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Supply-based superstructure synthesis of heat and mass exchange networks

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ABSTRACT

A new simultaneous mixed integer non-linear programing (MINLP) approach to heat exchange network synthesis (HENS) and mass exchange network synthesis (MENS) is presented. This supply-based superstructure (SBS) approach uses the supply temperatures/compositions of all the streams (including utilities) present in the synthesis problem to define heat/mass exchange superstructure intervals. The intermediate temperatures/compositions are variables used in the optimization of the network total annual cost (TAC). The ability of each stream to exchange heat/mass in any interval in the SBS is subject to thermodynamic/mass transfer feasibility. The paper presents the mathematical formulations for optimizing the TAC for HENS and MENS. The SBS synthesis technique has been applied to nine literature problems involving both HENS and MENS. The solutions obtained are in the same range as those in the literature, with one solution being the lowest of all.

1. Introduction

Energy and mass optimization in process plants have been accomplished using synthesis tools which are either sequential or simultaneous in nature, although most of the simultaneous mathematical optimization techniques do in fact involve more than one solution stage.

Pinch technology as a synthesis tool for heat exchanger networks (HENs) started in the late 1970s (Linnhoff & Flower, 1978). It is based on physical and thermodynamic insight and involves two stages: targeting and design. The first step is to determine the minimum energy consumption so as to obtain the annual operating cost (AOC) target. The network synthesis is then decomposed into sub-networks below and above the pinch, and the problem solved independently for each sub-network, using heuristics to evolve networks with minimum units. This may be compared with the annual capital cost (ACC) target obtained from the pinch curves (Linnhoff & Flower, 1978; Linnhoff & Hindmarsh, 1983). It has been the most dominant sequential method (El-Halwagi, 1997; Smith, 2005).

El-Halwagi and Manousiouthakis (1989) developed a mass exchange network (MEN) analogue of the pinch technology approach to heat exchange networks but their method can only target for the minimum mass separating agents (MSAs) needed for a separation task. Hallale and Fraser (2000a, 2000b) in their quest for capital cost targeting developed the y–y^* tool for targeting the mass exchanger area for both stage-wise and continuous contact columns.

Other developments in pinch based HENS and MENS (including some pinch related mathematical approaches for HENS) are contained in Shenoy (1995), Floudas (1995), El-Halwagi (1997), and Smith (2005).

The general problem with the pinch technique is its sequential nature. The simultaneous approaches on the other hand involve the use of mathematical programing models (Floudas, 1995) to optimize the total annual cost (TAC) in a single step. Costs which contribute to the TAC in heat and mass exchanger networks are annual operating cost (AOC, utility and mass separating agent costs) and annualized capital cost (ACC, heat and mass exchanger costs). Efforts have been made over the years to exploit the dynamic nature of mathematical programing to produce networks where the TAC can be optimized in a single step (Bagajewicz, Pham, & Manousiouthakis, 1998; Chen & Huang, 2005; Comeaux, 2000; Isafiade & Fraser, 2008a, 2008b; Papalexandri, Pistikopoulos, & Floudas, 1994; Szitkai, Farkas, Lelkes, Fonyo, & Kravanja, 2006; Yee & Grossmann, 1990). Note that none of these methods can guarantee globally optimum solutions, due to the inherent convexity of the HENS and MENS problems (Floudas, 1995).

One of the simultaneous approaches adopted by various workers to optimize the TAC in HENS and MENS is the use of superstructures. For instance, Yee and Grossmann (1990) presented a simplified stage wise superstructure (SWS) for HENS, which is an extended version of the superstructure developed by Grossmann and Sargent (1978) where, within each stage, heat exchange can

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occur between hot streams and cold streams. In the SWS, heat exchange can also occur between each hot stream and each cold stream within each stage in the superstructure. The SWS also bears resemblance to the spaghetti design concept of Linnhoff and co-workers (e.g. Linnhoff & Ahmad, 1990; Linnhoff, Mason, & Wardle, 1979) that shows division of the composite curves into sections, which is viewed by Yee and Grossmann (1990) as a series of stages.

Comeaux (2000) presented a reducible superstructure for MENS where the superstructure intervals were defined using the supply and target compositions of the rich streams and the equilibrium equivalent compositions of the lean streams in the rich phase. A stream extension rule (Comeaux, 2000) was adopted for the lean streams to ensure that each lean stream can match at least once with each rich stream in the superstructure. The superstructure made use of the branch flow rates to determine the existence or otherwise of matches between rich and lean streams. The superstructure was then modeled as a non-linear program (NLP) to determine the TAC of the networks.

Szitkai et al. (2006) applied the key idea of Yee and Grossmann (1990) along with the pinch technique and the mixed integer non-linear programing (MINLP) formulation of Papalexandri et al. (1994) to develop a MENS superstructure similar to Yee and Grossmann's HENS model. The authors verified their superstructure using the pinch designs of Hallale and Fraser (2000a, 2000b). The adapted superstructure retains most of the features of Yee and Grossmann's model and is referred to in this paper as 'SWS', although the authors did not call it this.

Emhamed et al. (2007) used a hybrid method for the optimization of mass exchange networks. The main idea of Emhamed et al. involves the use of integer cuts and bounds to the lean stream to exclude non-optimal solutions. The authors use the driving force plot (DFP) supertargeting method of Hallale (1998) to determine the initial flow sheet in the first step, and the flow sheet is then optimized using the MINLP formulation model of Szitkai et al. (2006) in the second step.

Isafiade and Fraser (2008a, 2008b) used a framework similar to the SWS of Yee and Grossmann (1990) and Szitkai et al. (2006) to optimize the design of heat and mass exchange networks. Their interval based MINLP superstructure (IBMS) model is constructed using the supply and target temperatures/compositions of either the hot/rich or cold/lean sets of streams. If the intervals are defined by hot/rich streams then the cold/lean streams are assumed to participate in all the intervals. The reverse is the case for a cold/lean stream based superstructure. The exchange of heat/mass between hot/rich streams and cold/lean streams in an interval is subject to thermodynamic feasibility, both for heat transfer and the equilibria that govern mass transfer.

The SWS technique and its derivatives, as well as the IBMS technique, all have isothermal mixing in common. In addition, the SWS of Yee and Grossmann (1990) is conceptually similar to a spaghetti design. In spaghetti design, however, the number of stages and enthalpy intervals are necessarily equal, but in SWS, the number of stages is typically much smaller than the number of enthalpy intervals. The choice of a larger number of stages is necessary for more combinations of stream matches (Shenoy, 1995).

Other workers have adopted an Evolutionary Algorithm (EA) method for the simultaneous synthesis of HENs. Lewin (1998) presented a generalized simultaneous method for the synthesis of heat exchanger networks based on a Genetic Algorithm (GA), a form of Evolutionary Algorithm (Goldberg, 1989), using NLP. In this formulation both the objective function and the constraints are non-linear. The author proposed a solution based on the observation that an optimal solution usually involves relatively few stream splits. The NLP problem was solved using a cascaded algorithm involving an upper level non-linear optimization of the stream split flows, and a lower level pseudo-linear optimization of the heat exchanger duties.

Krishna and Murty (2007) applied a modified differential evolution method (DEM), another form of EA, to HENS. The DEM is suitable for optimization problems with continuous variables so it needed to be modified to allow for the integer variables in HENS problems. The model considered stream splitting but did away with the simplifying assumption of isothermal mixing of the split streams of Yee and Grossmann (1990). Their model can also handle compulsory and forbidden matches in optimization of HENs. The DEM approach is more likely to find the true optimum than the Genetic Algorithm approach (Price & Storn, 1997).

The state space approach is another technique that has been adopted for the optimization of TAC in HENS and MENS. Bagajewicz et al. (1998) presented the application of the state space approach to HENS and MENS using NLP, demonstrating the flexibility of the approach in HENS and MENS formulation through the use of various operators. They showed that the state space approach contains a network superstructure as a special case but the approach can only guarantee local optimality.

Martin and Manousiouthakis (2001) also synthesized HENs and MENs using the state space approach. Martin and Manousiouthakis' work provides analytical proofs that, under certain assumptions, bypass streams and recycle streams can be set to zero without compromising the global optimality of the HEN/MEN minimum TAC problem. The resulting NLP formulation of the TAC HEN problem is solved to global optimality, using a hybrid algorithm with branch and bound underestimation and interval analysis. The two simple examples solved do not contain sufficient information to check the validity of their claim. A feature of this work is that two different streams, one hot and one cold, can be mixed to achieve the required outlet temperature (the same for both), as shown in their second example. While this may be helpful in certain situations, this is not generally applicable, and has not been implemented by any other workers in this field.

2. Problem statements

2.1. HENS

Given a number of hot and cold process streams (to be cooled and heated respectively), the task is to synthesize a heat exchanger network which can transfer heat from the hot streams to the cold streams in order to achieve a minimum total annual cost network. Given also are the heat capacity flowrates, supply and target temperatures and heat transfer coefficients of each process stream. Available for service are heating and cooling utilities whose costs, supply temperatures, target temperatures and heat transfer coefficients are also given, along with annual operating time, heat exchanger costs and the annual cost of capital.

2.2. MENS

Given a number of rich streams and a number of MSAs (lean streams), the task is to synthesize a network of mass exchangers that can preferentially transfer certain species from the rich streams to the MSAs in order to achieve a minimum total annual cost network. Given also are the flowrate of each rich stream and the supply and target compositions. In addition, the supply and target compositions for each MSA together with the mass transfer equilibrium relations are also given for each MSA. The flowrate of each MSA is unknown and is to be determined as part of the synthesis task. Also given are the annual operating time, mass exchanger sizing and cost information and the annual cost of capital.

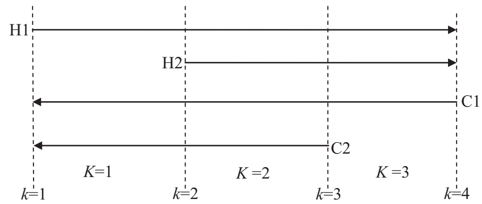

Fig. 1. Grid representation of the SBS superstructure for two hot and two cold streams.

The candidate MSAs can be classified as process and external MSAs. The process MSAs are available virtually free since they exist on site. However, the amount of each process MSA that can be used for mass exchange is bounded by its availability on site. On the other hand, the external MSAs can be purchased from the market and their flowrates are to be determined by economic considerations.

3. Motivation

Most approaches to heat exchanger networks have used temperature as the key variable for partitioning the system. This paper presents an alternative approach for the determination of temperature intervals in the superstructure-based synthesis of heat exchange networks that is similar to both the SWS and the IBMS approaches. Like the IBMS approach, this technique uses insights from pinch technology to generate the intervals for the superstructures for heat exchange network design. Noting that temperatures are the key parameters for the optimum use of driving forces in exchangers, the supply-based superstructure (SBS) is partitioned using the temperatures defined by the supply values of the all the process and utility streams. The temperatures of all other streams crossing the boundaries defined by the supply temperatures are variables to be used in the optimization. This is compared to the IBMS where the supply and target temperatures of either the hot streams or the cold streams are used to define the interval boundaries, and the SWS where a fixed number of intervals is defined and the boundary temperatures/compositions of all streams are variables. In all these approaches the exchange of heat is subject to thermodynamic feasibility.

Note that this approach also applies to mass exchange networks, with composition being the key partitioning variable.

