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Supply and target based superstructure synthesis of heat and mass exchanger networks

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ABSTRACT

This paper presents new methods for the optimisation of superstructures involving heat exchanger networks (HENs) and mass exchanger networks (MENs). The techniques developed in this study explore the use of key variables (namely supply temperatures/compositions and target temperatures/compositions) in HENs and MENs to define the intervals of superstructures. Such superstructures are modeled as mixed integer non linear programmes (MINLP) with the objective of minimisation of the total annual cost (TAC) for each network. The superstructures presented in this paper are derivatives of the interval and supply based superstructures (IBMS and SBS) developed previously. Two different superstructures are developed in this paper: the first uses the supply temperature/composition of hot/rich streams and the target temperature/composition of cold/lean streams (denoted supply and target based superstructure, S&TBS), while the second superstructure uses the target temperature/composition of hot/rich streams and the supply temperature of cold/lean streams (denoted target and supply based superstructure, T&SBS). Five HEN examples and three MEN examples are presented. The results obtained compare well with those in the literature.

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Keywords: Heat exchanger networks; Mass exchanger networks; Superstructure; Total annual cost

1. Introduction

The tasks of synthesizing cost effective heat exchanger networks (HENs) and mass exchanger networks (MENs) have become key aspects of process synthesis. Heat exchanger network synthesis (HENS) has received much attention over the years. For example, Lee et al. (1970) formulated HENS problems using the branch and bound technique of Lawler and Wood (1966) with the aim of optimal energy exchange to obtain a network of minimum cost. In their formulation, no stream splitting was considered. The technique of Lee et al., though helped in the reduction of combinatorial difficulty in HENS, but the highest number of streams that has been solved in the literature by this technique is ten (Pho and Lapidus, 1973). Another shortcoming of the method of Lee et al. is the difficulty in obtaining cyclic structures; as such optimality cannot be guaranteed (Rathore and Power, 1975). Nishida et al. (1977) presented an algorithmic evolutionary synthesis method that appears to be more suitable for more sizable HENS problems but the approach is sequential.

Linnhoff and Flower (1978) presented a thermodynamically based temperature interval synthesis method from which the pinch concept for HENS developed. The method is premised on the basis that a cost effective network should exhibit a high degree of energy recovery. They subdivided their approach into two stages: in the first stage, a preliminary network that gives the highest possible energy recovery was generated, in the second stage; the preliminary network generated in the first stage served as the initial point to search for the most satisfactory network from the view points of cost, safety, and control, among other considerations.

In the application of pinch technology to process synthesis, the design requirement is that there should be no heat flow across the pinch. The first step is to determine the minimum energy consumption 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 subnetwork, using heuristics to evolve networks with minimum units. This may be compared with the annual capital cost (ACC) target obtained from the pinch

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Nomenclature**Sets**

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

Indices

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

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
AFC	area cost coefficient for heat exchangers
b	equilibrium line intercept
$C_{j,k}$	represents the existence of cold stream j in interval K (i.e. 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	starting location for cold streams in the superstructure
CE	ending location for cold streams in the superstructure
CU	cost per unit of cold utility
D	area cost index for heat/mass exchangers
$H_{i,k}$	represents the existence of hot stream i in interval K (between temperature interval boundaries k and k + 1)
HS	starting location for hot streams in the superstructure
HE	ending location for hot streams 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 boundaries k and k + 1)
$RST_{r,k}$	rich stream r start at composition interval boundary k
$RED_{r,k}$	rich stream r end at composition interval boundary k
$S_{l,k}$	existence of lean stream l in interval K (between composition interval boundaries k and k + 1)
$SST_{l,k}$	lean stream l start at composition interval boundary k

$SED_{l,k}$	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
$T_{Hi,k}^s$	Supply temperature of hot stream i at interval boundary k
$T_{Cj,k}^s$	Supply temperature of cold stream j at interval boundary k
$T_{Hi,k}^t$	Target temperature of hot stream i at interval boundary k
$T_{Ci,k}^t$	Target temperature of cold stream j at interval boundary k
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
$Y_{Ri,k}^s$	supply composition of rich stream r at interval boundary k
$Y_{Ri,k}^t$	target composition of rich stream r at interval boundary k
$Y_{Si,k}^{s*}$	equilibrium supply composition of lean stream l at interval boundary k
$Y_{Si,k}^{*t}$	equilibrium target composition of lean stream l at 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

