IDEAS Approach to Process Network Synthesis: Application to Multicomponent MEN

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A novel method for the globally optimal solution of the general process network synthesis problem is first presented and then applied to the solution of the minimum utility cost (MUC) problem for mass exchange networks (MEN) with multicomponent targets (MT). Previous approaches that address the MUC MEN MT synthesis problem are discussed, and the novel conceptual framework, Infinite DimEnsionAl State-space (IDEAS), is then introduced. IDEAS allows the formulation of general process network synthesis problems as infinite convex (linear) programs whose local solutions are guaranteed to be globally optimal. In addition, an MUC MEN MT problem where conventional methods fail is probed. Then, the optimal network generated using IDEAS is discussed, together with the wide-ranging potential impact and flexibility of IDEAS.

Introduction

In recent years, investigation of rigorous design methods for generating optimal separation systems has become an important area of chemical process design research. One key subproblem of this area is the design of separation systems featuring minimum utility cost (MUC). The MUC problem is useful both as an end method in itself and also in iterative design methods where utility and capital cost tradeoffs are evaluated. The focus on rigorous design methods is currently driven by two forces. First is the classic rationale of enhanced plant economics. A MUC design by construction is the most efficient user of energy and material resources. Second, and potentially more important, is the need for reduction in emission of pollutants, while maintaining economic viability. Ever increasing environmental regulations continually lower the amounts and concentrations of pollutants allowed to be emitted from chemical plants. An overall MUC design methodology will allow for the creation of plants with positive economic valuation and optimal use of utilities, while meeting stringent environmental regulations.

Several different approaches have been pursued to address the MUC network design problem. Inspired by concepts in heat exchange network synthesis (HEN), Manousiouthakis proposed the concept of mass exchange network (MEN) synthesis (Manousiouthakis et al., 1986). Further development by Manousiouthakis lead to the use of concentration-mass load diagrams and the mass pinch concept which were used to solve the MUC problem for MEN with phase equilibrium based mass exchange, with El-Halwagi (El-Halwagi and Manousiouthakis, 1989, 1990). This work was further developed by Manousiouthakis and Gupta into a linear programming formulation for MUC for MEN with variable single component targets (Gupta and Manousiouthakis, 1993, 1996). El-Halwagi and Srinivas later addressed the MUC problem for a class of reactive MEN with fixed, single component targets (El-Halwagi and Srinivas, 1992, 1994; Srinivas and El-Halwagi, 1994).

Another approach to the MUC network design problem was the creation of the state space (SS) network framework by Manousiouthakis and coworkers. This new method allowed the inclusion of more complex process operations. Applications of SS were shown for complex distillation networks with Bagajewicz (Bagajewicz and Manousiouthakis, 1992; Bagajewicz, Pham and Manousiouthakis, 1998), for nonisothermal MEN with Roxenby (Roxenby and Manousiouthakis, 1993; Roxenby 1994), and for multicomponent MEN with Gupta (Gupta and Manousiouthakis, 1994).

In an attempt to gain understanding of the underlying phenomena, the MUC problem for a single mass exchanger (MEX) with multicomponent targets was also investigated. For a single MEX described by a Kremser-Souders-Brown

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(KSB) model, Wilson and Manousiouthakis (1998) derived the solution. This work was extended to allow recycle flows around a single MEX with a KSB model by Karvé and Manousiouthakis (2000).

Extension of each of these approaches to an overall MUC MEN with multicomponent targets (MT) design methodology has nevertheless eluded researchers. The key difficulty has been the inclusion of multicomponent phenomena. In this work, we present a conceptual breakthrough that not only succeeds in identifying the optimal MUC MEN MT network design, but can also be used to identify the globally optimal solutions to the general process network synthesis problem. An in-depth discussion of the previous approaches is presented. A description of the new design framework, the Infinite DimEnsionAl State-space (IDEAS) is provided. An application follows where conventional single component based MEN methods fail, and IDEAS is shown to identify the globally optimal MUC for this MEN MT design problem. Conclusions are drawn and the potential impact of IDEAS on process network synthesis is discussed.

Analysis of Previous Work

Single component MEN design

As is often the case with new areas of research, the beginning stages of MEN design can be seen as an application of HEN design technology with a different set of assumptions (Manousiouthakis et al, 1986). Under a restrictive set of assumptions, such as linear phase equilibrium, dilute concentrations of transferable components, and single component mass transfer (El-Halwagi and Manousiouthakis, 1989, 1990), the MEN design problem can be handled quite ably by HEN-like technology. Even with these restrictions, a useful set of real world problems, such as waste reduction, can be effectively handled (Wilson et al., 1998; Wilson and Manousiouthakis, 1998).

Key to early single component MEN design is the concept of *mass pinch*. Mass pinch is an expression of second law limitations analogous to heat pinch for HEN. As a lower bound of required mass utility use, it is rigorously valid in all cases. The usefulness of mass pinch in MEN design suggests that other results from HEN would also be valid. For single component MEN design, such results do apply. Unfortunately this is not the case for multicomponent MEN design.

The first additional result that causes difficulties in the multicomponent case is that the mass pinch curve has implications for the network of mass exchangers. One expression of this is the common statement mass (heat) should not be transferred across the pinch. Whenever a process exhibits a pinch, it is divided into two sub-processes and network generation is done on each separately. As will be outlined in the section on mass pinch analysis and synthesis, this can lead to inefficient and inconsistent designs that violate the goal of MEN.

A second result carried over that causes difficulties is the effect of a minimum allowable concentration difference $\Delta c_{\min}$. This offset is one expression of the limitation of equipment design and the tradeoffs between capital and operating costs. When used on single component MEN, where no streams are allowed to mix, $\Delta c_{\min}$ has the effects predicted by mass pinch on the overall network design. With multicomponent MEN and/or with sets of streams that are allowed to mix, the results can be nonoptimal processes.

Another nonobvious problem is that single component MEN design contains the implicit assumption that any thermodynamically feasible mass transfer is physically realizable. Even with a relatively simple model such as KSB, this can be seen not to be the case (Wilson and Manousiouthakis, 1998).