In the SWS, Yee and Grossmann (1990) fixed the number of stages required to model heat integration at max $[N_H, N_C]$ where N_H is the number of hot streams and N_C the number of cold streams. In the superstructure, all the hot process streams start at the first temperature location and end at the last temperature location; the opposite is the case for all the cold process streams. The utilities can be treated as process streams or placed at the ends of the superstructure. In the superstructure, all streams can participate in every stage. In each stage, each of the streams can split into the number of streams of the opposite kind for the purpose of heat exchange. The split streams are assumed to mix isothermally after leaving the heat exchangers in a stage before moving to the next stage. In the SWS the intermediate temperatures are all variables to be used in the optimization of the TAC.

The temperature locations in the IBMS model of Isafiade and Fraser (2008a) are defined by the supply and target temperatures of either the hot or cold set of streams. If the hot streams are used to define the superstructure (hot-based), then the cold streams are assumed to participate in all the intervals defined by the hot streams. In the IBMS, the intermediate temperatures are also variables to be used in the optimization. Every stream can split into the number of the streams of the opposite kind present in the interval concerned in order to exchange heat.

4. Construction of the hens supply-based superstructure (SBS)

Fig. 1 shows an illustration of a typical HENS SBS involving two hot and two cold streams. The supply temperatures of the all the hot and cold streams define the interval boundaries, with temperature decreasing from left to right. Streams are also arranged in descending order of supply temperature from top to bottom, with the hot

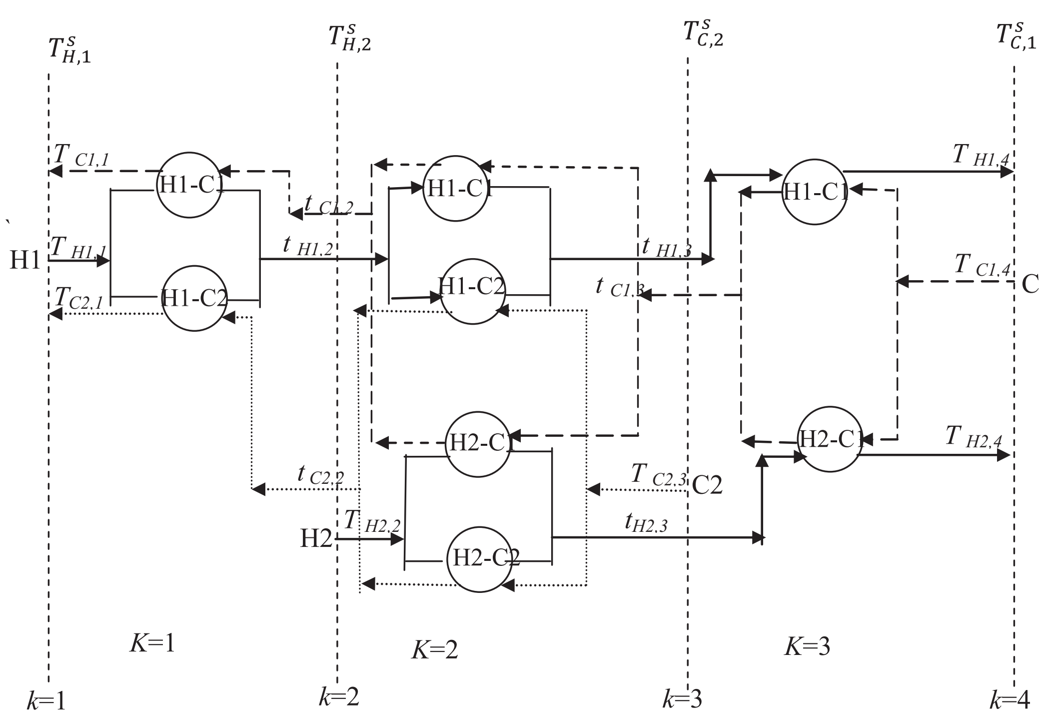

Fig. 2. The supply-based superstructure for HENS for two hot streams and two cold streams.

Table 1
Characteristics of the HENS superstructures.

SWS of Yee and Grossmann (1990)	IBMS of Isafiade and Fraser (2008a, 2008b)	SBS of this paper
Number of stages (intervals) defined by maximum of the number of hot streams or the number of cold streams	Number of intervals defined by the supply and target temperatures of either the hot streams or the cold streams (which normally gives more intervals than SWS)	Number of intervals defined by the supply temperatures of both the hot streams and the cold streams (this also normally gives more intervals than SWS)
The only boundaries fixed are the first and last: the first one is where all hot streams start and all cold streams end, while the last one is where all cold streams start and all hot streams end	Interval boundaries are fixed by the supply and target temperatures of either all the hot streams or all the cold streams	Interval boundaries are fixed by the supply temperatures of all the hot streams and all the cold streams
Exchange of heat between each hot stream and each cold stream is possible in all the stages of the superstructure	Exchange of heat by each hot stream is possible only in the intervals created by the supply and target values of that hot stream in a hot-based superstructure; the same applies to each cold stream in a cold-based superstructure (less opportunity for heat exchange within intervals than SWS)	Exchange of heat by each hot stream is possible in all intervals except those intervals with higher temperature values than the supply temperature of that stream; exchange of heat by each cold stream is possible in all intervals except those intervals with lower temperature values than the supply temperature of that stream (more opportunity for heat exchange within intervals than IBMS)
All streams exist across all the intervals	In a hot-based superstructure the hot streams exist in all the intervals between their supply and target temperatures, and the cold streams exist across all the intervals. The converse applies in a cold-based superstructure	Hot streams exist across all intervals at temperatures lower than their supply temperature. Cold streams exist across all intervals at temperatures higher than their supply temperature
MINLP formulation but NLP sub optimisation step often needed	MINLP formulation, NLP not needed	Same as IBMS
Stream splitting and (isothermal) mixing is possible in each of the stages of the superstructure	Stream splitting and (isothermal) mixing of streams in an interval is possible in each of the intervals of the superstructure	Same as IBMS

streams above the cold streams. In this illustrative problem, the order of the supply temperatures of the hot and cold sets of streams is as follows: $T^S_{H1} > T^S_{H2} > T^S_{C2} > T^S_{C1}$. Every hot stream terminates at the last temperature location ($k=4$, which is the lowest cold stream supply temperature) while every cold stream terminates at the first temperature location ($k=1$, which is the highest hot stream supply temperature).

In the SBS, each hot stream originates from the interval boundary that corresponds to its supply temperature and extends across all subsequent intervals so that it can exchange heat with all streams of the opposite kind in all these intervals, subject to thermodynamic heat transfer feasibility. Similarly, each cold stream originates from the interval boundary which corresponds to its supply temperature and participates in all the intervals having temperatures greater than its supply value. Note that, as with the IBMS, utility streams are included with the process streams in the SBS.

The participation and possible exchange of heat by streams in each interval of the SBS for the general system shown in Fig. 1 is illustrated in Fig. 2.

Fig. 2 shows that $T^S_{H,1}$ defines the first temperature location $k=1$, $T^S_{H,2}$ defines $k=2$, $T^S_{C,2}$ defines $k=3$, and $T^S_{C,1}$ defines the last temperature location $k=4$. Two or more supply temperatures that are the same share the same interval boundary. Circles are used to denote heat exchange between two streams; each pair of circles represents a heat exchanger.

Streams can only exchange heat in intervals where they are present, subject to thermodynamic feasibility constraints. In Interval 1 ($K=1$), Hot Stream 1 splits into two branches to potentially exchange heat with Cold Streams 1 and 2. The same split and heat exchange pattern occurs in Interval 2 for Hot Stream 1. Hot Stream 2 can potentially exchange heat with Cold Streams 1 and 2 in Interval 2. For Interval 3 Hot Stream 2 can potentially exchange heat only with Cold Stream 1. As can be seen in Fig. 2, Intervals 1–3 can have a maximum of two, four and two exchangers respectively.

Note that the temperatures of the hot and cold streams at temperature locations different from those which they define (i.e. intermediate temperatures) are variables to be used in the optimization of the objective function. This implies that the SBS does not adhere strictly to the vertical heat transfer concept of pinch technology. It is also important to note that the utility flows are treated as process streams with variable flow rates in SBS.

Tables 1 and 2 present the characteristics of the various HENS and MENS superstructure methods.

5. HENS and MENS SBS model variables

The indices, sets, parameters and variables which are used to describe and model the SBS for HENS and MENS are shown next.

5.1. Sets

C	cold process and utility streams
H	hot process and utility streams
R	rich process streams
S	lean streams (process and external mass separating agents)
K	temperature/composition intervals in the superstructure

5.2. Indices

i	hot process or utility stream
j	cold process or utility stream
k	index for temperature/composition boundary ($k=1, \ldots, NOK+1$)
l	lean stream (process or external mass separating agent)
r	rich process stream

5.3. Parameters

AC_l	annual cost per unit of lean stream l
ACH_{rl}	annual cost per height for continuous contact columns involving rich stream r and lean stream l
ACT_{rl}	annual cost per stage for staged columns involving rich stream r and lean stream l

Table 2
Characteristics of MENS superstructures.

'SWS' of Szitkai et al. (2006)	NLP of Comeaux (2000)	IBMS of Isafiade and Fraser (2008a, 2008b)	SBS of this paper
Number of stages (intervals) can be set arbitrarily or defined by the sum of number of rich streams and lean streams	Number of intervals defined by supply and target compositions of the rich streams and equilibrium equivalent of the lean streams	Number of intervals defined by the supply and target compositions of either the rich streams or the lean streams (which normally gives more intervals than SWS)	Number of intervals defined by the supply compositions of both the rich streams and the lean streams (this also normally gives more intervals than SWS)
All streams exist across all the intervals	The supply composition of rich and lean streams are fixed at the intervals defined by the supply composition values in the superstructure	In a rich-based superstructure the rich streams exist in all the intervals between their supply and target compositions, and the lean streams exist across all the intervals. The converse applies in a lean-based superstructure	Rich streams exist across all intervals at compositions lower than their supply composition. Lean streams exist across all intervals at compositions higher than their supply composition
Exchange of mass between rich and lean streams is possible in all stages of the superstructure	Lean stream is extended to match at least once with each rich stream in the superstructure	Exchange of mass by a rich stream is possible only between the intervals defined by the supply and target values of such stream in a rich based superstructure and same applies to a lean in a lean based superstructure (less freedom for mass exchange within intervals than SWS)	Exchange of mass with a stream is possible in all intervals except those intervals with lower composition values than the supply composition of such stream (more freedom for mass exchange within intervals than IBMS)
The target compositions of rich and lean streams are fixed at the last and first composition interval locations respectively in the superstructure	The target composition of rich stream is fixed at the interval defined by its target value while that of the lean is extended to match at least once with each rich stream	The supply and target compositions of lean streams are as in SWS in a rich based superstructure and similarly for rich streams in a lean based superstructure	The target compositions of rich and lean streams are as in SWS
Binary variables are used in the model to check the existence or otherwise of matches in the superstructure	No binary variables, instead branch flow rates are used to determine existence of matches	Same as SWS	Same as SWS
MINLP formulation but NLP sub optimisation step often needed	NLP formulation	MINLP formulation	Same as IBMS
Stream splitting and (iso-composition) mixing is possible in each of the stages in the superstructure	Stream splitting and mixing of a rich stream is possible only between the intervals created by supply and target of such stream. The converse applies to the lean stream	Stream splitting and (iso-composition) mixing is possible in any interval where a stream exists	Same as IBMS