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

Positive variables

dt_{ijk}	heat exchanger driving force for match i, j in temperature interval K
dy_{rlk}	mass 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}	mass exchanged between stream r and stream l in composition 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

curves (Linnhoff and Flower, 1978; Linnhoff and Hindmarsh, 1983). Other developments in pinch (thermodynamics) based HEN and other sequential techniques are contained in Nishida et al. (1977), Linhoff et al. (1979), Umeda et al. (1979), Linnhoff and Hindmarsh (1983), Linnhoff and Ahmad (1990), and Zhu et al. (1995). Some pinch related mathematical approaches in HENS have been presented by Papoulias and Grossmann (1983), Cerda et al. (1983), and Floudas et al. (1986).

MENS has received less attention than HENS. El-Halwagi and Manousiouthakis (1989) first applied the pinch concept of HENS to MENS for targeting the minimum mass separating agent (MSA) usage, while Hallale and Fraser (2000a,b) developed the y - y^* tool for capital cost targeting for MENS.

The shortcoming of the sequential pinch based technique (targeting followed by design) is the possibility of obtaining more than the minimum number of units which may lead to overestimation of the investment cost for the resulting network (Ciric and Floudas, 1990). Ciric and Floudas thus presented a pseudo-pinch formulation of the HEN with the aim of reducing the number of units in the heat exchanger network to the minimum. In this method, the assumption of no heat flow across the pinch was relaxed. Hallale and Fraser (2000a) demonstrated that for MENS, as opposed to HENS, a network with the minimum number of units does not necessarily lead to a minimum cost design. The approach of Ciric and Floudas is also sequential and Yee and Grossmann (1990) identified that a key shortcoming of the sequential techniques is that the different costs associated with the network design cannot be optimised simultaneously.

In order to overcome the shortcomings in pinch and pinch related techniques based HENS and MENS, different workers have adopted various simultaneous methods for HENS and MENS. For instance, the state space approach by Bagajewicz et al. (1998) and Martin and Manousiouthakis (2001), but, this approach can either give local optimum or the optimality only holds under the conditions that all the bypass streams and the recycle streams be set to zero at minimum TAC of the networks. Another approach that has been adopted is that of Evolutionary Algorithm (EA) as demonstrated by the Genetic Algorithm (GA) of Lewin (1998) and the differential evolution method (DEM) of Krishna and Murty (2007), even then, the EA approach can only guarantee local optimum, this is so since the DEM is only more likely to find the true optimum than the GA (Price and Storn, 1997).

An important development in process synthesis has been insight based superstructures for simultaneous optimisation of all the competing costs in HENS (Yee and Grossmann, 1990; Isafiade and Fraser, 2008a; Azeez et al., submitted for publication) and in MENS (Sztikai et al., 2006; Comeaux, 2000; Isafiade and Fraser, 2008b; Azeez et al., submitted for publication). Yee and Grossmann (1990) developed the stage-wise superstructure (SWS) for HENS, where the number of

stages was determined by the maximum of the number of hot or cold streams present in the synthesis task. Sztikai et al. (2006) used the key SWS idea of Yee and Grossmann (1990) to develop a similar superstructure for MENS. According to Sztikai et al., the number of stages in the superstructure can be set arbitrarily but in a manner that is large enough to accommodate the optimal structure. They thus suggested adding the number of rich and lean streams in the synthesis task to set the maximum number of stages in the superstructure, for moderate numbers of streams. Emhamed et al. (2007) used a hybrid method for the optimisation of mass exchange networks with an idea that involves the use of integer cuts and bounds to the lean stream to exclude non optimal solutions as an improvement of the MINLP model of Sztikai et al., but the approach of Emhamed et al., cannot guarantee global optimality.

Isafiade and Fraser (2008a) developed the interval based mixed integer non linear programming (MINLP) superstructure (IBMS) for HENS using either the supply and target temperatures of hot streams in a hot based superstructure or the supply and target temperatures of cold streams in a cold based superstructure. These authors also developed the mass exchange analogue of the IBMS for MENS (Isafiade and Fraser, 2008b). Subsequently, Azeez et al. (submitted for publication) presented the supply based superstructure (SBS) approach for both HENS and MENS, where the superstructure interval boundaries were defined using the supply temperatures of both the hot/rich and the cold/lean streams.