Advancement of MEN design to successfully handle the general multicomponent problem has been an area of active research. Two key ideas have arisen from past efforts. First, mass pinch analysis provides a rigorous lower bound on thermodynamically feasible mass transfer. Second, results from HEN design concerning network design are not generally applicable to the general MEN problem. A new methodology that is capable of expressing all possible network configurations is needed for MEN MT design to succeed.

State space

The task of constructing a completely generalized network representation has been pursued by many researchers over the years (Cerda et al., 1983; Duran and Grossmann, 1986; Papoulias and Grossmann, 1983). One of the frameworks for this task is the state space (SS) approach to process synthesis. SS was first introduced by Manousiouthakis and coworkers and was used to address the complex distillation network problem (Bagajewicz and Manousiouthakis, 1992), the separable MEN problem (Roxenby, 1994; Roxenby and Manousiouthakis, 1993), and the multicomponent MEN problem (Gupta and Manousiouthakis, 1994).

The key feature of SS is how it represents the process network. The network is decomposed into two blocks of operations. The first is called the distribution network (DN). It is here that all mixing, splitting, recycling, and bypassing of process streams occurs. The second is called the process operator (OP). Here, all other process unit operations take place. The process input streams feed into and the process outlet streams emerge from the DN. The OP is fed by a set of streams from the DN and in turn feeds the DN. Using this framework, it is very easy to construct all possible flows within the process.

The OP block can employ either detailed or aggregate representations of all the input operations in the process. In Bagajewicz and Manousiouthakis (1992) it was advocated that any complex distillation network can be represented as a mass/heat exchange network, using the state-space approach. Various operator representations (such as pinch, split-matching, and assignment) for both the MEN and HEN sub-networks were proposed and novel distillation network designs featuring MUC were identified. These MUC designs contained a number of innovative features, including feed-bypassing, heat pumping, reboiler-condenser heat integration, and side-stream interconnections between distillation towers. SS was shown to provide a sufficiently powerful and rich network topology to discover new designs that outmatched previous work (Bagajewicz and Manousiouthakis, 1992; Bagajewicz, Pham and Manousiouthakis, 1998).

In addition to providing a generalized network framework for processes, SS is also available as a conceptual framework within which rigorous theoretical results can be developed (Roxenby, 1994; Roxenby and Manousiouthakis, 1993). Here, the OP block is an embedded single component mass or heat pinch operator. Through a variation induced minimization proof technique, a significant series of results for single component MEN design were discovered. This resulted in a relatively tractable optimization problem. Nevertheless, the state-space approach in general yields nonconvexities in the optimization formulation that disallow a guarantee of global optimality for any answer found.

Single mass exchanger results

In an attempt to understand the phenomena present in multicomponent MEN design without any *a priori* assumptions, a single multicomponent mass exchange operation (MEX) was investigated (Wilson and Manousiouthakis, 1998). This single MEX was modeled by the KSB equations (King, 1981). Through mathematical manipulations, the authors were able to derive an analytical solution. With a proper set of concentration bounds and flow rate costs, a key result was shown. It was shown that in certain cases the minimum cost could depend on concentration bounds in a different component in each stream. This situation is a phenomena unique to multicomponent design. When this situation is present, the minimum flow rate is raised considerably over the single component minimum.

The next step was to expand the operation examined to a single MEX with recycles on both streams. In (Karvé and Manousiouthakis, 2000) it was shown that these additional flows can lower the required utility from that of (Wilson and Manousiouthakis, 1998) but that it may be significantly higher than predicted by mass pinch.

This work did provide several insights. One is that multicomponent mass exchange with even the relatively simple KSB model exhibits complex phenomena not found in single component mass exchange. Another was that the results are seen to approach the mass pinch limit as the network complexity is increased. Thus, a generalized network could conceivably attain the mass pinch limit.

Observations of previous work

In summary, while each of the above approaches has not been successful in generating a solution to the multicomponent MEN design problem, they have brought to light key features that any solution must address. Single component MEN design has highlighted the importance of the lower bound shown by mass pinch and the need for a generalized network. SS presented a generalized network framework, but failed to yield convex optimization formulations. Finally, studies of mass transfer in simple network elements has decisively shown that the multicomponent MEN design problem is inherently different from its single component counterpart.

Infinite DimEnsionAl State-Space Approach

Conceptual description

The *Infinite DimEnsionAl State space* (IDEAS) is a novel framework for the construction of a completely generalized process network. The key development behind this advancement is the use of a process operator whose domain and range lie in infinite (rather than finite) dimensional spaces. This process representation allows both consideration of all possible process networks for an *a priori* given set of technologies, and the formulation of convex (linear) process network synthesis problems that guarantee global optimality of the obtained solutions.

Traditionally, process operations have been considered to take inlet stream information (such as flows, component concentration, enthalpies, and so on) and transform it to similar outlet stream information. The resulting process operators were nonlinear, giving rise to nonconvex optimal network synthesis formulations.

IDEAS provides a radical departure from this approach. It considers that the process operator takes extensive (quantity) inlet stream information (that is, flow), available at any possible intensive (quality) inlet stream condition (that is, component concentration, enthalphy, and so on) and unit operation parameter conditions (that is, residence time, number of transfer units, and so on) and transforms it to extensive outlet stream information (that is, flow) available at the corresponding intensive outlet stream condition provided by the unit operation model. When viewed in this manner, it is easy for the reader to verify that the resulting IDEAS process operator OP is linear for any chemical process. This is the direct result of the following property of chemical processes: When their inlet flow rates are increased proportionally (without altering the other intensive inlet conditions), their outlet flow rates are also increased by the same proportion, while their intensive outlet conditions remain unaltered, as long as appropriately defined design parameters are kept constant. Heat exchangers, mass exchangers, reactors, distillation columns, and all other chemical processes satisfy this property.

Thus, having established the linearity of the IDEAS process operator OP, we are now in a position to justify the claim that the IDEAS representation gives rise to convex (linear) problem formulations. The constraints in the DN are solely mixing and splitting operations. The intensive (quality) information concerning any flow entering or leaving the DN is now fixed giving rise to DN constraints that are linear in the extensive (flow) variables. This combined with the linear OP results in a convex (linear) feasible region.