AFC	area cost coefficient for heat exchangers
b	equilibrium line intercept
$C_{j,K}$	is the existence of cold stream j in interval K (between temperature interval boundaries k and $k+1$
CB_{ij}	fixed charge for heat exchangers
CB_{rl}	fixed charge for mass exchanger columns involving rich stream r and lean stream l
CS	cold start in the superstructure
CU	cost per unit of cold utility
D	area cost index for heat/mass exchangers
$H_{i,K}$	is the existence of hot stream i in interval K (between temperature interval boundaries k and $k+1$)
HS	hot start in the superstructure
HU	cost per unit of hot utility
K_w	lumped mass transfer coefficient
m	equilibrium constant for the transfer of component from rich stream r to lean stream l
NOK	number of temperature/composition intervals
$R_{r,k}$	existence of rich stream r in interval K (between composition interval boundary k and $k+1$)
$RST_{r,k}$	rich stream r start at composition interval boundary k
$S_{l,k}$	existence of lean stream l in interval K (between composition interval boundary k and $k+1$)
$SST_{r,k}$	lean stream l start at composition interval boundary k
T_i^s	supply temperature of hot stream i
T_i^t	target temperature of hot stream i
T_j^s	supply temperature of cold stream j
T_j^t	target temperature of cold stream j
T_k	temperature of interval boundary k
X_l^s	supply composition of lean stream l
X_l^t	target composition of lean stream l
Y_r^s	supply composition of rich stream r
Y_r^t	target composition of rich stream r
Y_l^{*s}	equilibrium supply composition of lean stream l
Y_l^{*t}	equilibrium target composition of lean stream l
Y_k	composition of interval boundary k
Γ_H	upper bound for driving force in match i, j
Γ_M	upper bound for driving force in match r, l
ε_{min}	minimum composition difference in the lean phase
Ω_H	upper bound for heat exchanged in match i, j
Ω_Z	upper bound for mass exchanged in match r, l
$	conditional operator

5.4. Binary variables

Z_{ijk}	variable showing the existence of match i, j in interval K in the network
z_{rlk}	variable showing the existence of match r, l in interval K in the network

5.5. Positive variables

dt_{ijk}	heat exchanger driving force for match i, j in temperature interval K
dy_{rlk}	heat exchanger driving force for match r, l in composition interval K
F_i	flow rate of hot stream i
F_j	flow rate of cold stream j
G_r	rich stream flowrate
L_l	lean stream flowrate

M_{rlk} heat exchanged between stream i and stream j in temperature interval K
N_{rlk} number of stages in staged column rlk
q_{ijk} heat exchanged between stream i and stream j in temperature interval K
$t_{i,k}$ temperature of hot stream i at temperature boundary k
$t_{j,k}$ temperature of cold stream j at temperature boundary k
$y_{r,k}$ composition of rich stream r at composition boundary k
$y^*_{l,k}$ equilibrium composition of lean stream at composition boundary k

6. SBS model equations for HENS

The SBS model consists of balance equations, constraints, an objective function and stream existence conditionals.

6.1. Assignment of superstructure interval boundary temperatures

Referring to Fig. 2, the interval boundary temperatures are specified as follows (where lower case symbols represent variables to be optimized):

$$k = 1; \quad T^s_{H1,1} \quad T^s_{C1,1} = T^t_{C1}, \quad T_{C2,1} = T^t_{C2} \tag{1a}$$

$$k = 2; \quad T^s_{H2,2}, \quad t_{H1,2}, \quad t_{C1,2}, \quad t_{C2,2} \tag{1b}$$

$$k = 3; \quad T^s_{C2,2}, \quad t_{H1,2}, \quad t_{H2,2}, \quad t_{C2,2} \tag{1c}$$

$$k = 4; \quad T^s_{C1,4}, \quad T_{H1,4} = T^t_{H1}, \quad T_{H2,4} = T^t_{H2} \tag{1d}$$

Note that $T_{C1,1}$ and $T_{C2,2}$ are the target temperatures of the two cold streams, and $T_{H1,4}$ and $T_{H2,4}$ are the target temperatures of the two hot streams.

6.2. First set of stream existence conditionals

To ensure that a hot stream cannot exchange heat in any interval whose temperature is higher than its supply value while a cold stream cannot exchange heat in any interval where the temperature is lower than its supply value, the superstructure works with two stream existence conditionals, and one for the hot streams and one for the cold streams. The mathematical expressions for these conditionals are as follows:

$$H_{i,K}\$(T^s_i \geq T_k = 1) \tag{2}$$

$$C_{j,K}\$(T^s_j \geq T_k = 1) \tag{3}$$

6.3. Second set of stream existence conditionals

The second set of stream existence conditionals consists of the stream supply temperature conditionals which recognize the supply temperatures of the set of streams which define the interval boundaries in the superstructure. They are mathematically stated as follows:

$$HS_{i,K}\$(T^s_i = T_k) = 1 \tag{4}$$

$$CS_{j,K}\$(T^s_j = T_k) = 1 \tag{5}$$

6.4. Overall stream heat balance equations

The total heat exchanged by each stream over all matches in all intervals must equal the total enthalpy change of that stream. Eqs. (6) and (7) describe this for hot stream i and cold stream j respectively.

$$(T^s_i - T^t_i)F_i = \sum_{j \in c} \sum_{k \in K} q_{ijk}, \quad i \in H \tag{6}$$

$$(T^t_j - T^s_j)F_j = \sum_{i \in H} \sum_{k \in K} q_{ijk}, \quad j \in C \tag{7}$$

It should be noted that stream heat capacity flowrate F is modeled as a parameter for the process streams and as a variable for the utility streams.

6.5. Interval heat balance equations

The heat exchanged by each stream in each interval defines the temperature of that stream for the next interval. The heat exchanged between hot stream i and cold stream j in interval k is calculated using the interval heat balance equations for hot and cold streams respectively:

$$(t_{i,k} - t_{i,k+1})F_i = \sum_{j \in C} q_{i,j,k}, \quad i \in H \quad k \in K \tag{8}$$

$$(t_{j,k} - t_{j,k+1})F_j = \sum_{i \in H} q_{i,j,k}, \quad j \in C \quad k \in K \tag{9}$$

6.6. Temperature feasibility along the superstructure

Temperatures of hot streams need to decrease monotonically from left to right along the superstructure in order to reach their target values, whereas cold stream temperatures increase monotonically from right to left to reach their targets. This is ensured using the feasibility constraints shown in Eqs. (10) and (11) for hot and cold streams respectively:

$$t_{i,k} \geq t_{i,k+1}, \quad k \in K \quad i \in H \tag{10}$$

$$t_{j,k} \geq t_{j,k+1}, \quad k \in K \quad j \in C \tag{11}$$

6.7. Logical constraints

Binary variables $Z_{i,j,k}$, are used in logical constraint equations to ensure the existence or otherwise of match i, j in interval k. $Z_{i,j,k}$ takes on a value of '1' if match i, j exists in interval k and a value of '0' if not. The heat exchange between streams i and j is restricted to the smaller of the heat duties of the two streams involved in the match using the parameter Ω_{H}.

$$q_{ijk} - \Omega_H Z_{i,j,k} \leq 0, \quad i \in H \quad j \in C \quad k \in K \tag{12}$$

6.8. Heat exchanger driving force calculation

Approach temperatures dt_{ijk} are used together with the binary variable Z_{ijk} and the parameter Γ_H in logical constraint equations in order to calculate heat exchanger driving forces which are further used to calculate heat exchanger areas, as described by Eqs. (13) and (14). This is where thermodynamic feasibility is ensured (i.e. no negative driving forces are allowed).

$$dt_{ijk} \leq t_{i,k} - t_{j,k} + \Gamma_H(1 - Z_{ijk}), \quad k \in K, \quad i \in H, \quad j \in C \tag{13}$$

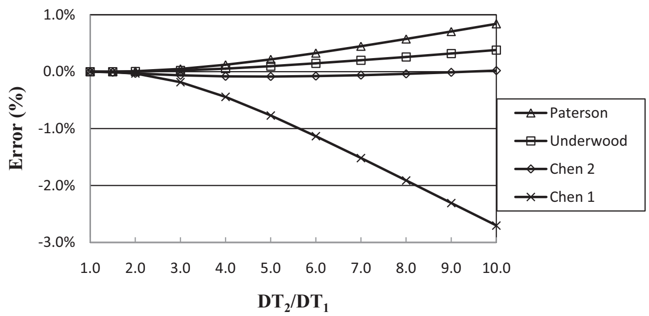

Fig. 3. Comparison of log-mean approximation errors.

$$dt_{ijk+1} \le t_{i,k+1} - t_{j,k+1} + \Gamma_H(1 - Z_{ijk}), \quad k \in K, \quad i \in H, \quad j \in C \tag{14}$$

The value Γ_H is set as the maximum of zero and the temperature differences between the hot and cold streams participating in the match concerned (Shenoy, 1995). This helps to avoid numerical errors due to negative temperature differences for matches which do not exist.

In order to avoid including exchangers of infinite areas in the calculations, an exchanger minimum approach temperature (EMAT) is included in the model. This is represented as:

$$dt_{ijk} \ge \delta \tag{15}$$

where δ is a small positive number.

6.9. Objective function

The objective function that is minimized in this study is the TAC of the network, as was used by all the other studies used for comparison of results. The TAC is given in Eq. (16). The capital cost of each exchanger is the sum of a fixed cost and an area cost. The objective function is given by:

$$\min \left(\sum_{i \in H}\sum_{k \in K} CUq_{ijk} + \sum_{j \in C}\sum_{k \in K} HUq_{ijk} + \sum_{i \in H}\sum_{j \in C}\sum_{k \in K} CB_{ij}Z_{ijk} + \sum_{i \in H}\sum_{j \in C}\sum_{k \in K} AFC \left[\frac{q_{ijk}}{U_{ij}} [LMTD_{i,j,k}] \right]^{D_{ij}} \right) \tag{16}$$

To avoid the singularity problem when calculating the logarithmic mean temperature difference, LMTD, if the driving forces are equal, Chen's first approximation is used (Chen, 1987), as given in Eq. (17). This has been done for comparison with other results which are based on it, rather than using Chen's second approximation which is more accurate.

$$LMTD_{ijk} = \left[\frac{(dt_{ijk})(dt_{ijk+1})(dt_{ijk} + dt_{ijk+1})}{2} \right]^{1/2} \tag{17}$$

Fig. 3 compares the errors of the various log-mean approximations over a range of $\Delta T_2/\Delta T_1$ between 1.0 and 10.0 (Chen, 1987; Paterson, 1984; Underwood, 1970). Note that Chen did not give errors for his two approximations, but noted out that his second approximation was better than Paterson's over the range of $\Delta T_2/\Delta T_1$ values from 1.5 to 10.0. Paterson (1987) subsequently pointed out that Chen's second approximation was slightly less accurate than Underwood's at a ratio of 1.5, but much more accurate around 10.0 (see Shenoy & Fraser, 2003). In fact, as may be seen in Fig. 3, Chen's second approximation is slightly worse than Underwood's below a ratio of 5.0, and quite a bit better from 5.0 upwards. Chen's first approximation is in fact worse than all the rest at ratios above 2.0. It is a pity that Yee and Grossmann (1990) chose the worst of all the approximations for their work, as everyone else has done the same for comparison purposes.

Table 3
Problem specifications for Example 1 (Lee et al., 1970).

Stream	T^s (°F)	T^t (°F)	F (Btu/(°F))
$H1$	320	200	16666.8
$H2$	480	280	20,000
$C1$	140	320	14450.1
$C2$	240	500	11,530
$S1$	540	540	–
$W1$	100	180	–

Hot utility ($S1$) cost = 12.76 \$kBtu^{-1} yr^{-1}, cold utility ($W1$) cost = 5.24 \$kBtu^{-1} yr^{-1}.
Heat exchangers annual cost = \$35 × area$^{0.6}$ (area in ft^2).
U = 150 Btu/ft^2 °F for all matches except those involving steam where U = 200 Btu/ft^2.