The SWS technique and its derivatives, the IBMS and the SBS technique all allow for splitting of streams within an interval, followed by isothermal mixing. None of these techniques allows for stream bypasses, nor for series exchange of split streams. The SWS of Yee and Grossmann (1990) is similar to the spaghetti design of pinch technology. In spaghetti design, the number of stages and enthalpy intervals are necessarily equal, but in SWS, the number of stages is selected as the maximum of the number of hot or cold streams present. It should be noted that Sztikai et al. (2006) observed that, in their implementation of the SWS for MENS, using the sum of the numbers of rich and lean streams led to more optimal solutions. This is in support of what Shenoy (1995) pointed out, that more stages are necessary for more combinations of stream matches. The IBMS and SBS techniques, and the techniques presented in this study, all use more intervals than the SWS.

2. Problem statements

2.1. HENS

Given a number, N_H of hot and N_C of 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 in addition are the heat capacity flowrates, supply and target temperatures and heat transfer coefficients of each process stream. Existing for service are heating and cooling utilities whose costs, supply temperatures, target temperatures and heat transfer coefficients are also known, given also are the 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 lean streams (MSAs), the task is to synthesize a network of mass exchangers that can preferentially relocate certain species from the rich streams to the MSAs so as to achieve a minimum total annual cost network. Available also are the flowrate of each rich stream and the supply and target compositions. Furthermore, the supply and target compositions for each MSA together with the mass transfer equilibrium relations are as well given for each MSA. The flowrate of each MSA is to be determined (unknown) as part of the synthesis task. Given also are the annual operating time, sizing and cost information of mass exchanger and the annual capital cost.

The candidate MSAs can be grouped as process and external MSAs. The process MSAs are available free, being on site. Nevertheless, the quantity of each process MSA that can be used in mass exchange process is subject to its availability on site. The external MSAs on the other hand can be purchased from the market and their flowrates shall be determined based on economic considerations.

3. Motivation

It would appear that the number of intervals used and the way they are partitioned does have an impact on the minimum TACs that have been obtained so far by various techniques, as indicated at the end of Section 1. It would appear that there is an inherent limitation of the solution space that occurs with any partitioning that is imposed on a problem. What is not clear is how problem-specific this limitation is, and to what extent the fact that the solvers used may have found local optima plays a part. The objective of this study is to explore whether a different partitioning technique could lead to consistently better results.

Temperatures of streams in HENS have been used over the years by various workers in partitioning the superstructure to achieve various objectives. One of the foremost is the Linear Programming (LP) and Mixed Integer Linear Programming transshipment model of Papoulias and Grossmann (1983) where supply temperatures of streams were used to partition a superstructure for the determination of utility cost and number of heat exchanger units. Even though the transshipment model derived its basis from the pinch technique, many other workers have based their models on the concept of the transshipment model for the synthesis of HENS. Examples include the NLP model of Floudas et al. (1986) for the generation of HENS with minimum investment cost and the NLP model of Colberg and Morari (1990) for the determination of minimum area required for a specified energy target. Other approaches that have used temperature partitioning include the following: the simultaneous-match pseudo pinch approach of Ciric and Floudas (1990), the MINLP model for simultaneous optimisation of utility consumption and stream matches of Ciric and Floudas (1991) and the interval based mixed integer non-linear programming (IBMS) of Isafiade and Fraser (2008a,b).

These temperature-based partitioning approaches guarantee feasible heat transfer in heat exchange network intervals (Papoulias and Grossmann, 1983). The present authors observed that in all the above transshipment-based models and other simultaneous optimisation techniques, none has exploited the use of a combination of either the sup-

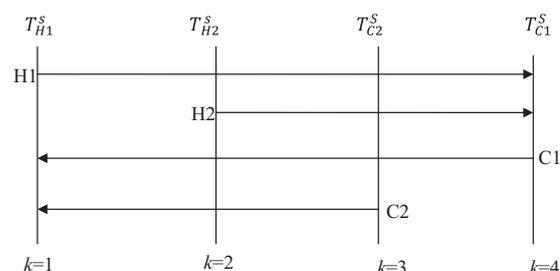


Fig. 1 – Grid representation of the superstructure for two hot and two cold streams.

ply temperatures of hot streams and target temperatures of cold streams or the target temperatures of hot streams and the supply temperatures of cold streams or the target temperatures of hot streams and the target temperatures of cold streams in HENS to develop superstructures that can optimise all the competing costs in HENS in a single step using MINLP. A similar observation may be made concerning MENS superstructures.