Having described the conceptual foundation of the IDEAS approach, we are now ready to present its mathematical formulation.

Mathematical formulation of the feasible region

The IDEAS approach is shown in Figure 1. The network contains a number of "families" or sets of streams which are allowed to mix only within their family. These families are indexed by $i \in \{1, \dots, N\}$ and interact inside the DN within their own sub-DN, DN_i. Each family has p_i external inlet and r_i external outlet streams. The information about the external inlet streams for family i is given by a sequence pair, (u_i, α_i). Let $(u_i(j), \alpha_i(j))$ be the jth term of this sequence pair for family i. Then, $u_i(j)$ represents the scalar extensive quantity (flow) variable at condition j, while $\alpha_i(j)$ represents the vector intensive quality (component concentration, enthalpy, and so on) information at condition j. Considering the total mass flow rate entering each family to be finite, and given that the number of inlet streams for each family, p_i is finite, it then holds that $u_i \in \phi_0^+ \subset l_1^+$. The number of qualities that are

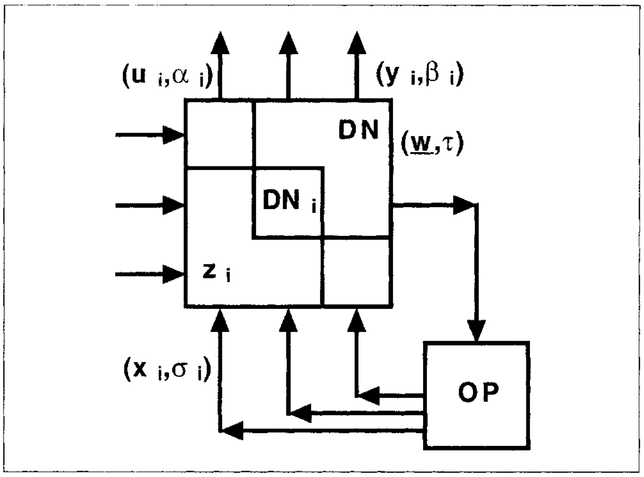

Figure 1. IDEAS network representation.

needed to describe a stream may vary from family to family and is given by n_i, yielding $\alpha_i \in l_\infty^{n_i}$. Without loss of generality and for mathematical simplicity, it is assumed that $\alpha_i(j) \in \mathbb{Q}^{n_i} \subset \mathbb{R}^{n_i}$. The external outlet streams are described in a similar manner by the sequence pair (y_i, β_i), where $y_i \in \phi_0^+ \subset l_1^+$, $\beta_i \in l_\infty^{n_i}$, and $\beta_i(j) \in \mathbb{Q}^{n_i} \subset \mathbb{R}^{n_i}$.

To capture the action of the OP requires a sequence pair in an inherently different space than the DN external inlets and outlets. To simplify discussion, the OP is restricted to a single unit operation technology and a single inlet stream from each family. The use of several different unit operations within a single process and multiple inlet streams from the same family is easily accomplished by the inclusion of either several OP blocks or modifications of the following description.

The information about the OP inlet streams is given by the sequence pair (w, τ). The first $\underline{w} = (w_1, \ldots, w_N)$ is a sequence of N-dimensional vectors whose jth term, $w(j)$, has entries $[w_i(j);\ i = 1, N]$, which represent the quantity (flow) variables from each of the $i = 1, N$ families entering OP at condition j. Considering the total mass flow rate entering OP from all families, over all conditions, to be finite, it then holds that $w_i \in l_1^+$ and $\underline{w} \in l_1^{+N}$. The second $\tau = (\gamma_1, \ldots, \gamma_N, \underline{\underline{R}}, D)$ is a sequence whose jth term consists of the following: $\gamma_i(j)$, $i = 1, N$ is a n_i-dimensional vector representing the quality (component concentration, enthalpy, and so on) information entering OP from the ith family at condition j; $\underline{\underline{R}}(j)$ is a $(N-1) \times N$ matrix representing the linear interrelations among the flow variables $[w_i(j);\ i = 1,N]$ entering OP at condition j; $D(j)$ is a d-dimensional vector whose entries represent the unit operation design parameters at condition j. Since the entries of $\tau(j)$ can be considered to be bounded, the following holds; $\gamma i \in l_\infty^{n_i}$; $i = 1, N$, $\underline{\underline{R}} \in l_\infty^{(N-1)\times N}$, and $D \in l_\infty^d$.

The information about the OP outlet streams for family i is given by the sequence pair (x_i, σ_i). To simplify the IDEAS description, all return flows to the same family at the same quality are combined before leaving the OP block. This creates N sequences of return flows that are given by the sequence pairs (x_i, σ_i). Since OP must obey a mass balance and the total OP inlet flow is finite, $x_i \in l_1^+$. The quality sequence for the OP outlet streams are in the same space as the external inlets and outlets for that family, that is, $\sigma_i \in l_\infty^{n_i}$, where $\sigma_i(j) \in \mathbb{Q}^{n_i} \subset \mathbb{R}^{n_i}$.

To more concisely describe the action of OP, an example is shown in Figure 2. Present are two families and a unit operation with two inlet flows, one from each family. Additionally, there are two qualities present in both families, and one design variable for the unit operation. This gives: $\gamma_i \in l_\infty^2$, $i = 1, 2$, $\underline{\underline{R}} \in l_\infty^{1\times 2}$, $D \in l_\infty$, $w \in l_1^{+2}$, $x_i \in l_1^+, i = 1,2$, and $\sigma_i \in l_\infty^2$, $i = 1, 2$. In this figure, only the first three inlet conditions, j, to OP are shown. Each condition specifies a unique unit operation. The conditions considered are such that the family 1 outlets for condition 1 and 2 have the same 'quality', as do the family 2 outlets for inlet conditions 1 and 3.