6.10. Application

Eqs. (1)–(17) which define the feasible space for the SBS model are all linear except for Eqs. (8), (9) and (16). The non-linearity in Eqs. (8) and (9) is due to the utility stream flows which are variables to be optimized. This does not, however, significantly affect the solution generation. Note that matches can easily be constrained in the network. Such constraints include preferred and forbidden matches. This can be accomplished by fixing the binary variables concerned or restricting the amount of heat to be exchanged in such exchangers.

The SBS model presented in this paper has been solved in the General Algebraic Modeling Systems (GAMS) environment (Rosenthal, 2007) with the solver DICOPT++, which uses CPLEX for the MILP and CONOPT for the NLP sub-problems. The solutions obtained with the use of SBS gave results which are in the same range as those reported in the literature, as will be shown in the examples which follow. The initialization approach is the one that was used by Isafiade (2008), which worked very well, and which was based on a similar approach by Shenoy (1995). This is done through the exchanger minimum approach temperature (EMAT), and setting upper bounds for heat capacity flowrates of hot and cold utilities.

7. HENS examples

7.1. Example 1: 4SP1 (Lee, Masso, & Rudd, 1970)

This example is the 4SP1 problem from Lee et al. (1970), which involves two hot and two cold streams, and one hot utility (steam) and one cold utility (water). It has also been solved for the situation where any match between $H1$ and $C1$ is forbidden (also termed a match restriction). The problem specifications are given in Table 3.

7.1.1. Case with no match restriction

Table 4 compares the results of workers who have solved this problem, listed in decreasing order of TAC (as is the case for all other tables comparing the results of different workers). In the SBS solution, Chen's first approximation was used to obtain the LMTD, this underestimates the real value of the LMTD (Krishna & Murty, 2007; Shenoy & Fraser, 2003), and hence overestimates the area and thus the capital cost. This accounts for the SBS and Krishna and Murty solutions being about 2% higher than those of Grossmann and Sargent (1978) and Bagajewicz et al. (1998). The grid representation of the SBS solution is shown in Fig. 4.

7.1.2. Case with match restriction

This case forbids any match between $H1$ and $C1$ (this may be required industrially for safety reasons, to avoid streams mixing if

Table 4
Comparison of results for Example 1.

Method	ΔT_{min} (°F)	Stream splits	No of units	TAC ($/year)	% difference
Two step targeting procedure of Papoulias and Grossmann (1983)	50	0	5	13,590[a]	28.45
Evolutionary development method of Linnhoff and Flower (1978)		0	5	13,587	28.42
Branch and bound method of Lee et al. (1970)	18	0	5	13,481	27.42
SBS of this study	1.9	1	5	10,794	2.02
DEM of Krishna and Murty (2007)	2.1	0	5	10,782	1.91
Mathematical optimization technique of Grossmann and Sargent (1978)	1	0	5	10,592	0.11
State space approach of Bagajewicz et al. (1998)	–	0	5	10,580	0.00

[a] Note this is the value was calculated by Bagajewicz et al. (1998).

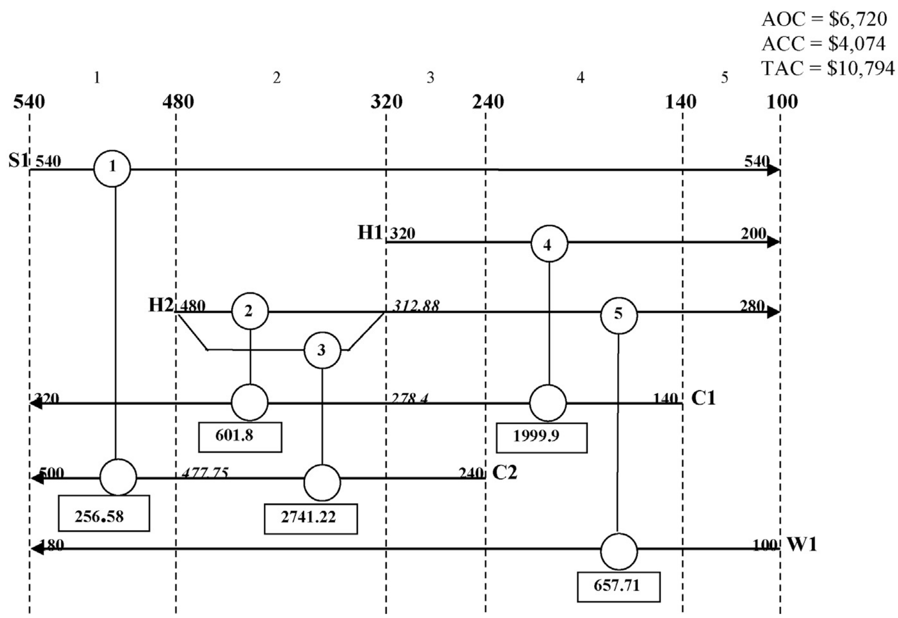

Fig. 4. The SBS network structure featuring five units with a TAC of $10,794.

there is an exchanger leak). Some workers incorporated cold–cold matching in their networks, although this option does not appear to be used in industry. Table 5 compares the results obtained by various workers: it may be noted that allowing for cold–cold matching yields much better solutions, and there is a large discrepancy without it (Figs. 5–7).

7.2. *Example 2: 4S1 (Shenoy, 1995)*

Another example involving two hot streams, two cold streams, one hot and one cold utility is the 4S1 problem of Shenoy (1995). It features equal heat transfer coefficients for all streams. Shenoy solved it using the SWS of Yee and Grossmann (1990) with the

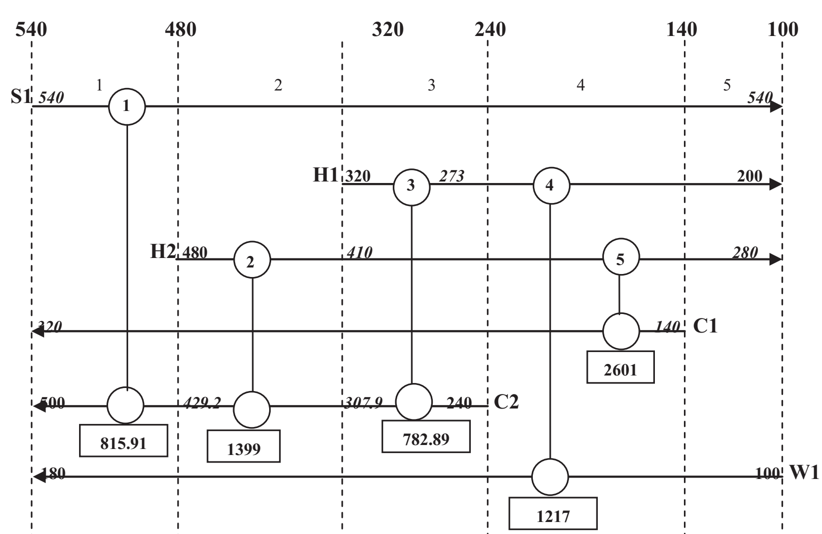

Fig. 5. The SBS network structure with match H1–C1 forbidden featuring five units with a TAC of $20,019.

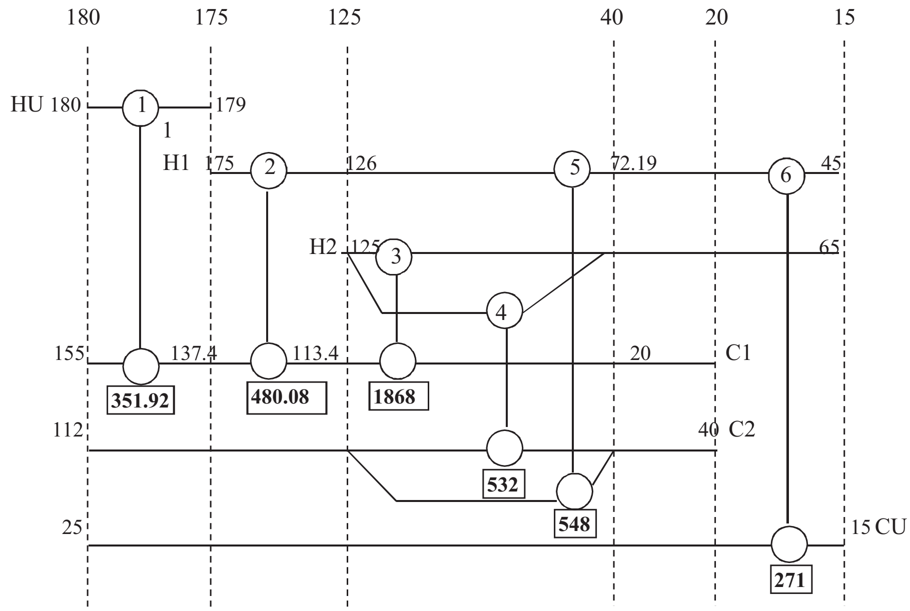

Fig. 6. SBS network structure for Example 2 featuring six units with TAC of $235,931.

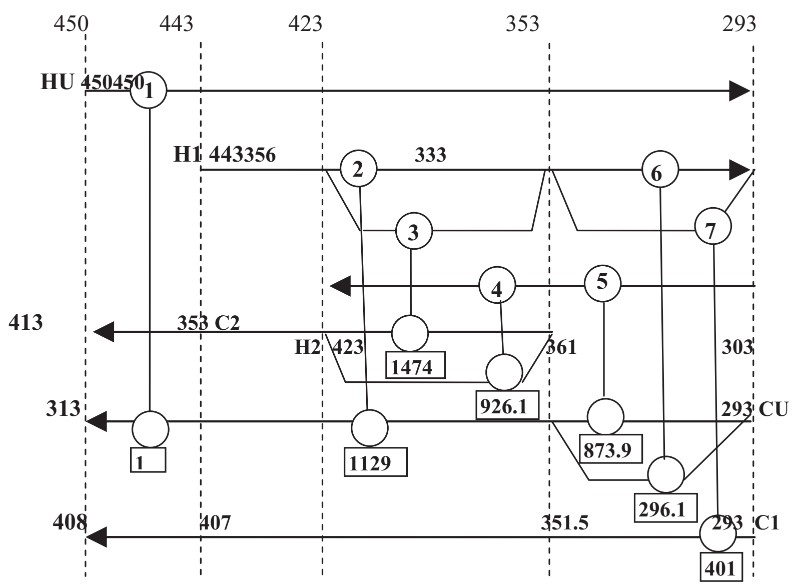

Fig. 7. SBS network structure for Example 3 featuring seven units with TAC of $90,521/yr.

Paterson (1984) approximation for LMTD. The problem specifications are shown in Table 6.

The results of this study are compared with those of other workers in Table 7. Note that all solutions involve six units and at least two splits, with $H2$ being always being one of the splits due to it large heat capacity flowrate. The SWS has the best solution, with the SBS close behind with an increase of 0.2% over the SWS, despite using an approximation that increased its costs.

7.3. *Example 3 (Linnhoff et al., 1982)*

Another example involving two hot streams and two cold streams, along with steam and cooling water as utilities was taken

Table 5
Comparison of results for Example 1 with match restriction.

Method	Cold–cold matching?	TAC ($/year)	% difference
Two step targeting procedure of Papoulias and Grossmann (1983)	No	21,100	52.9
SBS of this study	No	20,019	45.1
DEM of Krishna and Murty (2007)	No	18,705	35.5
SWS of Yee and Grossmann (1990)	Yes	13,800	0.0
Simulated annealing of Dolan, Cummings, and Le Van (1987)	Yes	13,800	0.0

Table 6
Problem specifications for Example 2 (Shenoy, 1995).