In the SBS of Azeez et al. (submitted for publication) supply temperatures/compositions of streams were used to define the interval partitioning of the superstructure. Each of the streams originates from its supply temperature/composition, and the hot/rich streams end at the last temperature interval boundary of the superstructure, while the cold/lean streams end at the first interval boundary of the superstructure. The HEN grid diagram of the SBS showing two hot streams (H1 and H2) and two cold streams (C1 and C2) is shown in Fig. 1, with the temperature decreasing from left to right along the superstructure. In Fig. 1, the supply temperature T_{H1}^s of H1 is higher than the supply temperature T_{H2}^s of H2 while the supply temperature T_{C2}^s of C2 is higher than that of C1, T_{C1}^s but lower than that of H2. In the SBS, both the process streams and the utilities are treated as process streams and all the streams fall within the superstructure as shown in Fig. 1. The superstructure was modeled as an MINLP for simultaneous optimisation of all the competing costs in HENS. An analogous structure exists for MENS (Azeez et al., submitted for publication).

This study presents three new ways of defining the superstructure partitioning and compares the effect on the total annual cost in both HENS and MENS. In a similar manner to the SBS, the superstructures presented in this study treat both streams and utilities as process streams.

Conceptual consideration of the SBS led to the realisation that any combination of supply and target temperatures/compositions could conceivably be used to define the boundaries of the intervals in the superstructure. This results in four possible combinations:

- Supply temperatures/compositions for the hot/rich streams and supply temperatures/compositions for the cold/lean streams (as in the SBS).
- Supply temperatures/compositions for the hot/rich streams and target temperatures/compositions for the cold/lean streams (a supply and target based superstructure, S&TBS).
- Target temperatures/compositions for the hot/rich streams and supply temperatures/compositions for the cold/lean streams (a target and supply based superstructure, T&SBS).
- Target temperatures/compositions for both sets of streams (a target based superstructure, TBS).

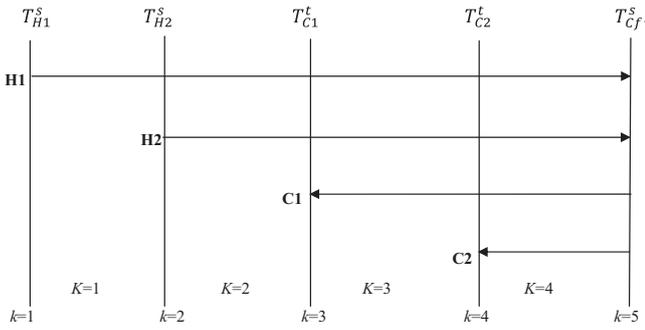


Fig. 2 – Grid diagram of a supply and target based superstructure (S&TBS) for two hot and two cold streams.

Each of the three new options will be examined in turn. Note that in all three cases one or more additional boundaries are introduced in order to create an interval or intervals at the extremes in order to cover all the possible stream conditions in the superstructure.

3.1. Supply and target based superstructure (S&TBS)

The first approach considered in this paper is the use of the supply temperatures of hot streams and the target temperatures of cold streams to define the interval boundaries of a HEN superstructure. The grid diagram in Fig. 2 shows two hot streams and two cold streams with the hot streams (H1 and H2) running between the interval boundaries that correspond to their respective supply temperatures (T_{H1}^s, T_{H2}^s) and the last (additional) interval boundary in the superstructure T_{Cf}^s while the cold streams (C1 and C2) run between the last (additional) interval boundary T_{Cf}^s and the interval boundaries that correspond to their respective target temperatures (T_{C1}^t, T_{C2}^t).