It should be emphasized at this point that the OP inlet flow rates at condition j, $[w_1(j), w_2(j)]$, are related by $\underline{\underline{R}}(j)$. For this example, the relationship would be $r_{1,1}(j)w_1(j) + r_{1,2}(j)w_2(j) = 0$, where $r_{1,1}(j)$ and $r_{1,2}(j)$ are fixed, finite values. Any change in one flow rate causes a proportional change in the other flow rate. Furthermore, the OP outlet flow rate contributions of inlet conditions j also change proportionally while the quality of the OP outlet condition is not altered.

The final set of variables needed to mathematically formulate IDEAS are the crossflow streams inside the DN. There are four sets of such streams corresponding to the DN inlet-OP inlet, DN inlet-DN outlet, OP outlet-DN outlet, and OP outlet-OP inlet connections. To describe each stream, information is needed about the flow rate, destination, and source. This information for the DN inlet-OP inlet streams is given by the sequence triplet $(z_{wui}, \tau, \alpha_i)$. Since the mass flow from the external inlets and the mass flow to OP are both finite and the DN must satisfy a mass balance at any point, $z_{wui} \in l_1^+(2)$. The other sets of streams are similarly defined by the sequence defined by the sequence triplets, $(z_{yui}, \beta_i, \alpha_i)$, $(z_{yxi}, \beta_i, \sigma_i)$, $(z_{wxi}, \tau, \sigma_i)$. Again, since the total mass leaving through the external outlets and the total mass entering the DN from OP are both finite, and since mass balances are

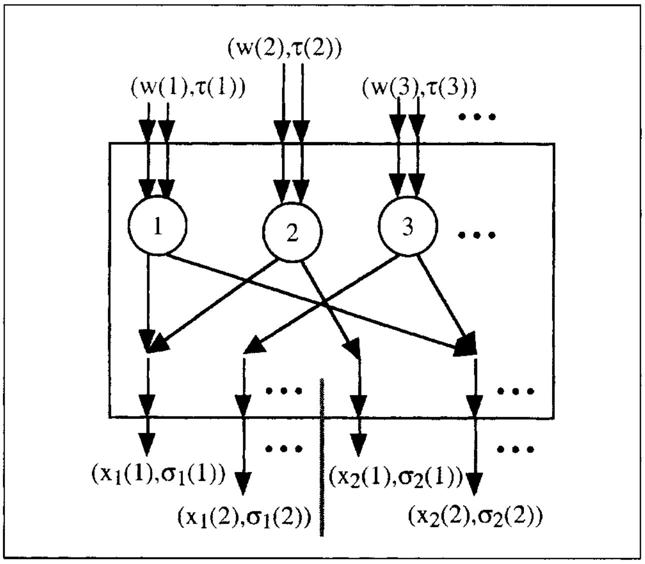

Figure 2. IDEAS OP representation.

required to be satisfied throughout the DN, it holds that $z_{yui} \in l_1^+(2)$, $z_{yxi} \in l_1^+(2)$, and $z_{wxi} \in l_1^+(2)$.

There are two classes of constraints present in the DN; conservation of mass and conservation of quality related entities. Examples of the latter are component balances, energy balances, and so on. Mass conservation equations are needed on all sides of the DN and are given by Eqs. 1—4 for the left, bottom, top, and right respectively. Quality related constraints are necessary only where mixing occurs, the top and right of the DN, and are given by Eqs. 5 and 6, where * is defined to be a multiplication of the corresponding elements of the sequences involved. The model equations for OP are given by Eqs. 7 and 8, where $F_i: l_1^N \rightarrow l_1$ is a linear operator that transforms the OP inlet flows into the ith family's OP outlet flows. F_i is defined so as to satisfy mass, energy, and design constraints for the unit operations. Equation 8 constrains the flows at each OP inlet condition j, $(\underline{w}_i(j),\ i=1, N)$, to have the specified ratios.

$$u_i = \left\{ \sum_{k=1}^{\infty} z_{wui}(k,j) + \sum_{k=1}^{\infty} z_{yui}(k,j) \right\}_{j=1}^{\infty} \quad i=1,\ldots,N \quad (1)$$

$$x_i = \left\{ \sum_{k=1}^{\infty} z_{wxi}(k,j) + \sum_{k=1}^{\infty} z_{yxi}(k,j) \right\}_{j=1}^{\infty} \quad i=1,\ldots,N \quad (2)$$

$$y_i = \left\{ \sum_{j=1}^{\infty} z_{yui}(k,j) + \sum_{j=1}^{\infty} z_{yxi}(k,j) \right\}_{k=1}^{\infty} \quad i=1,\ldots,N \quad (3)$$

$$w_i = \left\{ \sum_{j=1}^{\infty} z_{wui}(k,j) + \sum_{j=1}^{\infty} z_{wxi}(k,j) \right\}_{k=1}^{\infty} \quad i=1,\ldots,N \quad (4)$$

$$\beta_i^* y_i = \left\{ \sum_{j=1}^{\infty} \alpha_i(j) z_{yui}(k,j) + \sum_{j=1}^{\infty} \sigma_i(j) z_{yxi}(k,j) \right\}_{k=1}^{\infty} \quad i=1,\ldots,N \quad (5)$$

$$\gamma_i^* w_i = \left\{ \sum_{j=1}^{\infty} \alpha_i(j) z_{wui}(k,j) + \sum_{j=1}^{\infty} \sigma_i(j) z_{wxi}(k,j) \right\}_{k=1}^{\infty} \quad i=1,\ldots,N \quad (6)$$

$$x_i = F_i \underline{w} \quad i=1,\ldots,N \quad (7)$$

$$\underline{\underline{R}} * \underline{w} = \underline{0} \quad (8)$$

$$u_i,\ y_i,\ x_i \in l_1^+,\ z_{yui},\ z_{wui},\ z_{yxi},\ z_{wxi} \in l_1^+(2), \quad i=1,N, \quad \underline{w} \in l_1^{+N} \quad (9)$$