Stream	T^s (°C)	T^t (°C)	F (kW °C^{-1})	h (kW m^{-2} °C^{-1})	Costs (\$kW^{-1} yr^{-1})
$H1$	175	45	10	0.2	–
$H2$	125	65	40	0.2	–
$C1$	20	155	20	0.2	–
$C2$	40	112	15	0.2	–
$HU1$	180	179	–	0.2	120
$CU1$	15	25	–	0.2	10

Annualization factor = 0.322, utility costs in \$kW^{-1} yr^{-1}.
Capital cost (\$) = 30,000 + 750[area (m^2)]$^{0.81}$ for all exchangers.

Table 7
Cost comparison for Example 2.

Method	Stream splits	No of intervals	No of units	TAC ($/year)	% difference
Cold stream based IBMS of Isafiade and Fraser (2008a, 2008b)	3	5	6	239,332	1.67
Hot stream based IBMS of Isafiade and Fraser (2008a, 2008b)	2	5	6	237,800	1.02
SBS of this study	2	5	6	235,931	0.20
SWS of Shenoy (1995)	2	2	6	235,400	0.00

Table 8
Problem specifications for Example 3 (Linnhoff et al., 1982).

Stream	T^s (K)	T^t (K)	F (kW K^{-1})	Costs ($kW^{-1} yr^{-1})
$H1$	443	333	30	–
$H2$	423	303	15	–
$C1$	293	408	20	–
$C2$	353	413	40	–
$S1$	450	450	–	80
$W1$	293	313	–	20

$U = 0.8$ kW m^{-2} K^{-1} for all matches except one involving steam.
$U = 1.2$ kW m^{-2} K^{-1} for matches involving steam.
Annual cost = 1000 × [area (m^2)]$^{0.6}$.
Annual cost = 1000 × [(area (m^2)]$^{0.6}$.

Table 9
Cost comparison for Example 3.

Method	Stream splits	No of units	TAC ($/year)	% difference
SBS of this study	2	7	90,521	12.77
Magnet solution of Grossmann (1985)	–	6	89,832	11.91
Pinch technique of Linnhoff et al. (1982)	–	7	89,832	11.91
SWS of Yee and Grossmann (1990)	2	5	80,274	0.00

from Linnhoff et al. (1982). The problem specifications are shown in Table 8.

The results of various workers are shown in Table 9.

The SWS of Yee and Grossmann (1990) fixed two stages for this problem i.e. maximum of number of hot stream or cold stream to obtain a TAC of $80,274/yr using DICOPT++ in GAMS (Brooke et al., 1988). Grossmann (1985) obtained a TAC of $89,832/yr for this problem; the same TAC was reported for Linnhoff et al. (1982). SBS of this study obtained a TAC of $90,521/yr for this problem; this cost is less than 0.1% of the TAC obtained by Linnhoff et al., and that of Grossmann; but higher than the TAC of Yee and Grossmann by 12.77%.

7.4. Example 4 (MAGNETS problem)

This example is taken from MAGNETS User Manual for the analysis of SWS by Yee and Grossmann (1990). The problem involves five hot streams and one cold stream together with steam and cooling water. The problem specifications are shown in Table 10.

The network structure obtained for the present study is shown in Fig. 8 featuring eight units. The splits in all the networks are in line with the expectation of Yee and Grossmann (1990) because

Table 10
Problem specifications for Example 4.

Stream	T (K)	T (K)	F (kW K^{-1})	Cost ($kW^{-1} yr^{-1})
$H1$	500	320	6	–
$H2$	480	380	4	–
$H3$	460	360	6	–
$H4$	380	360	20	–
$H5$	380	320	12	–
$C1$	290	660	18	–
$S1$	700	700	–	140
$W1$	300	320	–	10

U (kW m^{-2} K^{-1}) = 1 for all matches, annualized area cost = 1200(A)$^{0.6}$ for all exchangers where A is the area (m^2).

of a single cold stream of fairly large size that matches with many hot streams. The network costs are shown in Table 11. The SBS network cost is 0.58% higher than Yee and Grossmann (1990) but lower than the best of Isafiade and Fraser (2008a). It is worthwhile to point out that the SWS has five stages defined by the number of hot streams, the IBMS has seven intervals defined by the supply and target temperatures of the hot streams and cold stream $C1$ splitting and mixing in the intervals created like this while the present study has six intervals and the cold stream $C1$ splitting and mixing in intervals created by the supply temperatures of streams where that of $C1$ is included. All the hot streams are constrained at both their supply and target temperatures in the IBMS while the SBS gives more freedom to both the hot and cold streams regarding the intervals where they could exchange heat. The reason for this is that in the IBMS network hot streams $H2$, $H3$ and $H5$ exist in two intervals each, while hot stream $H4$ exists in only one interval, whereas in SBS network hot stream $H2$ exists in four intervals, $H3$ in three intervals, and $H5$ and $H4$ exist in two intervals each (Fig. 9).

7.5. Example 5 (aromatic plant)

This problem involves the determination of a cost optimal network of exchangers for four hot streams and five cold streams having different heat transfer coefficients (Krishna & Murty, 2007; Lewin, 1998; Linnhoff & Ahmad, 1990). The stream data is shown in Table 12 and a comparison of costs with previous works is shown in Table 13. The cost obtained in the present study compares well with others. This shows that the new SBS is able to solve problems with different heat transfer coefficients. Krishna and Murty (2007) gave the linear nature of their objective function with respect to exchanger surface as the reason for not obtaining split streams while Lewin (1998) had to make adjustment to the hot oil effluent temperature to satisfy ΔT_{min} in his solution.

Table 11
Comparison of results for Example 4.

Method	No of intervals	Stream splits	No of units	Cost ($/year)	% difference
Cold stream based IBMS of Isafiade and Fraser (2008a, 2008b)	3	1	7	595,064	3.81
Hot stream based IBMS of Isafiade and Fraser (2008a, 2008b)	7	1	7	581,942	1.52
SBS of this study	6	1	8	580,023	1.19
SWS of Yee and Grossmann (1990)	5	1	7	576,640	0.60
GA of Lewin (1998)	–	2	9	573,205	0.00

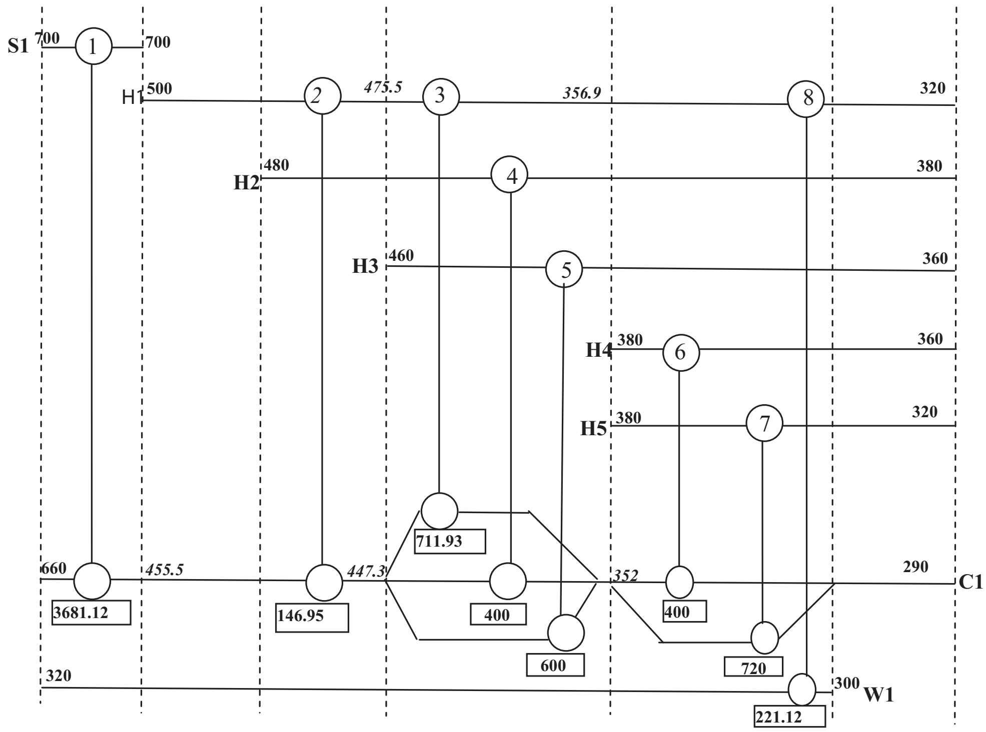

Fig. 8. The network structure for Example 4 of the SBS featuring eight units and one 3 way split and one 2 way split of the cold stream with, a TAC of $580,023.

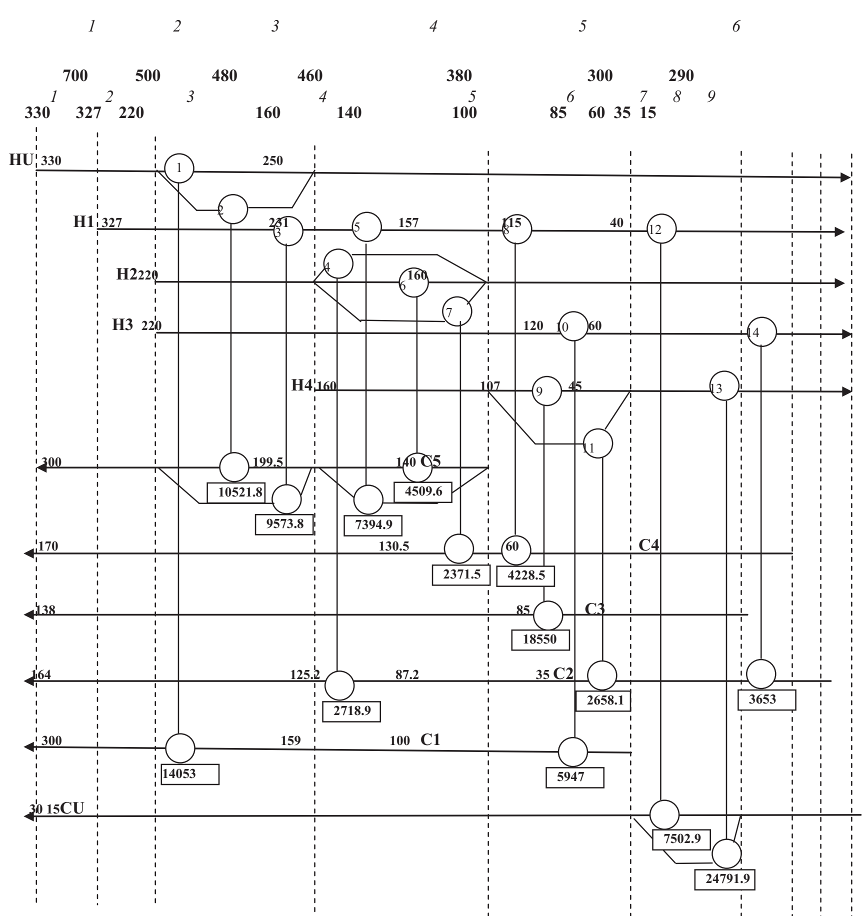

Fig. 9. SBS network structure for Example 5 featuring 14 units with six stream splits.

Table 12
Problem specifications for Example 5.