The combined set of the supply temperatures of the hot streams and the target temperatures of the cold streams are sorted in descending order, with only one value retained for any that are repeated. The resulting list defines the temperature interval boundaries in the superstructure, as shown in Fig. 2 for a HENS problem. Unlike in the SBS, where all the temperatures/compositions of the synthesis task automatically fall within the superstructure, there is the need to use the lowest supply temperature/composition of the cold/lean streams (which usually is the supply temperature/composition of the cold utility/external mass separating agent (MSA)) to define the last interval boundary in the superstructure. This is to ensure that all temperatures/compositions in the synthesis task fall within the superstructure. Thus, the last temperature boundary in S&TBS is an additional interval boundary. The exchange of heat between hot/rich streams and cold/lean streams in an interval within the superstructure is subject to the presence of such streams in that interval and to thermodynamic feasibility. An analogous structure to Fig. 2 represents the MENS counterpart.

Hot stream 1 can exchange heat in all intervals while hot stream 2 can exchange heat in all intervals except interval 1 (note that neither of them can exchange heat in either interval 1 or interval 2 because there are no cold streams in these intervals). Cold stream 1 cannot exchange heat in intervals 1 and 2 while cold stream 2 can only exchange heat in the last interval.

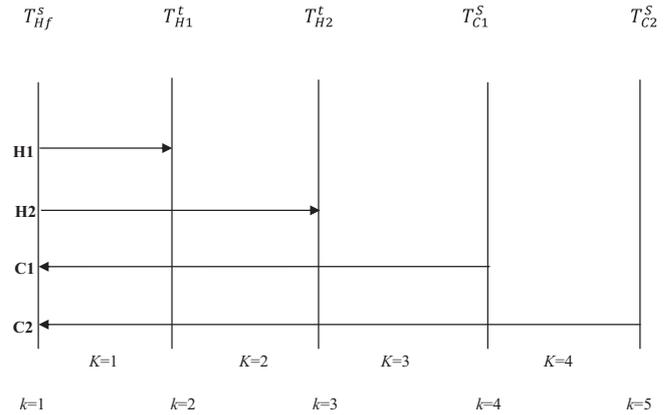


Fig. 3 – Grid diagram of a target and supply based superstructure (T&SBS) for two hot and two cold streams.

3.2. Target and supply based superstructure (T&SBS)

In the second approach, the target temperatures/compositions of hot streams and the supply temperatures/compositions of cold streams are used to define the interval boundaries of the superstructure. The grid diagram in Fig. 3 shows two hot streams and two cold streams in the superstructure. In the superstructure, the hot streams (H1, H2) run between the first (additional) temperature interval boundary T_{Hf}^s and the interval boundaries that correspond to their respective target temperatures (T_{H1}^t, T_{H2}^t) while the cold streams run between the interval boundaries that correspond to their supply temperatures and the additional interval boundary. The way Fig. 3 is set up is analogous to Fig. 2.

3.3. Target based superstructure (TBS)

The definition of a superstructure using the target temperatures/compositions of the hot/rich streams and the target temperatures/compositions of the cold/lean streams seems not to be feasible. This is because of the restriction imposed by the intervals defined by target values of all streams even when two additional interval boundaries are created to ensure that all available hot and cold stream conditions in the synthesis task fall within the superstructure. This is shown in Fig. 4, where it may be observed that heat exchange is only possible in interval 3, thus showing that such a structure cannot meet the energy requirements of all the streams.

Given that the TBS superstructure is not feasible, this paper will now consider the application of the S&TBS and

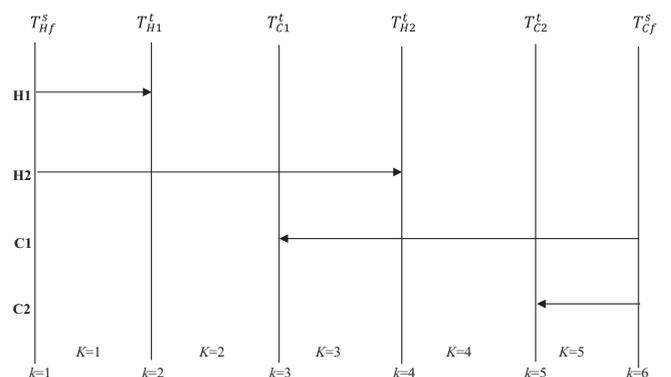


Fig. 4 – Grid diagram of a target based superstructure (TBS) for two hot and two cold streams.