Mathematical formulation of the objective function

Having presented the governing equations for the IDEAS conceptual framework, we are now in a position to describe the objective function that will be optimized. For this article, a linear objective function is used, as shown in Eq. 10. The term $\upsilon_i(j)y_i(j)$ is the linear contribution to the objective of the external inlet streams, where $\upsilon_i \in l_\infty$. Similarly, $\psi_i(j)y_i(j)$, $\chi_i(j)x_i(j)$, and $\omega_i(j)w_i(j)$ are the linear contributions to the objective of the external outlet, OP outlet, and OP inlet streams, where $\psi_i \in l_\infty$, $\chi_i \in l_\infty$, and $\omega_i \in l_\infty$. The final term is the linear contribution to the objective of the crossflow streams within the DN, $\zeta_{lmi}(k,j) z_{lmi}(k,j)$ where $\zeta_{lmi} \in l_\infty$(Eq. 2).

$$\sum_{i=1}^{N} \sum_{j=1}^{\infty} \left[\upsilon_i(j)u_i(j) + \psi_i(j)y_i(j) + \chi_i(j)x_i(j) + \omega_i(j)w_i(j) + \sum_{l=w,y} \sum_{m=u,x} \sum_{k=1}^{\infty} \zeta_{lmi}(k,j) z_{lmi}(k,j) \right] \quad (10)$$

This convex (linear) objective function is able to capture a variety of practically relevant objectives. For example, a utility cost objective is represented by setting $\psi_i = \chi_i = \omega_i = \zeta_{lmi} = \{0\}$, and $\upsilon_i = \{0\}$, except for the first p_i terms which represent the cost coefficients for each of the external inlet streams. The form of Eq. 10 is also capable of handling capital and total annualized cost objectives, as long as equipment cost is proportional to equipment size, by selecting ω_i appropriately. Other, possibly nonconvex, objective functions may also be considered, although in these cases the optimization problem may not remain convex.

IDEAS optimal network synthesis problem formulation

The combination of the objective function (Eq. 10) and the constraints (Eqs. 1–9) gives rise to the following infinite dimensional linear program defined over l_1 product spaces

$$\begin{aligned} \nu = \inf \quad & (10) \\ \text{subject to:} \quad & (1\text{–}9) \end{aligned} \quad (11)$$

This IDEAS formulation of the optimal process network synthesis problem possesses a number of important characteristics. First, it captures all possible process networks in its feasible region. Any given process network employs a fixed number of units with specific values for their design parameters, specific flows with associated quality conditions in and out of these units, and specific interconnections among the units. Given that the IDEAS OP inlets consider all possible combinations of quality conditions and unit design parameters that the OP outlets are then uniquely determined, and that the IDEAS DN considers all possible interconnections between external inlets/OP outlets and external outlets/OP inlets, it is then impossible for any particular process network to not be included in the IDEAS formulation.

Second, IDEAS provides a radical departure from all previous process network synthesis approaches. It is the only approach that considers all possible networks (for an *a priori* defined set of technologies) and yields a convex (linear) programming formulation. The traditional bilinearities, integer variables, and other nonconvexities plaguing other formulations are successfully eliminated. This results in the important result that a process network found by IDEAS is globally optimal.

The infinite dimensional nature of the IDEAS formulation (Eq. 11) necessitates a series of finite dimensional approximations for its solution. A number of approximations for problems with objective functions, that are continuous func-

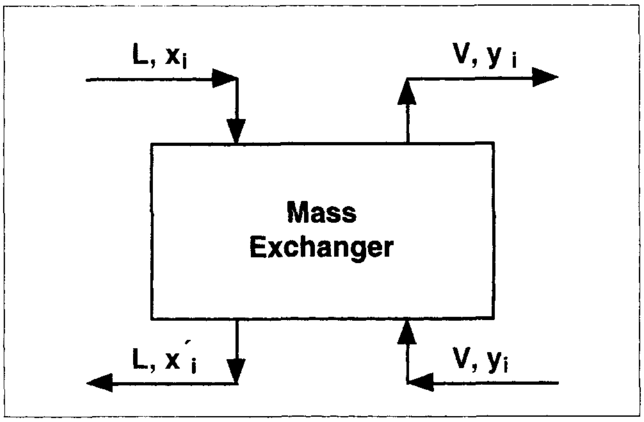

Figure 3. Single mass exchanger unit.

tionals on l_1 and constraints that are also described by maps from l_1 to l_1, have been shown to converge to the infimum ν of the infinite dimensional problem (Sourlas and Manousiouthakis, 1999). Since the functional presented in Eq. 10 is continuous (l_∞ is the dual space of l_1 and thus Eq. 10 is a bounded, and therefore continuous, linear functional) and the constraints defined in Eqs. 1—9 map l_1 to l_1, these convergence results are directly applicable to Eq. 11. In this work, we have chosen an approximation scheme that employs simultaneous constraint elimination and variable truncation.

MUC for Multicomponent MEN

Problem description

To demonstrate the capability of IDEAS to generate optimal process networks, we next illustrate the use of IDEAS in solving the MUC multicomponent MEN synthesis problem. To simplify and streamline the exposition and without loss of generality, we consider a MEN problem involving two families of streams with two transferrable components. The unit operation considered is a countercurrent mass exchanger, shown in Figure 3. The two families are assumed to be immiscible and the components are present in dilute concentrations. Chemical equilibria for the transferrable components are independent of the other component and linear. Under these assumptions, the mass-transfer unit operation can be successfully modeled by the KSB equations (King, 1981, pp. 361-366). The variables used in the KSB model are described in Table 1.

