}\right) \left(C_{j+1} - C_{\mathrm{w}}\right)}{C_{j+1} - C^{*}}$$
(2)

where, C_{j+1} is the concentration at the end of concentration interval j, C^* is the concentration of the water reused, C_w is the concentration of the water source, f_{wj} is the amount of fresh water consumed up to the interval j, $f_{r,j}$ is the amount of water reused from the previous time interval *via* storage tank in the beginning of the interval j.

On the basis of the comparison between $f_{r,j}$ and the amount of water available for reuse, if the amount of required water is higher than the amount of available water, then all the available water should to be reused. On the other hand, if $f_{r,j}$ is less than the amount of water that can be reused, the amount of water to be reused should be equal to $f_{r,j}$. It should be noted that, the amount of water available for reuse from the previous time interval must be identified using the network design method, thus the target process should be performed using the design process.

For this example, concentration interval 3 in between the time intervals 0.5—1.0h and 1.0—1.5h require to reuse water of 12.5t and 25t, respectively, with 200mg·L⁻¹ from time interval 0—0.5h, and these details are provided in column 7 and 12 in Table 4.

Chin. J. Ch. E. 15(3) 369 (2007)

General de la C								Tim	ie, h						_
interval	$C_j,$ mg·I ⁻¹		0-	-0.5				0.5	-1.0			1.0	—1.5		$f_{\rm w}$
milervar	ing L	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\mathrm{w},j}$		F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\mathrm{w},j}$	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\mathrm{w},j}$	
					40					37.5				25	102.5
	400								17.5				15		
3							50	10			50	10			
	200			8	40	12.5			7.5	37.5 12.5			5	25	
2		40	4				75	7.5			50	5			
	100			4	40										
1		40	4												
	0														

 Table 4
 The CIT involving the reuse of water between different time interval for example

Note that, the target of water reuse between the time intervals should be started from the first concentration interval. After the identification of the amount of water reused, the water-using system involving the reuse should be target again using the improved CIA proposed in Part I, by considering the reused water as the one inner water source or as the fictitious water treatment process. The targeting procedure presented in this section should be repeatedly applied for every concentration interval until the availability of water and the requirement of water reuse is over.

The minimum amount of water usage is equal to the sum of minimum water usage in all time intervals. As shown in Table 4, the minimum amount of freshwater consumed is 102.5t: 19t fresh water is not consumed for water reuse in different time intervals.

3.2.3 *Targeting the minimum amount of freshwater consumption in the repeated batch*

Most industrial batch processes are repeated on a regular cycle, and water can be recovered between the batches as well as within a single batch through an intermediate storage. It has been demonstrated that the target for repeated batch process can be considered to be same as that for a continuous process[18], which is analogous to the energy integration of repeated batch process[25]. On the basis of this principle, this article gives the following time-dependent CIT (Table 5) for targeting the minimum amount of freshwater consumption in the repeated batches.

In contrast to the targeting for a single batch, the $\Delta m_{\text{cum},j}$ value is obtained by the summation of all time interval contaminant load Δm_j , further, the amount of freshwater consumption $f_{w,j}$ can be obtained using CIA technique. These details are provided in column 9 and 10 of Table 5.

For the example, the minimum freshwater requirement for repeated batch process is similar to that in the single batch, and the value is 102.5t.

3.2.4 Network design

On the basis of the network design approach proposed by part I, by introducing storage tank for the reuse of water between the time intervals, the network of single batch and repeated batch process can be constructed for all the time intervals.

For the single batch process, only the water from the previous time interval can be reused by the latter time interval, so similar to the target process, the water network design should be started from the first time interval, and it should follow the time interval sequence of water network design the last time interval.

Figure 3 shows the network design of a batch for the example, which requires one storage tank, and the storage capacity is 37.5t. Fig.4 shows the design by Kim and Smith[2] on the basis of "time pinch analysis"[1]. According to their studies, two storage tanks are required and the total storage capacity is 100 t. Comparison shows that the method proposed by the

Concen-	<u> </u>				Tim	ie, h				
tration	C_j , mg·I ⁻¹	0—	-0.5	0.5-	-1.0	1.0-	-1.5	Total s	system	$f_{ m w}$
interval	ing L —	F_{j}	Δm_j	F_{j}	Δm_j	F_{j}	Δm_j	$\Delta m_{\operatorname{cum},j}$	$f_{\mathrm{w},j}$	
										102.5
	400							40.5	101.25	
3				50	10	50	10			
	200							20.5	102.5	
2		40	4	75	7.5	50	5			
	100							4	40	
1		40	4							
	0									

 Table 5
 The CIT involving the reuse of water between different time interval for example



Figure 3 Water network design using CIA technique for the example



Figure 4 Water network design using Wang and Smith's approach for the example

present article describes a storage tank of preferable capacity to solve this problem.

