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Separation network design with mass and energy separating agents

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ABSTRACT

The mathematical model developed in this paper deals with simultaneous synthesis of the integrated separation network, where both mass separating agents (MSAs) and energy separating agents (ESAs) are taken into account. The proposed model formulation is believed to be superior to the available ones. Traditionally, the tasks of optimizing ESA-based and MSA-based processes were either performed individually or studied on a heuristic basis. In this work, both kinds of processes are incorporated into a single comprehensive flowsheet and a novel state-space superstructure with multi-stream mixings is adopted to capture all possible network configurations. By properly addressing the issue of interactions between the MSA and ESA subsystems, lower total annualized cost (TAC) can be obtained by solving the corresponding mixed-integer nonlinear programming (MINLP) model. A benchmark problem already published in the literature has been investigated to demonstrate how better conceptual designs can be generated by our proposed approach.

1. Introduction

Separation operations, which transform chemical mixtures into new mixtures and/or essentially pure components, are of central importance in process industries. Separations involve different modes and one way of classifying these separation processes is based on the nature of separating agents, which take the form of MSAs and ESAs. Typical ESA and MSA processes, especially distillation sequences and the mass exchange networks (MEN), have been the subject of extensive investigations due to the significant capital and operating costs associated with such processes.

In the past decades, a number of approaches have been proposed for the systematic synthesis of distillation sequences, including heuristic methods (Seader & Westerberg, 1977), evolutionary techniques (Stephanopoulos & Westerberg, 1976), hierarchical decomposition (Douglas, 1998), explicit and implicit enumerations (Chavez, Seader, & Wayburn, 1986; Fraga & McKinnon, 1995), stochastic methods (An & Yuan, 2009; Fraga & Matias, 1996; Wang, Li, Hu, & Wang, 2008), matrix based methods (Ivakpour & Kasiri, 2009; Shah & Agrawal, 2010), temperature collocation approaches (Ruiz et al., in press; Zhang & Linninger, 2004) and superstructure based optimization (Andrecovich & Westerberg, 1985; Bagajewicz & Manousiouthakis, 1992; Caballero & Grossmann, 2001, 2004; Floudas & Paules, 1988; Proios & Pistikopoulos, 2005; Yeomans & Grossmann, 2000a, 2000b). As observed by Yeomans and Grossmann (1999), while there are relative merits and shortcomings of these different approaches, superstructure optimization can provide a systematic framework with which the various subsystems can be simultaneously optimized and interconnected in a natural way. For instance, a superstructure optimization model for distillation can be readily incorporated as part of the optimization of a process flowsheet. As we will demonstrate later in this paper, our research fully takes such advantage and is specifically aimed at addressing the formulation and interactions of distillation system with MEN design.

Compared to the extensive investigations on distillation sequences, it was not until late 1980s that pollution preventions and economic considerations had drawn attention to a more specialized separation problem, MEN synthesis. In the early development, a systematic sequential procedure that can synthesize MEN was first proposed by El-Halwagi and Manousiouthakis (1989). In this work, preliminary network featuring maximum mass exchange was generated and then improved to obtain a final cost effective configuration which satisfies the assigned exchange duty. Later, El-Halwagi and Manousiouthakis (1990a) introduced the linear transshipment model (Papoulias & Grossmann, 1983) to the synthesis of MEN with single-component targets. Their work was further developed to incorporate the associate mass-exchange regeneration networks which deal with lean stream recycling (El-Halwagi & Manousiouthakis, 1990b). In recent studies, Hallale and Fraser (2000a, 2000b, 2000c, 2000d) presented a series of papers for targeting the capital and operating cost estimates with

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Nomenclature

Sets and indices

RS^{IN} initial inlet nodes of rich streams to DN
PLS^{IN} initial inlet nodes of process lean streams to DN
ELS^{IN} initial inlet nodes of external lean streams to DN
RLS^{IN} initial inlet nodes of regenerating agents to DN
RS^{OUT} final outlet nodes of rich streams from DN
PLS^{OUT} final outlet nodes of process lean streams to DN
ELS^{OUT} final outlet nodes of external lean streams to DN
RLS^{OUT} final outlet nodes of regenerating agents to DN
ME set of mass exchange units (including regenerating units) in the system
DIS set of distillation columns in the system
RIN_{ME} mixing node of rich streams leading to the inlet of mass exchange unit *me*
$ROUT_{ME}$ splitting node of the rich stream from the outlet of mass exchange unit *me*
LIN_{ME} mixing node of lean streams (including regenerating agents) leading to the inlet of mass exchange unit *me*
$LOUT_{ME}$ splitting node of the lean streams (including regenerating agents) from the outlet of mass exchange unit *me*
DIN_{DIS} node denoting the inlet of the distillation columns *dis*
$TOUT_{DIS}$ node denoting the outlet from the top of distillation unit *dis*
$BOUT_{DIS}$ node denoting the outlet from the bottom of distillation unit *dis*
MX all mixing nodes in the system, $MX = RS^{OUT} \cup PLS^{OUT} \cup ELS^{OUT} \cup RLS^{OUT} \cup RIN_{ME} \cup LIN_{ME} \cup DIN_{DIS}$
SP all splitting nodes in the system, $SP = RS^{IN} \cup PLS^{IN} \cup ELS^{IN} \cup RLS^{IN} \cup RIN_{ME} \cup LIN_{ME} \cup TOUT_{DIS} \cup BOUT_{DIS}$
N_{SP} all forbidden mixing nodes of stream from splitting node *sp*