Streams	T^s (°C)	T^t (°C)	F (kW K^{-1})	h (kW m^{-2} K^{-1})
$H1$	327	40	100	0.50
$H2$	220	160	160	0.40
$H3$	220	60	60	0.14
$H4$	160	45	400	0.30
$C1$	100	300	100	0.35
$C2$	35	164	70	0.70
$C3$	85	138	350	0.50
$C4$	60	170	60	0.14
$C5$	140	300	200	0.60
Hot oil	330	250	–	0.50
Water	15	30	–	0.50

Plant Lifetime is five years, rate of interest = 0%.
Exchanger cost (US$) = 10,000 + 350 × S (S is area in m^2).
Hot oil cost = 60 US$kW^{-1} yr^{-1}; water cost = 6US$kW^{-1} yr^{-1}.

8. Construction of the MENS supply-based superstructure

The SBS has also been applied to MENS. A typical MENS problem with two rich streams ($R1$ and $R2$) and two lean streams ($S1$ and $S2$) is represented in Fig. 10, which is the MENS analogue of Fig. 2. The superstructure is partitioned using the supply compositions of all the streams.

In Fig. 10, the composition intervals are defined by the supply compositions of all streams arranged in descending order. The supply composition Y^s_{R1} of rich stream $R1$ is higher than the supply composition Y^s_{R2} of rich stream $R2$. The supply composition Y^{s*}_{S2} of lean stream $S2$ is higher than the supply composition Y^{s*}_{S1} of lean stream $S1$ but lower than the supply compositions of $R1$ and $R2$. All the other characteristics of the superstructure in Fig. 10 for MENS are the same as those discussed for Fig. 2 for HENS, with the appropriate terminology changes. The process and external lean streams are given equal opportunity to exchange mass in the superstructure based on economics. This is unlike pinch technology, where external lean streams are only used below the pinch.

9. SBS model equations for MENS

The sets of equations which are used to model the MENS SBS are similar to those presented for the HENS SBS.

9.1. Assignment of superstructure interval boundary compositions

The model equations are presented below:

$$k = 1; \quad Y^s_{R1,1}, \quad Y^*_{S1,1} = Y^{s*}_{S1} \tag{18a}$$

$$k = 2; \quad Y^s_{R2,2}, \quad Y^*_{R1,2}, \quad Y^*_{S1,2}, \quad Y^*_{S2,2} \tag{18b}$$

$$k = 3; \quad Y^s_{S2,3}, \quad Y_{R1,3}, \quad Y_{R2,3}, \quad Y^*_{S1,3} \tag{18c}$$

$$k = 4; \quad Y^{s*}_{S1,4}, \quad Y_{R1,4} = Y^{s*}_{R1}, \quad Y_{R2,4} = Y^{s*}_{R2} \tag{18d}$$

9.2. First set of stream existence conditionals for MENS

In a similar manner to HENS SBS, stream existence conditionals are used to ensure that a rich stream cannot exchange mass in any interval whose composition is higher than its supply value while a lean stream cannot exchange mass in any interval where the composition is lower than its supply value:

$$R_{r,x}\$(Y^s_r \geq Y_k) = 1 \tag{19}$$

$$S_{l,x}\$(Y^{*s}_r \leq Y_k) = 1 \tag{20}$$

9.3. Second set of stream existence conditionals

The second set of stream existence conditionals is the stream supply composition recognition conditionals:

$$RST_{r,k}\$(Y^s_r = Y_k) = 1 \tag{21}$$

$$SST_{l,k}\$(Y^{*s}_l = Y_k) = 1 \tag{22}$$

9.4. Overall stream mass balance equations

The total mass exchanged by each stream over all matches in all intervals must equal the total component mass change of that stream. Eqs. (23) and (24) describe this for rich stream i and lean stream j respectively.

$$(Y^s_r - Y^t_r)G_r = \sum_{k \in K}\sum_{j \in S} M_{rlk}, \quad r \in R \tag{23}$$

$$(Y^{*t}_l - Y^{*s}_l)L_l = \sum_{k \in K}\sum_{r \in R} M_{rlk}, \quad l \in S \tag{24}$$

Note that the rich stream flowrate G_r is modeled as a parameter in Eq. (23), whereas the lean stream flowrate L_l in Eq. (24) is modeled as a variable. Note that the stream flowrates are all taken to be constant throughout the network, which is true if mass ratios are used (provided there is minimal evaporation, if a liquid stream is involved), and a good assumption for low concentrations when mass fractions are used.

9.5. Interval mass balances

The mass exchanged by each stream in each interval defines the composition of that stream for the next interval. Both are

Table 13
Comparison of results for Example 5.

Method	Stream splits	No of units	Cost (M$/year)	% difference
DEM of Krishna and Murty (2007)	2	–	3.146	8.30
Block decomposition technique of Zhu, O'Neill, Roach, and Wood (1990)	0	10	2.980	2.58
SBS of this work	6	14	2.976	2.44
Linnhoff and Ahmad (1990)	0	13	2.960	1.89
GA of Lewin (1998)	0	11	2.946	1.41
DEM of Krishna and Murty (2007)	0	15	2.942	1.27
GA of Lewin (1998)	2	12	2.936	1.07
Petersen (2005)	7	17	2.905	0.00

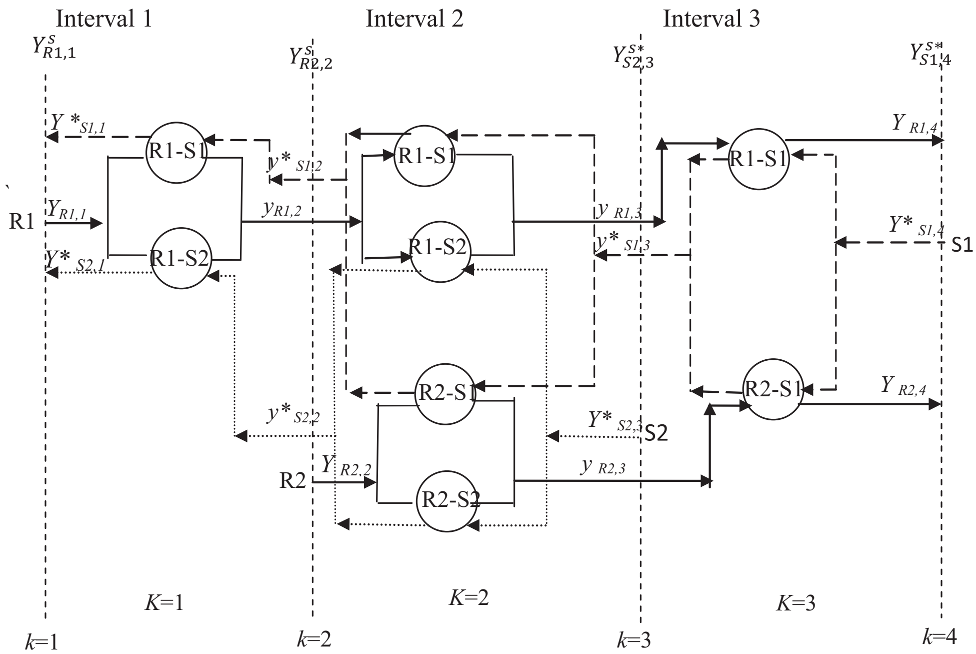

Fig. 10. Supply based superstructure for MENS with two rich streams and two lean streams.

determined using the interval mass balance equations for rich and lean streams which are presented in Eqs. (25) and (26).

$$(y_{r,k} - Y_{r,k+1})G_r = \sum_{a \in S} M_{rlk}, \quad k \in K \tag{25}$$

$$(y^*_{l,k} - Y^*_{r,k+1})L_l = \sum_{r \in R} M_{rlk}, \quad k \in K \tag{26}$$

9.6. Composition feasibility along the superstructure

Constraints are used to ensure monotonic decrease of composition from the first composition location to the last composition location in the superstructure, this translates to a decrease in composition from supply to target and target to supply for rich and lean streams respectively.

$$y_{r,k} \geq y_{r,k+1}, \quad k \in x, \quad r \in R \tag{27}$$

$$y^*_{l,k} \geq y^*_{l,k+1}, \quad k \in x, \quad l \in S \tag{28}$$

9.7. Logical constraints

The existence of a match r, l in interval k is modeled using a binary variable, Z_{rlk}. If a match exists Z_{rlk} takes on a value of '1' and otherwise it is '0'. An upper bound, Ω, is used to restrict the amount of mass which can be exchanged in each match to the lesser of the mass loads of the rich and lean streams participating in each match.

$$M_{rlk} - \Omega Z_{rlk} \leq 0, \quad r \in R \quad l \in S \quad k \in K \tag{29}$$

9.8. Calculation of exchanger driving forces

The variables dy_{rlk} and dy_{rlk+1}, which are the exchanger rich and lean end composition differences respectively, are used together with the logical constraint Z_{rlk} in the equations to calculate exchanger driving forces. These equations also incorporate the parameter Γ_M which is set as the maximum of '0' and the composition differences between rich stream r and lean stream l in interval k (Shenoy, 1995), to avoid numerical errors due to negative composition differences for matches that do not exist.

$$dy_{rlk} \leq y_{r,k} - y^*_{l,k} + \Gamma_M(1 - Z_{rlk}), \quad k \in K, \quad r \in R, \quad l \in S \tag{30}$$

$$dy_{rlk} \leq y_{r,k} - y^*_{l,k} - \Gamma_M(1 - Z_{rlk}), \quad k \in K, \quad r \in R, \quad l \in S \tag{31}$$

$$dy_{rlk+1} \leq y_{r,k+1} - y^*_{l,k+1} + \Gamma_M(1 - Z_{rlk}), \quad k \in K, \quad r \in R, \quad l \in S \tag{32}$$

$$dy_{rlk+1} \leq y_{r,k+1} - y^*_{l,k+1} - \Gamma_M(1 - Z_{rlk}), \quad k \in K, \quad r \in R, \quad l \in S \tag{33}$$

As in the HENS SBS, an exchanger minimum approach composition (EMAC) ϵ is included in the model so as to avoid having exchangers of infinite sizes:

$$dy_{rlk} \geq \varepsilon \tag{34}$$

where ε is a small positive value.

The integer infeasible path MINLP (IIP-MINLP) formulation of Sorsak and Kravanja (2002) which enables the solver also to search for feasible solution through infeasible solutions (as used by Szitkai et al., 2006) is used in SBS model. The equation for this is:

$$w_{r,l,k} = dw_{r,l,k} + ew_{r,l,k} - fw_{r,l,k}, \quad r \in R, \quad l \in S, \quad k \in K \tag{35}$$

where $w_{r,l,k}$ is the relaxed form of the real variable $dw_{r,l,k}$ while $ew_{r,l,k}$ and $fw_{r,l,k}$ are positive and negative tolerances respectively, which eventually equal zero.

9.9. Objective function

The objective function, which is the minimum network TAC, is as shown in Eqs. (36) and (37). Note that the exchanger mass based calculation method of Hallale (1998) is used in this study for continuous contact columns, while the per stage costing method of Papalexandri et al. (1994) is used for costing stage-wise columns.

For continuous contact columns the objective function is as follows:

$$\min\left(\sum_{l\in S}(AC_l)(L_l)+\sum_{r\in R}\sum_{l\in S}\sum_{k\in K}CB_{rl}Z_{rlk}+\sum_{r\in R}\sum_{l\in S}\sum_{k\in K}ACH_{rl}\left[\frac{M_{rlk}}{K_w}[LMCD]\right]^{D_{rl}}+VT\right) \quad (36)$$

where

$$VT=VF\cdot\sum_{r\in R}\sum_{l\in S}\sum_{k\in K}(ew_{r,l,k}+fw_{r,l,k})$$

For stage-wise columns, the expression is:

$$\min\left(\sum_{l\in S}(AC_l)(L_l)+\sum_{r\in R}\sum_{l\in S}\sum_{k\in K}CB_{rl}Z_{rlk}+\sum_{r\in R}\sum_{l\in S}\sum_{k\in K}ACT_{rlk}(N_{rlk})\right) \quad (37)$$

where N_{rlk} is the number of stages for match i, j in interval k.