Table 1. KSB Model Variable Definitions

x_j	inlet concentration of j in phase 1
y_j	inlet concentration of j in phase 2
x'_j	outlet concentration of j in phase 1
y'_j	outlet concentration of j in phase 2
L	flow of the first phase
V	flow of the second phase
m_j	coefficient in the equilibrium relation
b_j	intercept in the equilibrium relation
N	number of 'stages' in exchanger
j	component

Table 2. Example 1 Data

$\alpha_{1,1}(1)$	0.0	$\beta_{1,1}(1)$	0.008	$\alpha_{1,2}(1)$	0.0	$\beta_{1,2}(1)$	0.025
$\alpha_{2,1}(1)$	0.040	$\beta_{2,1}(1)$	0.016	$\alpha_{2,2}(1)$	0.042	$\beta_{2,2}(1)$	0.002
$\alpha_{2,1}(2)$	0.024	$\beta_{2,1}(2)$	0.016	$\alpha_{2,2}(2)$	0.042	$\beta_{2,2}(2)$	0.010
$\alpha_{2,1}(3)$	0.024	$\beta_{2,1}(3)$	0.008	$\alpha_{2,2}(3)$	0.074	$\beta_{2,2}(3)$	0.010
m_1	4.0	b_1	0.0	m_2	2.0	b_2	0.0
$u_2(1)$	0.125	$u_2(2)$	0.375	$u_2(3)$	0.125	$v_1(1)$	1.0

$$\frac{y'_j - m_j x_j - b_j}{y_j - m_j x_j - b_j} = \frac{1 - \dfrac{L}{m_j V}}{1 - \left(\dfrac{L}{m_j V}\right)^{N+1}} \tag{12}$$

$$\frac{y_j - m_j x'_j - b_j}{y_j - m_j x_j - b_j} = \frac{\left(\dfrac{L}{m_j V}\right)^{N}\left(1 - \dfrac{L}{m_j V}\right)}{1 - \left(\dfrac{L}{m_j V}\right)^{N+1}} \tag{13}$$

Considering the first (second) family to have one (three) external inlet(s) and one (three) external outlet(s), the inlet(s) and outlet(s) specifications are shown in Table 2. The notation used is explained in Table 3. For family 2, the external outlet streams are required to have the same flow rate as the external inlets, $y_2 = u_2$. The utility cost for the network is proportional to the flow rate of family 1, with cost coefficient $v_1(1)$. The objective is to minimize the utility cost of the network $v_1(1)u_1(1)$ while meeting the outlet specifications.

Mass pinch analysis and synthesis

Given the data in Table 2, we can now proceed to use single component MEN techniques for both analysis and synthesis of process networks. The analysis stage of single component MEN design, mass pinch, provides an important, rigorous, thermodynamic lower bound on the MUC for MT MEN. Construction of the mass load diagrams for components 1, Figure 4, and component 2, Figure 5, yields the location of any mass pinches present. In these figures, the numbers above each linear segment of the rich curves refer to the streams involved. For both components, mass pinch analysis identifies the minimum utility cost as 1.0, and each component exhibits a mass pinch.

For component 1, the mass pinch occurs at $y_1 = 0.024$. This pinch occurs between rich stream 1 and the lean stream on one side and rich streams $1+2+3$ and the lean stream on the other. Employing standard mass pinch network generation, the problem is decomposed into two subproblems at the pinch since mass should not be transferred across it. This

Table 3. MEN Variable Definitions

$\alpha_{1,j}(i)$	Lean stream i inlet condition for component j
$\alpha_{2,j}(i)$	Rich stream i inlet condition for component j
$\beta_{1,j}(i)$	Lean stream i outlet condition for component j
$\beta_{2,j}(i)$	Rich stream i outlet condition for component j
$u_2(i)$	Flowrate of rich stream i
$v_1(i)$	Cost per unit flow rate for lean stream i

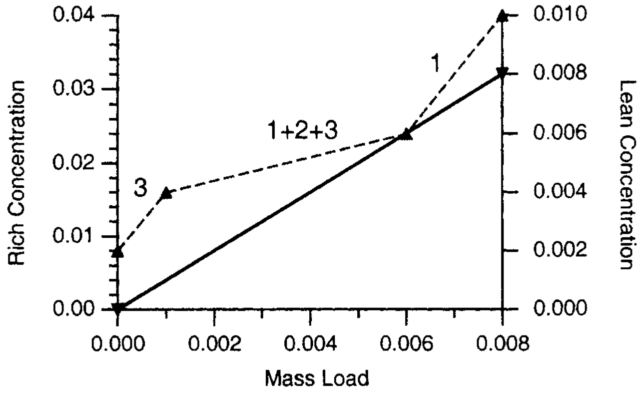

Figure 4. Mass load diagram for Component 1.

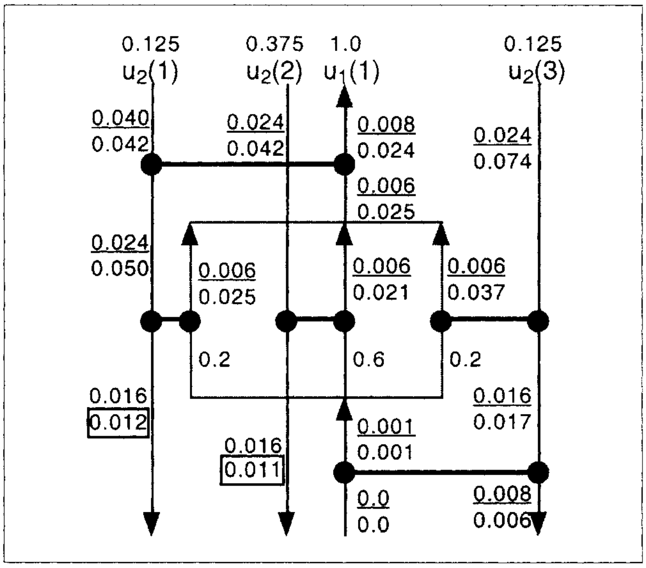

Figure 6. Mass pinch optimal network for Component 1.

design method results in network 6, where the concentrations are shown next to each stage. The concentrations of the second component are computed simultaneously and displayed below that of the first component. This network clearly violates the outlet conditions in component 2 for rich streams 1 and 2.

A similar result occurs for analysis of component 2. The mass pinch here occurs at $y_2 = 0.42$ and the subproblems involve rich stream 3/lean utility and rich streams $1+2+3$/lean utility. Network 7 results. In this case, the outlet concentrations of the first component, shown above that of component 2, are seen to violate their bounds for rich streams 2 and 3.

