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Study on the Optimization of Completely Batch Water-using Network with Multiple Contaminants Considering Flow Change

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***Abstract*—**This work addresses the problem of optimizing completely batch water-using network with multiple contaminants where the flow change caused by mass transfer is taken into consideration for the first time. A mathematical technique for optimizing water-using network is proposed based on source-tank-sink superstructure. The task is to obtain the freshwater usage, recycle assignments among water-using units, wastewater discharge and a steady water-using network configuration by following steps. Firstly, operating sequences of water-using units are determined by time constraints. Next, superstructure is simplified by eliminating the reuse and recycle from water-using units with maximum concentration of key contaminants. Then, the non-linear programming model is solved by GAMS (General Algebra Model System) for minimum freshwater usage, maximum water recycle and minimum wastewater discharge. Finally, numbers of operating periods are calculated to acquire the steady network configuration. A case study is solved to illustrate the applicability of the proposed approach.

***Keywords*—**Completely batch process, flow change, multiple contaminants, water-using network.

I. Introduction

WATER-USINGnetwork synthesis (WNS) plays a more and more important role in the development of industrial processes and it should be taken seriously, due to the globally increasing concern about the environmental and economic issues associated with water usage and wastewater discharge. The studies on optimization of water-using network in literatures mainly focus on continuous processes. To date, batch processes occupy a considerable proportion in industries including pharmaceutical, fine chemical, especially food processes, which has drawn growing attention to the synthesis of batch water-using network. Most of the methodologies on water-using network synthesis can be broadly classified as graphical and mathematical techniques. The advantage of mathematical techniques is that it can handle multiple-contaminant problems and get globally optimal solution, whereas graphical techniques are limited to single contaminant problems.

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Wang and Smith [1] developed a graphical technique called time pinch technology for water minimization in batch processes, which proved to be restricted to semi-batch rather than strictly batch processes. References [2]-[4] have shown the studies on the water cascade analysis techniques to minimize water usage. The graphical techniques above are applicable to batch water-using network with singe contaminant and can not ensure global optimization. On the other hand, mathematical techniques have been developed in a set of literatures, as [5]-[9]. Most of the mathematical approaches proposed are confined to single contaminant system. Reference [10] hasshows a methodology for wastewater minimization in multiple contaminant system,considering whether central reusable water storage exists and solving the MINLP problem for minimizing wastewater.

In this work, a mathematical technique is introduced for the optimization of completely batch water-using network with multiple contaminants. The source-tank-sink network superstructure is set up to represent all possibilities of water recycle among water-using units, and a non-linear programming model base on the superstructure is built, by which flow change between the inlet and outlet of water-using units is taken into consideration for the first time. Next, the key contaminants of water-using units are identified, the limiting outlet concentration of which can be comparable and the superstructure is simplified through eliminating water recycle from the water-using units with maximum outlet concentration of key contaminants to other units. The network complexity is reduced and the mathematical model is solved by GAMS to determine the minimum freshwater utilization and water-using network configuration in a single period and multiple periods.

II. Problem Statement

The water-using units studied in this work are operated in completely batch process mode, in which water inflows and outflows only at the start time and end time respectively, and can be stated as follows:

1) A set of water-using units are given, the operating time (start time and end time) of which and varieties of contaminants included as well as mass loads to be removed are set, and the units tolerates limiting concentrations (maximum inlet and outlet concentrations).
2) The outlets of water-using units are considered as water sources that could supply recycle water, and inlets as water sinks that require water.

3) Storage tanks are used to bridge the time gaps, in which water from sources may be stored and recycled to sinks when needed in the same operating period or over operating periods.

Also available for service is a fresh water source without any contaminants from an external tank to supplement the water sinks requirements.

III. Design Approach

The design approach is described in the following sections.

A. Water-using Network Superstructure

Fig.1 represents a superstructure of batch water-using network, which involves water sources (ellipses), water sinks (rectangles), and storage tanks (cylinders). Water sources may be stored in a number of storage tanks for water recycle to water sinks or released as wastewater to a specified tank which collects wastewater. The maximum number of needed storage tanks is equal to the number of water sinks, so that it is sufficient to provide a single batch of water to each water sink.

