



# Optimal design of batch mass exchange networks with multipurpose exchange units



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## ARTICLE INFO

### Article history:

Received 15 March 2015

Received in revised form

23 September 2015

Accepted 2 October 2015

### Keywords:

Batch process

Mass exchange network

Simultaneous optimization

Multipurpose mass exchanger

Mixed-integer nonlinear optimization

## ABSTRACT

A novel mathematical model for simultaneous optimization of batch mass exchange networks with multipurpose mass exchange units that can be shared by more than one match in different periods is presented in this work. It can be shown that both utility cost and capital investment can be reduced simultaneously with the use of multipurpose mass exchangers and mass storage tanks. Specifically, state-space superstructure that does not contain any structural simplification is proposed to capture the entire characteristics of the network configuration and a mixed-integer nonlinear optimization model is then formulated accordingly to generate the optimal batch operating policies and the corresponding flowsheet. Two examples are presented in this paper to demonstrate the validity and advantages of the proposed approach.

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## 1. Introduction

Mass transfer operations, which transfer single or multiple components from rich streams into relatively lean mass separating agents (MSAs) to conduct the separations, are ubiquitous and indispensable in chemical industries. A mass exchange network (MEN), which consists of several mass-exchange units arranged in a specific configuration, is widely used in the process industry to reduce pollution, recover valuable materials, and meet product specifications (El-Halwagi, 2012).

The importance of continuous MEN synthesis was first brought to attention by El-Halwagi and Manousiouthakis (1989). Since then, continuous MEN design has long been the research focus of process systems engineering community. The techniques to synthesize continuous MEN can be classified into the following three categories: the insight-based pinch and graphical techniques (El-Halwagi and Manousiouthakis, 1990a; Hallale and Fraser, 2000a, 2000b, 2000c, 2000d; Gadalla, 2015), the mathematical-based optimization approaches (Papalexandri et al., 1994; Papalexandri and Pistikopoulos, 1994; Sztikai et al., 2006; Chen and Hung, 2005, 2007; Liu et al., 2013a) and the hybrid methods (El-Halwagi and

Manousiouthakis, 1990b; El-Halwagi and Srinivas, 1992; Srinivas and El-Halwagi, 1994a, 1994b; Alva-Argaez et al., 1999; Isafiade and Fraser, 2008; Wagialla, 2012; Azeez et al., 2012, 2013; Liu et al., 2013b). However, relative few studies have been carried out for batch MEN synthesis due to the inherent time dimension. MEN synthesis for batch process systems are industrially very common and important since (1) batch MEN design explicitly considers MSAs and therefore is a more generalized procedure of batch water network design and (2) the process configuration of a batch process is more flexible and can be easily adjusted to meet the product specifications. The techniques to synthesis batch MEN can be broadly classified into two classes: the insight-based pinch analysis (Foo et al., 2004, 2005) and the mathematical-based optimization techniques (Chen and Ciou, 2006, 2007). Foo et al. (2004) first proposed time-dependent composition interval table and calculated the consumption of external utilities of the batch MEN with three operating modes, including the single operation without storage tanks, the single operation with storage tanks, and the cyclic operation with storage tanks. Later, Foo et al. (2005) introduced the method for setting the minimum number of mass exchange units target and a procedure for designing a maximum mass recovery network that features the minimum utility targets. On the other hand, without using any heuristics that are based on the concepts of pinch limitation, Chen and Ciou (2006, 2007) proposed a sequential strategy for synthesizing the batch MEN and its associated mass storage policy based on the stage-wise superstructure (Yee and Grossmann,

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**Notations***Superscripts*

in inlet to distribution network  
out outlet from distribution network

*Sets and indices*

$E$  set of multipurpose exchange units  
 $LS$  set of lean process sources and external MSAs  
 $ME$  set of mass exchange tasks  
 $ME_e$  set of separation tasks that can be performed in unit  $e$   
 $N_{sp}$  all forbidden mixing nodes of stream from  $sp$   
 $R_{me}^{out}, L_{me}^{out}$  mixing node of rich and lean streams at  $me$   
 $R_{me}^{in}, L_{me}^{in}$  splitting node of the rich and lean at  $me$   
 $RS$  set of all rich process sources  
 $SINK$  set of all process and waste sinks  
 $ST$  set of mass storage units  
 $st^{out}, st^{in}$  mixing and splitting nodes around tank  $st$   
 $T$  set of time intervals during the time horizon  
 $SP$  set of all splitting nodes in distribution network,  
 $SP = R_{me}^{in} \cup L_{me}^{in} \cup RS \cup LS \cup ST^{in}$   
 $MX$  set of all mixing nodes in distribution network,  
 $MX = R_{me}^{out} \cup L_{me}^{out} \cup SINK \cup ST^{out}$