Examination of the two networks (Eqs. 6 and 7) shows that they cannot be superimposed. The order of the mass-transfer operations is completely different. One common solution for this situation is to increase the utility stream flow rate until all separation criteria are met. For network 6, the utility flow rate must be increased to 1.21, a 21% increase, to meet the outlet bounds for all streams. Network 7 needs an even higher utility cost of 1.94, a 94% increase, before it satisfies all outlet concentration bounds.

IDEAS based MEN synthesis

To proceed with the use of IDEAS for the MUC for MT MEN design, a detailed description of OP is required. To this end, the first term of the sequence pair $(\underline{w},\tau)$ is analyzed in some detail. The first term of $\underline{w}$ has one flow from each of the two families present, $\underline{w}(1) = [w_1(1), \underline{w}_2(1)]$. The first term of the other sequence τ consists of information about the inlet and outlet quality conditions, the ratio of the flow rates, and the design variables. For the two component system in this application modeled by the KSB equations (Eqs. 12 and 13), this gives $\tau(1) = [\gamma_1(1), \gamma_2(1), \underline{\underline{R}}(1), D(1)]$. Each mass exchanger is required to receive flow from both families (no mass exchanger takes flow from one family only), giving $\underline{\underline{R}}(1) = (1, -r_{1,2}(1))^T$, where $w_1(1) = r_{1,2}(1)w_2(1)$. The KSB model, when the ratio of flow rates is fixed, has one remaining degree of freedom, the number of transfer units, giving $D(1) = N(1)$. Collecting this information gives

$$\underline{w}(1) = (w_1(1), w_2(1)) \tag{14}$$

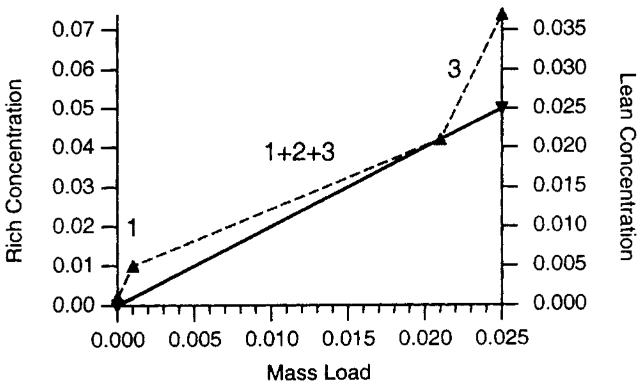

Figure 5. Mass load diagram for Component 2.

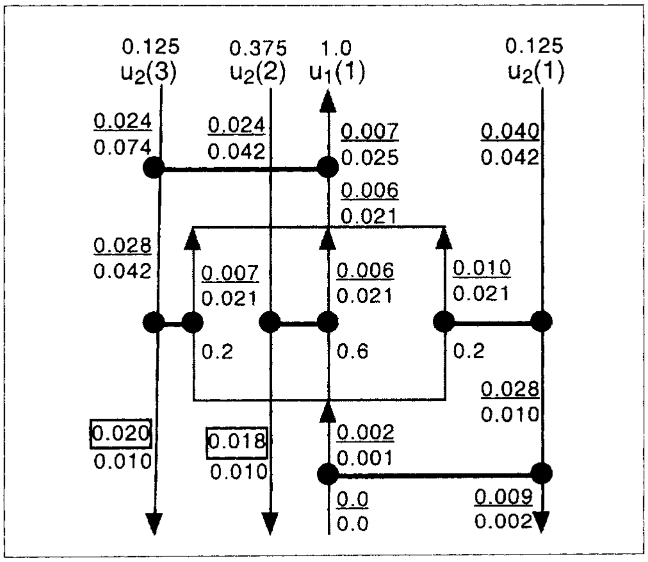

Figure 7. Mass pinch optimal network for Component 2.

$$\tau(1)=\left(\begin{bmatrix}\gamma_{1,1}(1)\\ \gamma_{1,2}(1)\end{bmatrix},\ \begin{bmatrix}\gamma_{2,1}(1)\\ \gamma_{2,2}(1)\end{bmatrix},\ [1\quad -r_{1,2}(1)],\ N(1)\right) \tag{15}$$

$$w_1(1)-r_{1,2}(1)w_2(1)=0 \tag{16}$$

For the KSB model, the outlet flow rates are identical to the inlet flow rates; only the component concentrations are changed. Equations 12 and 13 determine the outlet conditions given the inlet conditions, flow rate ratio, and number of transfer units. Substituting Eqs. 14–16 into Eqs. 12 and 13 yields

$$\frac{\sigma_{2,i}(1)-m_i\gamma_{1,i}(1)-b_i}{\gamma_{2,i}(1)-m_i\gamma_{1,i}(1)-b_i}=\frac{1-\dfrac{r_{1,2}(1)}{m_i}}{1-\left(\dfrac{r_{1,2}(1)}{m_i}\right)^{N(1)+1}},\ i=1,2 \tag{17}$$

$$\frac{\gamma_{2,i}(1)-m_i\sigma_{1,i}(1)-b_i}{\gamma_{2,i}(1)-m_i\gamma_{1,i}(1)-b_i}=\frac{\left(\dfrac{r_{1,2}(1)}{m_i}\right)^{N(1)}\left(1-\dfrac{r_{1,2}(1)}{m_i}\right)}{1-\left(\dfrac{r_{1,2}(1)}{m_i}\right)^{N(1)+1}},\quad i=1,2 \tag{18}$$

The contribution of $\underline{w}(1)$ to $x_i(1)$, $i=1,2$, which are at the quality conditions $\sigma_i(1)=(\sigma_{i,1}(1)\ \sigma_{i,2}(1))^T$, $i=1,2$, is captured by

$$F_1(1,1)=[1\quad 0] \tag{19}$$

$$F_2(1,1)=[0\quad 1] \tag{20}$$

The globally optimal network discovered by IDEAS is shown in Figure 8. This network has a MUC of 1.0 and is thus a globally optimal solution. There are several salient features to this network. One feature is the heavy use of splitting and mixing operations to achieve the desired outlet concentration for the rich streams. Mixing and splitting operations are not considered at all by the single component mass pinch methods. Another feature is the use of only 4 MEX to accomplish the separation. The minimum number of necessary MEX predicted by mass pinch is 5. Also, the first MEX encountered by rich stream 1 raises the concentration of the second component rather than lowering it. This is in direct contradiction to mass pinch methods which state components should always move towards their outlet concentration.