Parameters

Fs_{max}, Fs_{min} upper and lower bounds of the flow rates in DN
$M_{me}^{max}, M_{me}^{min}$ upper and lower bounds of the mass exchanged in unit *me*
ΔC_{me}^{min} minimum composition difference for unit *me*
h_{me}, b_{me} Henry coefficient and constant in mass exchange unit *me*
$K_{re}a$ overall mass transfer coefficient
$\alpha_{dis}^{LK,HK}$ relative volatility of the light key component to the heavy key component
r_{dis} unit latent heat of the mixtures in distillation unit *dis*
$Q_{dis}^{max}, Q_{dis}^{min}$ maximum and minimum inlet flow rate to unit *dis*
C_{els}, C_{rls} annualized cost coefficients for mass separating and regenerating agents
C_{me}, C_{dis} annualized cost factors for mass exchange unit *me* and distillation unit *dis*
C^{h}, C^{c} annualized cost coefficients for hot and cold utilities

Continuous variables

f_{mx}^{out} total outlet flow rate from mixing node *mx*
c_{mx}^{out} composition at mixing node *mx*
f_{sp}^{in} total inlet flow rate to splitting node *sp*
c_{sp}^{in} composition at splitting node *sp*
$fs_{sp,mx}$ flow rate from splitting node *sp* to mixing node *mx*
fr_{me} flow rate of the rich stream passing through mass exchange unit *me*
cr_{me}^{in} composition of the rich stream leading to the inlet of mass exchange unit *me*
cr_{me}^{out} composition of the rich stream from the outlet of mass exchange unit *me*
fl_{me} flow rate of the lean stream passing through mass exchange unit *me*
cl_{me}^{in} composition of the lean stream leading to the inlet of mass exchange unit *me*
cl_{me}^{out} composition of the lean stream from the outlet of mass exchange unit *me*
m_{me} mass exchanged of unit *me*
$\Delta c_{me}^{1}, \Delta c_{me}^{2}$ composition driving forces at both ends of the mass exchanger *me*
Δc_{me} logarithmic mean composition difference for mass exchanged of unit *me*
A_{me} the area of mass exchange unit *me*
NTU_{me}, HTU_{me} the number of transfer units and the height of a transfer unit for packed column *me*
H_{me} the height of packed column *me*
NH_{me} number of the trays in the tray column *me*
q_{dis}^{in} inlet flow rate to distillation unit *dis*
c_{dis}^{in} composition of the heavy key component in stream to distillation unit *dis*
q_{dis}^{tout} outlet flow rate from the top of distillation unit *dis*
c_{dis}^{tout} composition of the heavy key component in stream from the top of distillation unit *dis*
q_{dis}^{bout} outlet flow rate from the bottom of distillation unit *dis*
c_{dis}^{bout} composition of the heavy key component in stream from the bottom of distillation unit *dis*
N_{dis}^{min} minimum number of equilibrium stages of distillation unit *dis*
NP_{dis} number of equilibrium stages of distillation unit *dis*
R_{dis}^{min} minimum reflux ratio of the of distillation column *dis*
R_{dis} actual reflux ratio of distillation column *dis*
x_{dis}^{e}, y_{dis}^{e} the mass fractions of the heavy key component in liquid and vapor at the feed plate in distillation unit *dis*
$\Phi_{dis}^{R}, \Phi_{dis}^{C}$ the heat duty for reboilers and condenser for unit *dis*

Binary and integer variables

$nfs(sp, mx)$ binary variables denoting the existence/nonexistence of the flow rate between nodes *sp* and *mx*
$w(me), w(dis)$ binary variables denoting the existence/nonexistence of the mass exchange unit *me* and distillation unit *dis*
N_{me} final number of trays after rounding up NT_{me} to the nearest integer
N_{dis} final number of plates after rounding up NP_{dis} to the nearest integer

simple approximations when calculating annualized costs. Apart from the aforementioned sequential procedures based on pinch technique, mathematical optimization techniques for MEN have been used to handle more complex trade-offs of all cost factors. Papalexandri, Pistikopoulos, and Floudas (1994) first developed an MINLP model based on a hyperstructure representation. The two-way balance between operating cost and investment cost was explored and this model was also extended to include regenera-