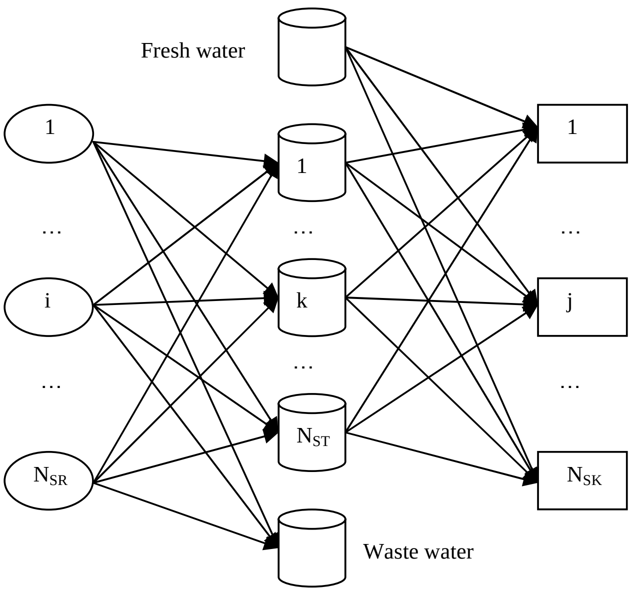

Fig.1. Superstructure of batch water-using network.

B. Mathematical Model

Object: minimize F_{FW} (1)

Subject to:

$$F_{FW} = \sum_j F_{fw}(j) \quad (2)$$

$$F_{SK}(j) = \sum_k F_{ST,SK}(k) + \sum_i F_{SR,SK}(i) + F_{fw}(j) \quad (3)$$

$$F_{SR}(i) = \sum_k F_{SR,ST}(k) + \sum_j F_{SR,SK}(j) + F_{SR,WW}(i) \quad (4)$$

$$F_{ST}(k)_P = \sum_i F_{SR,ST}(i) + F_{ST}(k)_{P-1} \quad (5)$$

$$F_{ST}(k)_{P-1} = 0 \text{ when } P = 1 \quad (6)$$

$$F_{SK}(j) * C_{in,c}(j) = \sum_k F_{ST,SK}(k) * C_{ST,c}(k) + \sum_i F_{SR,SK}(i) * C_{out,c}(i) \quad (7)$$

$$F_{ST}(k)_P * C_{ST,c}(k)_P = \sum_i F_{SR,ST}(i) * C_{out,c}(i) + F_{ST}(k)_{P-1} * C_{ST,c}(k)_{P-1} \quad (8)$$

$$F_{SR}(i) * C_{out,c}(i) - F_{SK}(i) * C_{in,c}(i) = m_c(i) \quad (9)$$

$$F_{SR}(i) = F_{SK}(i) + \sum_c m_c(i) \quad (10)$$

$$F_{SR}(i) \le Q_{out}^{\max}(i) \quad (11)$$

$$F_{SK}(i) \ge Q_{in}^{\min}(i) \quad (12)$$

$$Q_{out}^{\max}(i) = \max_c \left(m_c(i) \Big/ \left(C_{out,c}^{\max}(i) - C_{in,c}^{\max}(i) \right) \right) \quad (13)$$

$$Q_{in}^{\min}(i) = \max_c \left(m_c(i) \Big/ C_{out,c}^{\max}(i) \right) \quad (14)$$

$$C_{in,c}(i) \le C_{in,c}^{\max}(i) \quad (15)$$

$$C_{out,c}(i) \le C_{out,c}^{\max}(i) \quad (16)$$

$$F_{WW} = \sum_i F_{SR,WW}(i) \quad (17)$$

$$t_{i,s} \le t_i \le t_{i,e} \quad (18)$$

$$F_{key}(i) = \max_c \left(m_c(i) \Big/ \left(C_{out,c}^{\max}(i) - C_{in,c}(i) \right) \right) \quad (19)$$

$i = 1,2,\dots,N_{SR}$, $j = 1,2,\dots,N_{SK}$, $k = 1,2,\dots,N_{ST}$, $c = 1,2,\dots,S$, $P = 1,2,\dots$

The first set of constraints represents that the total freshwater flow is the sum of the freshwater sent to each water sink. The second constraint represents the flow balance for each water sink where water recycles from tanks during the discontinuous operating time and from water sources when the operating time of a unit and the next one is continuous, and fresh water supplements when needed. The third set of constraints represents the flow balance for each water source where water available is distributed to a number of tanks, water sinks, and the waste water tank when water source is not allocated for recycle. The fourth constraint shows the flow balance for each tank in the operating period P , which is the sum of recycle water from water sources and water remaining in the previous period, and the initial condition is given by(6).The next three constraints represent the mass balance of each contaminant for each sink, tank and source by (7), (8) and (9). Considering the flow change between the inlet and outlet of water-using units caused by mass transfer, the outflow is the sum of the inflow and mass loads of all contaminants, which given by (10) improves the accuracy compared to the dilute solution hypothesis. The low limit of inflow and high limit of outflow are added in this work, represented by(13) and (14) respectively, which could accelerate convergence. The constraints given by (15) and (16) ensure that the inflow and outflow should satisfy the constraint of concentration for each contaminant in water sinks and sources. The total amount of wastewater collected in a specified tank is the sum of individual wastewater from the water sources, represented by (17). As assumed, the constraint of the operating time of each unit is given by (18).