This example demonstrates that IDEAS generates globally optimal MUC MEN MT networks. By use of this novel conceptual framework, all inlet streams were transformed into their desired outlet streams with the MUC.

Discussion and Conclusions

It is important to not that the assumptions and restrictions used in the MEN synthesis problem above in no way restrict

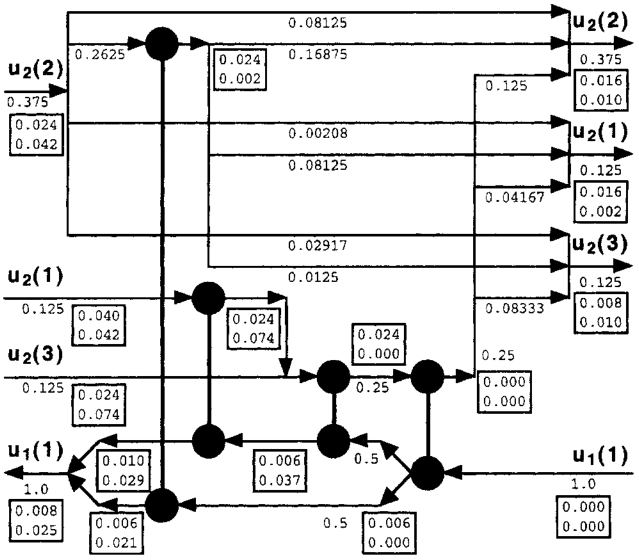

Figure 8. Globally optimal IDEAS network.

the capabilities of IDEAS. There are several, rather restrictive, assumptions inherent in the use of the KSB model, but it should be emphasized that this is an example application of IDEAS. Changes in the modeling equations would be handled through appropriate changes in $(\underline{w},\tau)$, $F_i, i=1,N$, and $\sigma_i, i=1,N$. For example, removal of the assumption of constant flow rates through the mass exchanger can be handled by changing the entries of $F_i(1,1)$ from ones and zeros to whatever ratios of outlet to inlet flow rates are predicted by the mass exchanger model employed. Modifications of the modeling equations would cause corresponding changes in τ and its functional relationship to σ_i. Incorporation of additional, different, unit operations is also easily accomplished.

Also, there are many equivalent ways to describe τ. After the inlet conditions are specified, a given unit operation model contains several remaining degrees of freedom. Any consistent set of undetermined variables can be chosen to remove these degrees of freedom. In the application above, the choice was to fix the ratio of the flow rates and the number of transfer units. It is very easy to change this to a choice of two outlet conditions, one in each family. The flow rate ratio, remaining outlet conditions, and the number of transfer units can then be calculated from Eqs. 17 and 18.

There are several alternative representations of IDEAS that can be employed at the discretion of the designer. For example, to keep n_i, the number of qualities needed to describe a stream in the ith family, as low as possible, it is sometimes beneficial to preprocess a stream through an operator before it enters the DN. This may be done, for example, in distillation, where it is reasonable to consider that streams entering and exiting mass exchange units are either saturated vapors or liquids, in which case their enthalpic condition is fully determined by their component concentration condition. Thus, a HEN operator may be used to preprocess streams and bring them to a saturated state prior to entry to the DN. Also under other circumstances (such as when multiple technologies are considered), it may be desirable to consider some mixing and splitting operations to take place outside the DN and as part of the OP action.

To sum up, this article introduces the IDEAS conceptual framework for process network synthesis. IDEAS is then employed in solving the MUC MEN MT synthesis problem. The IDEAS method creates infinite dimensional convex (linear) optimization formulations, which in turn allow determination of globally optimal solutions. Through examination of an application of IDEAS, the power of this new approach is demonstrated. Previous methods applied to this application are shown to produce nonoptimal solutions. IDEAS is shown to identify a globally optimal, simple network that meets the known lower bound on utility cost. The obtained network features structures were not identified before by current design methods.

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Notation

Sets of infinite sequences

ϕ_0^+ = finite number of nonzero nonnegative elements
l_∞ = absolute value of any element is finite, $\sup_{i=1,\ldots,\infty}|a(i)| < \infty$
l_1 = absolute sum of elements is finite, $\sum_{i=1}^{\infty}|a(i)| < \infty$
l_1^+ = all elements nonnegative and sum of elements finite $\sum_{i=1}^{\infty}a(i) < \infty$, $\inf_{i=1,\ldots,\infty}a(i) \geq 0$
l_∞^N = N-dimensional vectors with absolute value of any element finite, $\sup_{i=1,\ldots,\infty}\sum_{j=1}^{N}|a_j(i)| < \infty$
l_1^{+N} = N-dimensional nonnegative vectors with sum of elements finite, $\sum_{i=1}^{\infty}\sum_{j=1}^{N}a_j(i) < \infty$, $\inf_{i=1,\ldots,\infty, j=1,\ldots,N}a_j(i) \geq 0$
$l_\infty^{M\times N}$ = $M \times N$ matrices with all elements finite $\sup_{i=1,\ldots,\infty, m=1,\ldots,M, n=1,\ldots,N}|a_{m,n}(i)| < \infty$
$l_1^+(L)$ = nonnegative L-tuples, $f(k_1,\ldots,k_L)$, with sum of elements finite, $\sum_{k_1=1}^{\infty}\ldots\sum_{k_L=1}^{\infty}f(k_1,\ldots,k_L) < \infty$, $\inf_{k_1,\ldots,k_L \in \mathcal{Z}^+}f(k_1,\ldots,k_L) \geq 0$

Other sets

$\mathcal{Q}^N$ = N-dimensional vectors with all elements real and rational
$\mathcal{R}^N$ = N-dimensional vectors with all elements real

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