*Parameters*

$F_{sp}^{in,max}$  upper bound of the mass flow rates at node  $sp$  in DN  
 $F_s^{max}, F_s^{min}$  upper and lower bounds of the mass flow rates in DN  
 $M^{max}, M^{min}$  upper and lower bounds of the mass exchange rate  
 $\Delta C^{min}$  minimum composition difference  
 $h, b$  Henry coefficient and constant  
 $cost_{ls}, cost_{st}$  annualized cost coefficients for lean stream  $ls$  and storage  $st$   
 $cost^{fix}, cost^{var}$  annualized fixed and variable cost coefficients for mass exchangers  
 $D_t$  the elapse time for time interval  $t$  per batch cycle  
 $NC$  the number of batch operation cycle per year  
 $V^{max}$  maximum size of storage tank

*Continuous variables*

$f_{mx,t}^{out}$  total mass flow rate at mixing node  $mx$  at time interval  $t$   
 $c_{mx,t}^{out}$  composition at mixing node  $mx$  at time interval  $t$   
 $f_{sp,t}^{in}$  total mass flow rate at splitting node  $sp$  at time interval  $t$   
 $c_{sp,t}^{in}$  composition at splitting node  $sp$  at time interval  $t$   
 $f_{sp,mx,t}$  mass flow rate from splitting node  $sp$  to mixing node  $mx$  at time interval  $t$   
 $m_{me,t}$  mass exchange rate of task  $me$  at time interval  $t$   
 $\Delta c_{me,t}^1, \Delta c_{me,t}^2$  composition driving forces for task  $me$  in time interval  $t$   
 $NT_{me,t}$  number of trays needed for task  $me$  in interval  $t$   
 $N_e$  number of trays for equipment  $e$   
 $v_{st,t}$  the mass in tank  $st$  at the end of interval  $t$   
 $v_{st}$  the size for storage tank  $st$

*Binary and integer variables*

$nfs_{sp,mx,t}$  binary variables denoting the existence/nonexistence of the flow between nodes  $sp$  and  $mx$  in time interval  $t$   
 $w_{me,t}$  binary variables denoting whether task  $me$  is performed in interval  $t$

$z_{e,t}$  binary variables denoting whether equipment  $e$  is occupied in interval  $t$   
 $z_e$  binary variables denoting the existence/nonexistence of equipment  $e$

1990) for batch cyclic production. The network configurations and the operational rates of all streams were obtained first by minimizing the total annual cost (TAC). Then, cost of stream storage was minimized based on results obtained from the first design phase. Despite considerable contributions accomplished by Chen and Ciou's works, there are several limitations that inevitably lead to the suboptimal designs of the batch MEN networks. One serious limitation is that extra processing capacities of mass exchange units are essentially wasted since a single mass exchanger was used to satisfy the separation need of one particular pair of streams. Another equally serious problem is that the established policies for the use of storage tanks based on stage-wise superstructure are far from optimal. A much larger class of design alternatives is eliminated from the stage-wise superstructure as streams are only allowed to enter to or exit from the storage tanks at both ends of each stage. As a result, the economic optimality of those resulting networks cannot be guaranteed since (1) many design features, such as time-sharing usage of mass exchanger, are left out of consideration and (2) the trade-offs among all cost terms (i.e., cost of storage devices, cost of utilities and cost of mass exchange units) cannot be properly balanced based on the sequential approach.

The aforementioned drawbacks of the traditional batch MEN designs have been circumvented in this study by introducing the state-space framework and multipurpose mass exchange units. In particular, a state-space representation is proposed to capture all possible structural characteristics of batch MEN and to give maximum flexibility on the usage of storage tanks. Moreover, to avoid the capacity waste in earlier works, time-sharing schemes and multi-purpose mass exchangers that can be shared by more than one pair of match in different time intervals are introduced. With this approach, it can be shown that (1) the number of mass exchange units needed as well as processing capacities can be saved and (2) both total operating cost (TOC) and total capital cost (TCC) can be simultaneously reduced. To illustrate the overall design methods developed in this work, the rest of this paper is organized as follows. The batch MEN design problem is formally defined in the next section. The MINLP model and solution strategy are described in Sections 3 and 4, respectively. Encouraging results and improvements against the benchmark examples from the literature are reported in Section 5. Conclusions and future works are provided in Section 6.

## 2. Problem statement

To facilitate the concise formulation of the mathematical model, several important assumptions are first made to simplify this problem: the mass flow rates and composition of each stream remain unchanged throughout the network within its time duration; the equilibrium relation governing the transferable component is independent of time and the entire network operates at constant pressure; mass exchange takes places in a tray column and the mass exchange units are of the counter-current type; multipurpose mass exchange units can be utilized to perform different mass transfer tasks without solvent contamination; the working capacity of the multipurpose mass exchanger is adjustable according to the way suggested by Sekine and Kusakabe (1992); mass storage tanks are allowed to be used but the initial and final operating conditions

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