For the repeated batch process, water reuse between any time intervals can be realized through introducing the storage tank. This repeated batch process can be considered as a continuous process[18], and the network design is on the basis of the continuous process approach proposed in Part I. For the specific case of the example problem, the obtained network for the repeated batch process is the same as that the single batch process, and it is shown in Fig.3.

3.3 Example analysis

As shown above, the optimal solutions for freshwater target and network design for both the single batch and the repeated batch process of the example problem are found to be same. However, for some example in reality, the target and network design for single batch and repeated batch process may be different. For the same example, if the time data are given as in Table 6 instead of those given in Table 1.

 Table 6
 Limiting water data for the example

Process	Demand	Concentration	Time, h		
number	flowrate, $t \cdot h^{-1}$	$C_{i,\mathrm{in}}^{\mathrm{max}}$	$C_{i,\mathrm{out}}^{\mathrm{max}}$	ts	t _e
1	100	100	400	0	1.0
2	80	0	200	1.0	1.5
3	50	100	200	0	0.5

Using the target procedure and network design approach proposed in Part I, for the single batch process, the freshwater target is found to be 121.25t, and the resulted network design is shown in Fig.5. For the repeated batch process, the freshwater target becomes 102.5t, and the network is shown in Fig.6. It is demonstrated that the target and network design for single and repeated batch process can be different The reason is that, in single batch process, the water in the latter time interval cannot be reused by the previous time interval because of time constraints, such as the water released by operation unit 2, whereas in repeated batch process, the water can be stored and can be reused by the operation units in the previous time interval of the next batch.

4 CONCLUSIONS

This article solves the synthesis problem of single and repeated batch/discontinuous water-using system. A time-dependent CIA method was proposed to solve the problems involving both non-mass-transfer-based and mass-transfer-based operation. Case study illustrated that the proposed method can effectively identify the water reuse opportunities and the amount of water reused under time constraints for reducing freshwater usage, thus the minimum freshwater consumption for single batch /discontinuous water-using systems can be targeted. Moreover, by comparing with the results obtained by Wang and Smith[1], this method obtains different flowsheet structure with less storage tank, and thereby reduces the cost of the system. The targeting for repeated batch process has also been performed.



Figure 5 Water network design of single batch process



Figure 6 Water network design of repeated batch process

NOMENCLATURE

C^{*}	the concentration of water to be reused, mg L^{-1}
C_i	the concentration up to the concentration inter-
5	val j, mg·L ⁻¹
$C_{ m w}$	the concentration of water source, $mg \cdot L^{-1}$
F_i	the sum of the limiting water flow rates through
	the interval j, $t \cdot h^{-1}$
$f_{\mathrm{r},j}$	the amount of water reused through the stor-
	age tank, $t \cdot h^{-1}$
f_{w}	the amount of freshwater consumption for enti-
	tle water system, $t \cdot h^{-1}$
$f_{\mathrm{w},j}$	the fresh water amount up to interval j , t·h ⁻¹
m_i	the load to be removed in interval j of operation
	unit <i>i</i> , kg·h
$\Delta m_{\text{cumulative}, j}$	the cumulative mass transferred up to the con-
	centration interval j , kg·h ⁺
Δm_j	the amount of mass transferred in interval j ,
	kg·h '
$N_{\rm du,t}$	the duplicate number of the starting and ending
	time of the operation
$N_{\text{in,t}}$	the number of time interval
No	the number of operation unit
Subscripts	
<i>i</i> , <i>n</i>	operation unit
j, k	concentration interval

REFERENCES

- 1 Wang, Y.P., Smith, R., "Time pinch analysis", *Trans. IChemE A*, **73**, 905–914(1995).
- 2 Kim, J.K., Smith, R., "Automated design of discontinuous water system", *Trans. IChemE B*, **82**(B3), 238– 248(2004).
- 3 Alva-Argaez, A., Kokossis, C., Smith, R., "Wasterwater minimization of industrial systems using an integrated approach", *Comput. Chem. Eng.*, 22(Suppl), 741—

744(1998).