The key contaminant of a unit is identified by (19), and then the superstructure can be simplified through eliminating water recycle of the unit with maximum concentration of key contaminant as shown in [11] to reduce the complexity, the advantage of which may be more obvious especially in a large water-using network.

This mathematical model is a non-linear program (NLP), which can be solved to determine the target of minimum usage of freshwater, and the assignment of recycle water allocated among water sources, tanks, and water sinks. In this work, binary variables that identify the existence of storage tanks are not taken into account, which further decreases the complexity of solving the model compared to the mix-integer non-linear program. If the flow of recycle water stored in a tank is small (close to zero), it can be concluded that this tank is nonexistent. The minimum usage of freshwater and a steady water-using network configuration can be acquired by the single period and multi-period procedures. In order to demonstrate the applicability of the approach afore-mentioned, a case is solved as follows.

IV. Case Study

Table 1 shows the water-using data for a case study (adapted from [12]).

TABLE I
WATER-USING DATA

i	c	$C_{i,in,c}^{max}$	$C_{i,out,c}^{max}$	$t_{i,s}$	$t_{i,e}$	$m_{i,c}$
	1	1000	4000			300
A	2	2000	4000	6	18	200
	3	500	2000			150
	1	0	2000			80
B	2	0	1000	6	18	40
	3	0	500			20
	1	1000	2000			25
C	2	500	1000	0	5	10
	3	500	1500			20

Following the proceduresof solving the problem proposed in this work, the order of operation is C, A (B) in a single period, and the unit B should consume freshwater completely rather than recycle water due to the limiting inlet concentration of contaminants. The outflow of unit A is discharged directly to the wastewater tank because of its maximum concentration of key contaminant 3, and the superstructure is simplified. The water from the unit C could be stored in tanks and reused. A single period mathematical model is solved by GAMS and the result is that minimum freshwater usage 124.29t, wastewater discharged 125.14t, one tank needed to store recycled water, and the water-using network is shown in Fig.2.

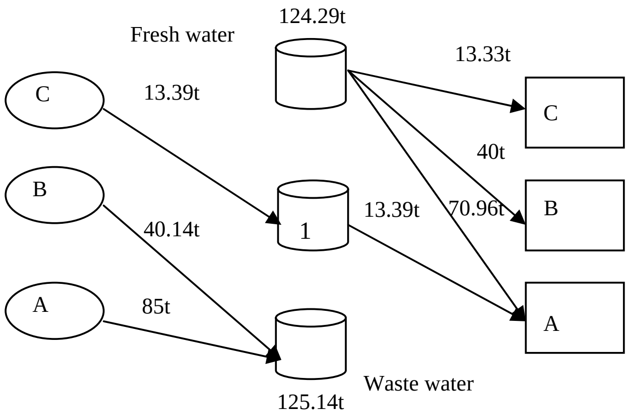

Fig. 2 Water-using network in a single period

Taking multiple periods into account, the outflow of water-using units in a single period could be reused in the following period and the usage of freshwater could decrease accordingly. The multi-period procedures are employed and a steady water-using network is determined through calculation in two operating periods with minimum freshwater usage 101.87t, wastewater discharged 87.93t, a storage tank of capacity 49.66m^3 needed, shown in Fig.3. The minimum usage of freshwater in this work corresponds to a reduction of 20.6%, compared to that without water recycle among water-using units.