To avoid the problem of singularities associated using the LMCD for mass exchanger sizing the first approximation of Chen (1987) is used, as was done for LMTD in HENS. A detailed comparison of the various log-mean approximations and the errors associated with them is given in Section 6.9.

$$LMCD_{rlk}=\left[\frac{(dy_{rlk})(dy_{rlk+1})(dy_{rlk}+(dy_{rlk+1}))}{2}\right]^{1/3} \quad (38)$$

To avoid the singularity in calculating the number of stages using the Kremser equation, Shenoy and Fraser (2003) presented the following approximation:

$$N_{rlk}=\left(\frac{\Delta y^n+\Delta y^{*n}}{\Delta y_1^n+\Delta y_2^n}\right)^{1/n} \quad (39)$$

where Δy and Δy^* are the rich stream concentration difference and the lean stream equilibrium concentration difference respectively; Δy_1 is the driving force at the rich end of the exchanger; Δy_2 is the driving force at the lean end of the exchanger; and n is given as 1/3 by Underwood (1970) and 0.3275 by Chen (1987).

It is important to note that the approximation of Shenoy and Fraser (2003) to obtain the number of stages was obtained from the logarithmic mean approximations of Underwood (1970) and the second approximation of Chen (1987). The error in using Eq. (39) for calculating the number of stages is a function of the ratio of the driving forces $(((\Delta y)1)/(\Delta y2))$. At a ratio of 15.85, the Underwood and second Chen approximations gave errors of 0.73% and 0.29% respectively, while at a ratio of 76, the errors are 3.48% and 2.43% respectively (Shenoy & Fraser, 2003). Fraser and Shenoy (2004) give a detailed analysis of errors in terms of the absorption and effectiveness factors.

10. MENS examples

10.1. Example 6: ammonia removal (Hallale, 1998)

This example is taken from Hallale (1998). Note that Hallale did not present an optimal solution for this problem (unlike has been assumed by others (Emhamed et al., 2007; Szitkai et al., 2006). In this problem ammonia is to be removed from five gaseous streams (composed mainly of air). Two process MSAs, $S1$ and $S2$, and one external MSA, $S3$, are available for the removal. The problem specifications are given in Table 14.

Table 14
Problem specifications for Example 6 (Hallale, 1998).

Rich stream	G (kg/s)	Y (s)	Y (t)
$R1$	2	0.005	0.0010
$R2$	4	0.005	0.0025
$R3$	3.5	0.011	0.0025
$R4$	1.5	0.010	0.0050
$R5$	0.5	0.008	0.0025

Lean stream	L^c (kg/s)	X (s)	X (t)	m	b	Cost ($/kg)
$S1$	1.8	0.0017	0.0071	1.2	0	0
$S2$	1.0	0.0025	0.0085	1	0	0
$S3$	∞	0.0	0.017	0.5	0	0.001

Packed column exchangers, K_W = 0.02 kg NH_3/(s kg), shell cost = \$618$M^{0.66}$, where M is exchanger mass.
Annualization factor = 0.225; annual operating time = 8150 h.

Table 15
Comparison of costs for Example 6 with previous workers.

Method	Splits: rich/lean	No of units	TAC ($/yr)	% difference
Hybrid method of Emhamed et al. (2007)	3/2	10	134,399	3.46
'SWS' of Szitkai et al. (2006)	0/1	8	134,000	3.16
IBMS of Isafiade and Fraser (2008b)	1/1	7	133,323	2.63
SBS of this study	1/2	9	129,900	0.00

Table 15 compares the results of present study with those of previous workers, and the network structure is shown in Fig. 11. The solution obtained using the SBS has a TAC which is lower than any of the others at \$129,900, which is 2.63% below the next best solution.

10.2. Example 7: dephenolization of aqueous wastes (El-Halwagi, 1997)

This example is taken from El-Halwagi (1997). Phenols from two aqueous streams, $R1$ and $R2$ are to be absorbed by solvent extraction. Gas oil ($S1$) and lube oil ($S2$) are available free as process MSAs along with an external MSA, light oil ($S3$). It was specified that the entire gas oil stream $S1$ should be used. Problem specifications for the problem can be found in Table 16.

Results for this example are compared in Table 17, and the SBS network for it is shown in Fig. 12. Comeaux (2000) has the two best solutions for this problem, followed by the IBMS (Isafiade & Fraser, 2008b) and then the SBS, which is 2.28% above the best solution.

10.3. Example 8: coke oven gas problem (El-Halwagi & Manousiouthakis, 1989)

This example was taken from El-Halwagi and Manousiouthakis (1989). The problem involves the removal of hydrogen sulfide and

Table 16
Problem specifications for Example 7 (El-Halwagi, 1997).

Rich Stream	R (kg/s)	Y (s)	Y (t)
$R1$	2	0.050	0.010
$R2$	1	0.030	0.006

Lean stream	L^c (kg/s)	X (s)	X (t)	m	b	Cost ($/kg)
$S1$	5	0.005	0.015	2.00	0	0
$S2$	3	0.01	0.030	1.53	0	0
$S3$	∞	0.0013	0.015	0.71	0.001	0.01

Sieve tray columns, cost per equilibrium stage per year = \$4552/yr (Papalexandri et al., 1994).

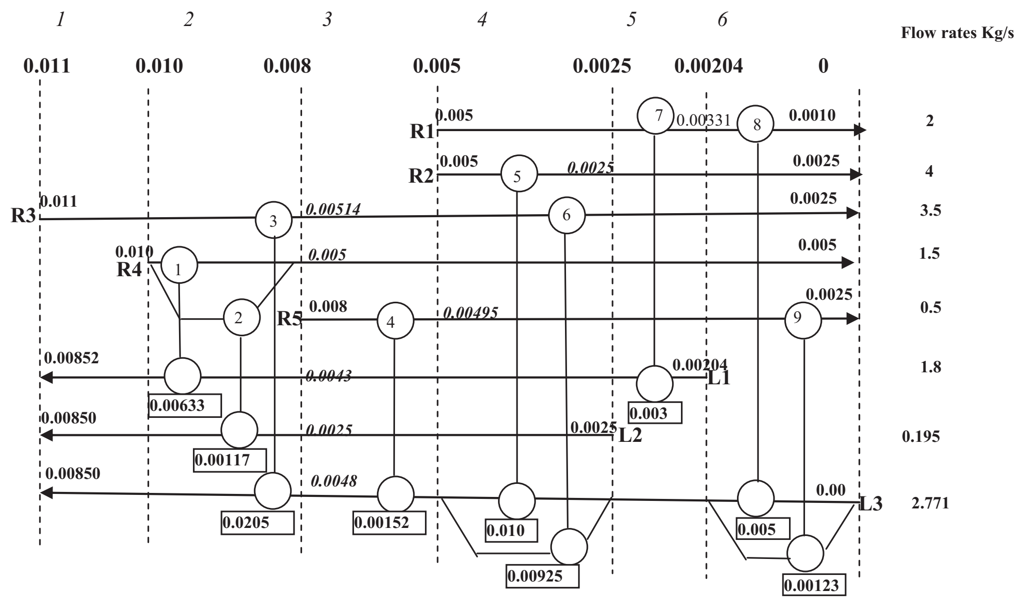

Fig. 11. Network structure for Example 6 of SBS featuring nine units with a split of rich stream and two separate 2 way splits of a lean stream with TAC of $129,901/yr.

Table 17
Summary and comparison of TAC for Example 7.

Method	Splits: rich/lean	No of units	Total cost ($/yr)	% difference
Lean based IBMS of Isafiade and Fraser (2008b)	0/0	5	358,292	7.92
Pinch technique of Hallale and Fraser (2000a, 2000b, 2000c)	0/2	7	345,416	4.04
SBS of this study	0/0	6	339,579	2.28
Rich based IBMS of Isafiade and Fraser (2008b)	0/0	6	338,168	1.86
First option of Insight based technique of Comeaux (2000)	0/2	7	333,300	0.39
Second option of Insight based technique of Comeaux (2000)	0/2	8	332,000	0.00

carbon dioxide from two rich streams, namely coke-oven gas, $R1$, and tail gas from a Claus unit, $R2$. One process MSA (aqueous ammonia), $L1$, and one external MSA (chilled methanol), $L2$, are available for this removal. Comparable targets for this problem were established by El-Halwagi and Manousiouthakis (1990). These led Hallale and Fraser (2000c) to point out that H_2S controls the MSA flow rate and the number of stages in the exchanger, so that this problem can be treated as though H_2S were the only transferred component. Others who treated this problem as a multicomponent problem (i.e. including the CO_2) generated the same MEN as that found by El-Halwagi and Manousiouthakis (Chen & Huang, 2005; Papalexandri et al., 1994). The problem specifications are shown in Table 18.

The comparison of results with previous workers is as shown in Table 19, and the SBS network in Fig. 13. In this case the best solution was the 'SWS' of Chen and Huang (2005),

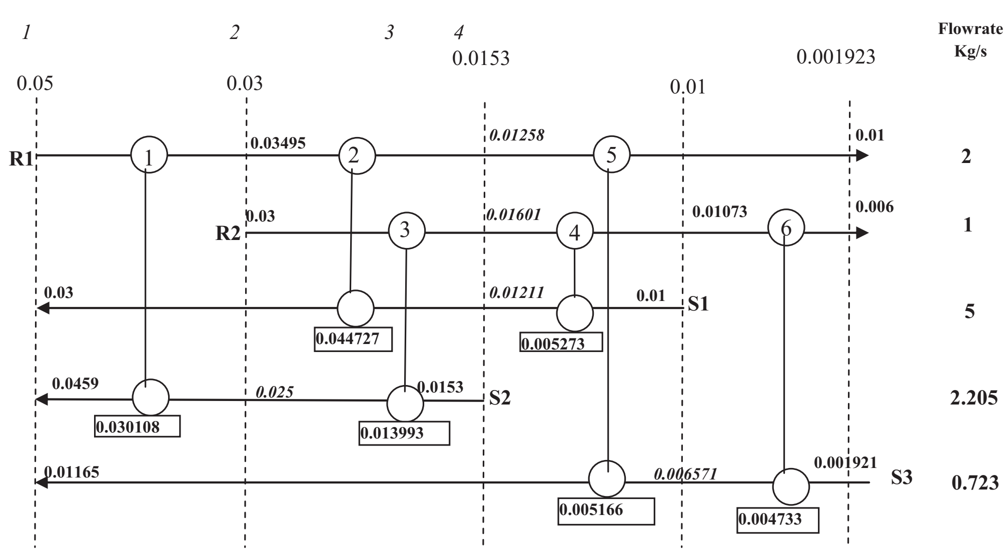

Fig. 12. SBS network for Example 7 featuring six units with a TAC of $339,579.