- 4 Alva-Argaez, A., Kokossis, C., Smith, R., "A multi-contaminant transhipment model for mass exchanger networks and wastewater minimization", *Comput. Chem. Eng.* 23, 1439–1453(1999).
- 5 Savelski, M.J., Bagajewicz, M., "On the use of linear models for the design of water utilization systems in process plants with a single contaminant", *Trans. IChemE*, A(79), 600–610(2001).
- 6 Yang, Y.H., Lou, H.H., Huang, Y.L., "Synthesis of an optimal wastewater reuse network", *Waste Manag.*, 20(4), 311—319(2000).
- 7 El-Halwagi, M.M., Gabriel, F., Harell, D., "Rigorous graphical targeting for resource conservation *via* material recycle/reuse network", *Ind. Eng. Chem. Res.*, **42**(19), 4319—4328(2003).
- 8 Huang, C.H., Chang, C., Ling, H.C., Chang, C.C., "A mathematical programming model for water usage and treatment network design", *Ind. Eng. Chem. Res.*, 38(7), 2666–2679(1999).
- 9 Wang, B., Feng, X., Zhang, Z.X., "A design methodology for multiple-contaminant water networks with single internal water main", *Comput. Chem. Eng.*, 27(7), 903– 911(2003).
- Wang, Y.P., Smith, R., "Wastewater minimization", *Chem. Eng. Sci.*, **49**(7), 981–1006(1994).
- 11 Wang, Y.P., Smith, R., "Wastewater minimization with flowrate constraints", *Trans. IChemE A*, **73**, 889— 904(1995).
- 12 Dhole, V.R., Ramchandani, N., Tainsh, R.A., Wasilewski, M., "Make your process water pay for itself", *Chem. Eng.*, (1), 100–103(1996).
- 13 Olesen, S.G., Polley, G.T., "A simple methodology for the design of water networks handing single contaminant", *Trans. IChemE A*, **75**, 420–426(1997).
- 14 Polley, G.T., Polley, H.L., "Design better water networks",

June, 2007

Chem. Eng. Prog., 96, 47-52(2000).

- 15 Castro, P., Matos, H., Fernandes, M.C., Nunes, C.P., "Improvement for mass-exchange networks design", *Chem. Eng. Sci.*, 54, 1649—1665(1999).
- 16 Prakash, P., Shenoy, U.V., "Targeting and design of water networks for fixed flowrate and fixed contaminant load operations", *Chem. Eng. Sci.*, **60**(1), 255–268(2005).
- operations", Chem. Eng. Sci., 60(1), 255–268(2005).
 Foo, C.Y., Manan, Z.A., Yunus, R.M., Aziz, R.A., "Sythesis of mass exchage network for batch processes (1) Utility targeting", Chem. Eng. Sci., 59, 1009–1026(2004).
- 18 Foo, C.Y., Manan, Z.A., Yunus, R.M., Aziz, R.A., "Sythesis of maximum water recovery network for batch processes systems", *J. Clean Prod.*, **13**(15), 1381— 1394(2005).
- 19 Hallale, N., "A new graphical targeting method for water minimization", Adv. Environ. Res., 6(3), 377–390(2002).
- 20 Almato, M., Sanmati, E., Espuna, A., Puigjaner, L., "Rationalizing the water reuse in batch process industries", *Comput. Chem. Eng.*, 21, 971–976(1997).
- 21 Almato, M., Espuna, A., Puigjaner, L., "Optimization of

water use in batch process industries". Comput. Chem. Eng., 23, 1427-1437(1999).

- 22 Almato, M., Sanmati, E., Espuna, A., Puigjaner, L., "Economic optimization of the water reuse network in batch process industries", *Comput. Chem. Eng.*, 23, 157–160(1999).
- 23 Majozi, T., "An effective technique for wastewater minimization in batch processes", *J. Clean Prod.*, **13**(15), 1374–1380(2005).
- 24 Majozi, T., "Wastewater minimization using central reusable water storage in batch plants", *Comput. Chem. Eng.*, 29(7), 1631—1646(2005).
- 25 Liu, Y.J., Yuan, X.G., Luo, Y.Q., "Synthesis of water utilization system using concentration interval analysis method (I) Non-mass-transfer-based operation", *Chin. J. Chem. Eng.*, **15**(3), 361–368(2007).
- 26 Kemp, I.C., Deakin, A.W., "The cascade analysis for energy and process integration of batch processes (I) Calculation the energy target", *Trans. IChemE*, 67, 495–509(1989).