Table 1 – Characteristics of the HENS superstructures.

SWS of Yee and Grossmann (1990)	IBMS of Isafiade and Fraser (2008a)	SBS of Azeez et al. (submitted for publication)	S&TBS of this paper	T&SBS of this paper
Numbers of intervals (stages) depend on maximum of the number of hot streams or the number of cold streams.	Numbers of intervals depend on the values of supply and target temperatures of either the hot streams or the cold streams (this normally gives more intervals than SWS).	Numbers of intervals depend on the supply temperatures of both the hot streams and the cold streams (this also normally gives more intervals than SWS).	Number of intervals depend on the supply temperatures of hot streams and target temperatures of cold streams (this also normally gives more intervals than SWS).	Number of intervals depend on the target temperatures of hot streams and supply temperatures of cold streams (this also normally gives more intervals than SWS).
The boundaries fixed are the first and last: the first one being where the hot streams start and the cold streams end, whereas the last one is where the hot streams end and cold streams start.	Interval boundaries are determined by the supply and target temperatures of either the hot streams or the cold streams.	Interval boundaries are determined by the supply temperatures of the hot streams and the cold streams.	Interval boundaries are determined by the supply temperatures of the hot streams and the target temperatures of the cold streams.	Interval boundaries are determined by the target temperatures of the hot streams and the supply temperatures of the cold streams.
Every stream exists across all the intervals.	The hot streams exist in all the intervals between their supply and target temperatures in a hot based superstructure, while the cold streams exist across all the intervals. Converse is the case in a cold-based superstructure.	The hot streams exist across all intervals defined by temperatures lower than their supply temperatures. The cold streams exist across all intervals defined by temperatures higher than their supply temperature.	Hot stream existence across intervals is as in SBS. Cold streams exist across all intervals at temperatures lower than their target values.	Hot streams exist across intervals at temperatures higher than the target values. Cold streams existence across intervals is as in SBS.
Thermal exchange between each hot stream and each cold stream is feasible in all the stages of the superstructure.	Thermal exchange by each hot stream is feasible only in those intervals created by the supply and target values of that hot stream in a hot-based superstructure; the same goes for each cold stream in a cold-based superstructure.	Thermal exchange by each hot stream is possible in all intervals except those intervals with higher temperature values than the supply temperature of such stream; thermal exchange by each cold stream is possible in all intervals except intervals with lower temperature values than the supply temperature of such stream.	Thermal exchange by each hot stream is same as in SBS; exchange of heat by each cold stream is possible in all intervals except those intervals with higher temperature values than the target temperature of that stream.	Thermal exchange by each hot stream is possible in all intervals except those intervals with lower temperature values than the target temperature of that stream; exchange of heat by each cold stream is as in SBS.
MINLP model formulation but includes NLP sub optimisation step.	MINLP model formulation.	Same as IBMS.	Same as IBMS.	Same as IBMS.
Splitting and isothermal mixing of stream is possible in every stage of the superstructure.	Splitting and isothermal mixing of streams is possible in every interval created in the superstructure.	Same as IBMS.	Same as IBMS.	Same as IBMS.

T&SBS superstructures to the solution of HENS and MENS problems. Detailed comparisons of the characteristics of the various HENS and MENS superstructures are presented in Tables 1 and 2 respectively, in terms of how the number of intervals is determined, how the boundaries of the intervals are specified, the possibility of exchange in the various intervals, the existence of streams in the various intervals, the model formulation, and how stream splitting and mixing are handled.

4. Advantages of the new superstructures

In the superstructures presented in this study, the utilities in HENS are treated as process streams, and so are the external lean streams in MENS. This has the advantage that both process and external lean streams are considered simultaneously.

Moreover, in a similar manner to the SWS technique and its derivatives, as well as the IBMS and the SBS techniques,

Table 2 – Characteristics of MENS superstructures.