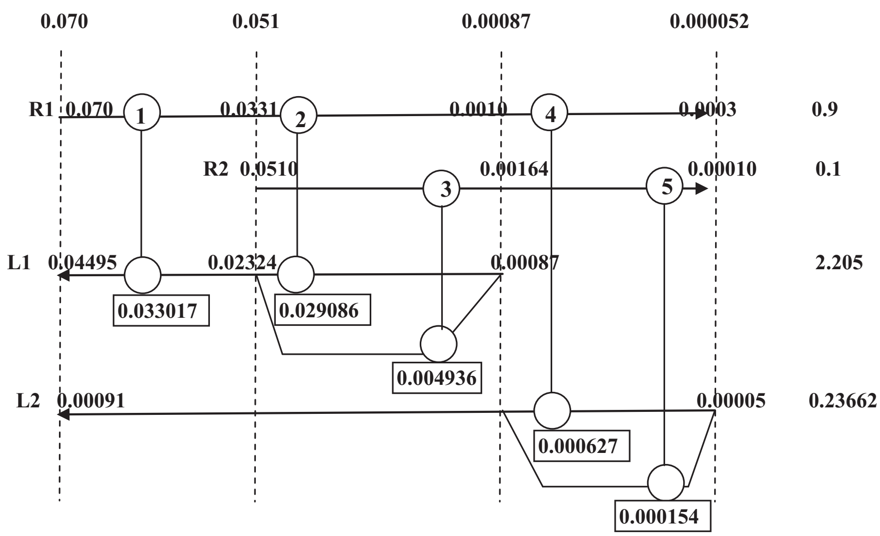

Fig. 13. The SBS superstructure for Example 8 with TAC of 469,968 $/yr.

Table 18
Problem specifications for Example 8 (El-Halwagi & Manousiouthakis, 1989).

Rich stream	R (kg/s)	Y^s	Y^t
$R1$	0.9	0.070	0.0003
$R2$	0.1	0.051	0.0001

Lean stream	L^c (kg/s)	X (s)	X (t)	m	b	Cost ($/yr) (kg/s)
$S1$	2.3	0.0006	0.031	1.45	0	117,360
$S2$	∞	0.0002	0.0035	0.26	0	176,040

Sieve tray columns, cost per equilibrium stage per year = $4552/yr (Papalexandri et al., 1994).

followed by Hallale's pinch technique, and then the IBMS (Isafiade, 2008). Here the SBS solution is 9.37% above the best solution, but still considerably better that the hyperstructure solution of Papalexandri et al. (1994).

10.4. Example 9: dephenolization of coal conversion waste (Papalexandri et al., 1994)

This example involves simultaneous mass exchange and regeneration of one of the MSAs. Phenol is removed from four aqueous streams, $R1$–$R4$. Two MSAs are available for this removal, light oil, $S1$ (used on a once-through basis), and activated carbon, $S2$ (which is regenerated using caustic soda, $H1$, as the regenerant in a stripping process, and recycled). The inlet and outlet compositions of the regenerable MSA, X_2^s and X_2^t are not given, and have to be determined in the synthesis task, but those of $S1$ and the regenerating agent Z^s and Z^t are given. The problem specifications are shown in Table 20. Note that for $S2$, the cost shown in Table 20 refers to the actual usage of the stream and not to the circulating flow, but nobody has used this value because a ratio of make-up flow to circulating flow has not been specified.

Table 19
Summary and comparison of TAC for Example 8.

Method	Splits: rich/lean	No of units	Total cost ($/yr)	% difference
Hyperstructure technique of Papalexandri et al. (1994)	0/1	3	917,880	113.61
Rich based IBMS of Isafiade (2008)	0/0	4	530,471	23.45
SBS of this study	0/0	5	469,968	9.37
Lean based IBMS of Isafiade (2008)	0/2	4	446,840	3.99
Pinch technique of Hallale and Fraser (2000a)	0/1	5	431,613	0.44
'SWS' of Chen and Huang (2005)	0/2	4	429,700	0.00

Table 20
Problem specifications for Example 9 (Papalexandri et al., 1994).

Rich streams	G (kg/s)	Y^s (mass fraction)	Y^t (mass fraction)
$R1$	3.3	0.05	0.0015
$R2$	0.6	0.07	0.003
$R3$	1.4	0.02	0.003
$R4$	0.2	0.03	0.002

MSAs	L^c (kg/s)	X^s (mass fraction)	X^t (mass fraction)	m	b	Cost ($/yr)/(kg/s)
$S1$	10	0.0013	0.025	0.71	0.001	58,680
$S2$	10			0.13	0.001	417,060

Regent	M^c (kg/s)	Z^s (mass fraction)	Z^t (mass fraction)	m	b	Cost ($/yr)/(kg/s)
$H1$	10	0	0.005	1.38	0.0	88,020

Sieve tray columns for $S1$, cost per equilibrium stage per year = $4552/yr (Papalexandri et al., 1994).
Packed columns for $S2$ and $H1$, cost per year = $4245H/yr, with H = packed height (m) (Papalexandri et al., 1994).

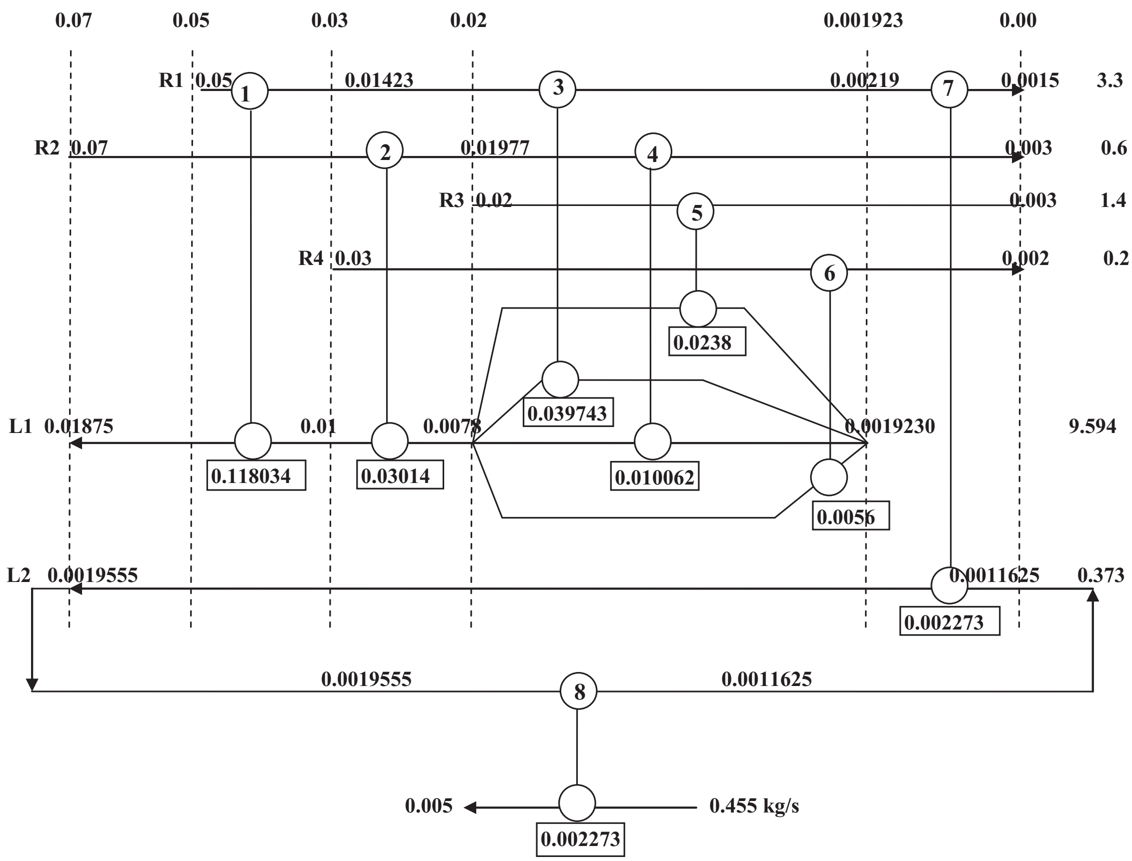

Fig. 14. SBS network structure for Example 9 featuring 8 units with TAC of 693,976 $/yr.

Table 21
Comparison of results for Example 9.

Method	Number of units	TAC ($/yr)	% difference
Hyperstructure technique of Papalexandri et al. (1994)	6	957,000	39.10
'SWS' of Szitkai et al. (2006)	NA	720,000	4.66
Pinch technique of Hallale and Fraser (2000a, 2000b, 2000c)	8	706,000	2.62
'SWS' of Chen and Huang (2005)	7	694,000	0.87
SBS	8	693,976	0.86
Rich based IBMS of Isafiade and Fraser (2008b)	8	689,300	0.19
Insight based technique of Comeaux (2000)	6	688,000	0.00

Table 22
Comparison of results over all nine examples.

Example	Number of streams	Best technique (out of n)	TAC ($/yr)	Next best solution (%)	SWS (%)	IBMS (%)	SBS (%)
1. 4SP1	2 H, 2 C, 1 HU, 1 CU	State space (7)	10,580	+0.11	–	–	+2.02
2. 4S1	2 H, 2 C, 1 HU, 1CU	SWS (4)	235,400	+0.20	0.00	+1.67	+0.20
3. Linnhoff problem	2 H, 2 C, 1 HU, 1 CU	SWS (4)	80,274	+11.91	0.00	–	+12.7
4. MAGNETS problem	5 H, 1 C, 1 HU, 1 CU	GA (5)	573,205	+0.60	+0.60	+1.52	+1.19
5. Aromatic plant	4 H, 5 C, 1 HU, 1 CU	Sequential match reduction (8)	2,900,000	+1.07	–	–	+2.44
6. Ammonia removal	4 R, 3 L (2 process MSAs, 1 external MSA)	SBS (4)	129,901	+2.63	+3.16	+2.63	0.00
7. Dephenolization	2 R, 3 L (2 process MSAs, 1 external MSA)	Insight based (6)	332,000	+0.39	–	+1.86	+2.28
8. Coke oven gas problem	2 R, 2 L (1 process MSA, 1 external MSA)	'SWS' (6)	429,700	+0.44	0.00	+3.99	+9.37
9. Dephenolization of coal conv. waste	4 R, 2 L, 1 H (2 process MSAs, 1 regenerant)	Insight based (7)	688,000	+0.19	+0.87	+0.19	+0.86

The results for this example are shown in Table 8, and the SBS network in Fig. 14. The result that was obtained with SBS now is TAC of $693,976/year, this consists of AOC of $618,181/yr and annual ACC of $75,795/yr. The trend of TAC is as shown in Table 21.

11. Conclusion

Supply temperatures/compositions of streams have been used to develop new superstructures for optimization of the total annual cost in HENS and MENS. This technique is similar to the SWS of

Yee and Grossmann (1990) and Szitkai et al. (2006) and the IBMS of Isafiade and Fraser (2008a, 2008b), differing mainly in how the interval boundaries are defined. The SBS creates a relatively large number of intervals for HENS and MENS, which provides more opportunity for matches between particular streams (Shenoy, 1995).

The examples presented have costs that are within the range of previous results, with easy initialization, and solutions that were found quickly. As shown in Table 22, no single technique has found the best solution for all of the problems presented. Table 22 lists the best technique for each of the nine problems investigated, with its TAC, plus the difference to the next best solution. It also compares each of the three interval-based techniques (SWS, IBMS and SBS) with the best solution. From Table 22 it appears that the SWS is best suited to smaller problems, whereas the SBS seems to perform better for larger problems.

Although this method assumes isothermal and iso-composition mixing of split streams at the interval boundaries, as in the SWS and IBMS, this does not appear to be a significant limitation in obtaining good solutions for the examples presented. The SBS has been shown to handle both HENS and MENS problem, including forbidden matches, problems with different heat transfer coefficients, and problems involving MSA regeneration.

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