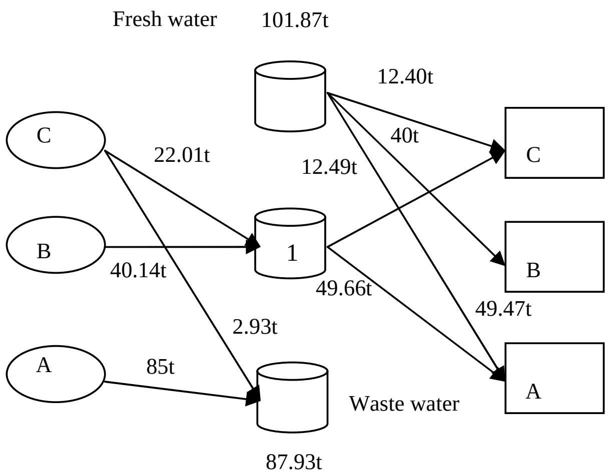

Fig. 3 The steady water-using network in multiple periods

V. Conclusions

A mathematical approach considering the flow change for minimizing freshwater utilization in completely batch water-using processes with multiple contaminants has been proposed in this work. Firstly, a source-tank-sink water-using network superstructure is built, and a non-linear programming (NLP) model taking flow change into consideration is represented. Secondly, the superstructure is simplified through eliminating water recycle of water-using units with maximum concentration of key contaminants. Finally, minimum usage of freshwater and a steady water-using network are determined through solving the mathematical model by GAMS in a single period and multiple periods. The approach proposed in this paper is applicable to both single period and multi-period batch facilities with multiple contaminants. The main advantages of the approach lie in its ability to decrease the complexity of solving mathematical models involving time constraints and multi-contaminant system, applicability of considering the flow change to be more realistic for mass transfer. A case study has been solved to illustrate the effectiveness of the proposed approach.

NOMENCLATURE

TABLE II
CHARACTERS

Symbol	Annotation	Conversion units to SI [a]
C	concentration	1 ppm→ 10^{-6}kg/kg
F	flow	1 t→10^3kg
m	mass load	1 kg
N	counting number	1
P	operating period	1
Q	flow	1 t→10^3kg
t	operating time	1 h→3.6×10^3s

TABLE III
SUPERSCRIPTS

Symbol	Annotation
max	maximum
min	minimum

TABLE IV
SUBSCRIPTS

Symbol	Annotation
c	varieties of contaminants
e	end of operating
FW, fw	freshwater
i, j	water-using units
in	inlet
k, ST	storage tanks
key	key contaminant
out	outlet
s	start of operating
SK	water sink
SR	water source
WW, ww	wastewater

ACKNOWLEDGMENT

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TABLE VI
EDUCATIONAL BACKGROUND

Degree	Major	Institution	Earned year
Doctor	Chemical Process Systems Engineering	DUT, Dalian, Liaoning, PRC	2004
Master	Chemical Engineering	DUT, Dalian, Liaoning, PRC	1989
Bachelor	Chemical Engineering	DUT, Dalian, Liaoning, PRC	1986

TABLE VII
PUBLICATIONS

Articles
Du Jian, Meng Xiaoqiong,Du Hongbing,Yu Hongmei, Fan Xishan,Yao Pingjing，"Optimal design of water utilization network with energy integration in process industries (Periodicalstyle),"*Chinese Journal of Chemical Engineering*, Vol. 12, No. 2, pp. 247-255, 2004.
XIAO Feng,DU Jian,LIU Linlin,LUAN Guoyan,YAO Pingjing ，" Simultaneous Optimization of Synthesis and Scheduling of Cleaning in Flexible Heat Exchanger Networks (Periodical style),"*Chinese Journal of Chemical Engineering*,Vol. 18, No.3, pp.402-411, 2010.
Lin-lin Liu, Jian Du, Feng Xiao, Li Chen, Ping-jing Yao, "Direct heat exchanger network synthesis for batch process with cost targets (Periodical style),"*Applied Thermal Engineering*, Vol. 31, No.14-15, pp. 2665-2675, Oct. 2011.

TABLE VIII
AWARDS

Award	Identified Insitution	Earned year
The Third-class Rewarding of Excellent Teaching Progress of Liaoning Province	Construction and Reform of Laboratory of Principle of Chemical Engineering	2005
The Second-class Rewarding of Science and Technology Progress of Petroleum and Chemistry Industry Association of China (01II-2-005-1)	The Technology of Process Systems Energy Integration	2001

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Jian Du was born on December 3 in1964 in Benxi city of Liaoning province in China, and studied in Dalian University of Technology from 1982 to 1989 for Bachelor degree and Master degree majoring in Chemical Engineering, and then earned the Doctor degree in 2004 majoring in Chemical Process Systems Engineering since 2000. She has been working in Chemical Engineering Department of Dalian University of Technology since 1989 from an Assistant to a Lecturer and to an Associate Professor and then to a Professor. She has publications in the form of books and articles, and her research interests are Process Systems Engineering, Energy Integration and Mass Integration.Prof. Du has been awarded the Technology of Process Systems Energy Integration, identified by the Ministry Education of China in 2000, and the Second-class Rewarding of Science and Technology Progress of Petroleum and Chemistry Industry Association of China (01II-2-005-1) in 2001, and the First-class Rewarding of Excellent CAI of DUT in the Net Class of Principle of Chemical Engineering in 2004, and the Third-class Rewarding of Excellent Teaching Progress of Liaoning Province in the Construction and Reform of Laboratory of Principle of Chemical Engineering in 2005.

TABLE V
PERSONAL INFORMATION

Birthdate	Birthplace	Sex
December 3, 1964	Benxi, Liaoning, PRC	female