'SWS' of Szitkai et al. (2006)	NLP of Comeaux (2000)	IBMS of Isafiade and Fraser (2008b)	SBS of Azeez et al. (submitted for publication)	S&TBS of this paper	T&SBS of this paper
Number of intervals (stages) can be defined arbitrarily or by the sum of number of rich streams and lean streams.	Numbers of intervals depend on the values of supply and target compositions of the rich streams and equilibrium equivalent of the lean streams.	Numbers of intervals depend on the values of supply and target compositions of either the rich streams or the lean streams (this normally gives more intervals than SWS).	Numbers of intervals depend on the values of supply compositions of both the rich streams and the lean streams (this also normally gives more intervals than SWS).	Numbers of intervals depend on the values of supply compositions of the rich streams and the target composition of the lean streams.	Numbers of intervals depend on the values of the target compositions of rich streams and the supply composition of lean streams.
The boundaries fixed are the first and last: the first one being where the rich streams start and the lean streams end, whereas the last one is where the rich streams end and lean streams start.	Interval boundaries are fixed between supply and target compositions, but the target is extended for lean streams.	Interval boundaries are determined by the supply and target compositions of either the rich streams or the lean streams.	Interval boundaries are determined by the supply compositions of the rich streams and the lean streams.	Interval boundaries are determined by the supply compositions of the rich streams and the target compositions of the lean streams.	Interval boundaries are determined by the target compositions of the rich streams and the supply compositions of the lean streams.
The target compositions of rich streams are fixed at the last interval location while those of lean streams are fixed at the first interval locations in the superstructure.	The target composition of each rich stream is set at the interval defined by its target value while the target of each lean stream is extended to match at least once with each rich stream.	The supply and target compositions of rich streams are as in SWS in a lean based superstructure and likewise for lean streams in a rich based superstructure.	The target compositions of all the rich and the lean streams are as in SWS.	The target compositions of the rich and the lean streams are as in SWS.	The target compositions of the rich and the lean streams are as in SWS.
Every stream exists across all the intervals.	Every stream exists between the supply and extended target composition values of rich and lean stream respectively in the superstructure.	The rich streams exist in the intervals between their supply and target compositions values. In a rich-based superstructure, while the lean streams exist across all the intervals. Converse is the case in a lean-based superstructure.	Rich streams existence is across all intervals at compositions lower than their supply composition. Lean streams existence is across all intervals at compositions higher than their supply composition.	Rich streams exist across all intervals as in the SBS. Lean streams exist across all intervals at compositions lower than their target compositions.	Rich streams exist across all intervals at compositions higher than their target composition. Lean streams exist across all intervals as in SBS.
Mass exchange between rich and lean streams is feasible in all stages of the superstructure.	Extension of lean stream is used to ensure a match at least with each rich stream in the superstructure.	Mass exchange by a rich stream is feasible only between the intervals defined by the supply and target values of such stream in a rich based superstructure. The same goes for a lean in a lean based superstructure (reduced opportunity for mass exchange within intervals than SWS).	Mass exchange with a stream is feasible in all intervals except those intervals with lower composition values than the supply composition of such stream, (more opportunity for mass exchange within intervals than IBMS).	Exchange of mass by a rich stream is as in SBS but for a lean stream, it is possible in all intervals except those intervals with higher composition values than its target composition value.	Exchange of mass by a stream is possible in all intervals except those intervals with lower composition values than the target composition of such stream. Exchange of mass by a lean stream is as in SBS.

– Table 2 (Continued)

'SWS' of Szitkai et al. (2006)	NLP of Comeaux (2000)	IBMS of Isafiade and Fraser (2008b)	SBS of Azeez et al. (submitted for publication)	S&TBS of this paper	T&SBS of this paper
The existence or otherwise of matches in the superstructure model are checked using binary variables.	Branch flow rates are used to determine existence of matches rather than binary variables.	Same as SWS.	Same as SWS.	Same as SWS.	Same as SWS.
MINLP model formulation but NLP sub optimisation step usually required.	NLP model formulation.	MINLP model formulation.	Same as IBMS.	Same as IBMS.	Same as IBMS.
Splitting and iso-composition mixing of streams is possible in every stage in the superstructure.	Splitting and mixing of a rich stream is possible only between the intervals created by supply and target of such stream. The converse goes for the lean stream.	Splitting and iso-composition mixing of stream is possible in any interval where a stream exists.	Same as IBMS.	Same as IBMS.	Same as IBMS.

the present superstructures assume isothermal mixing at the boundary junctions in HENS and MENS to be able to do away with non linear heat/mass balances at these junctions. It should be noted that the conception of the SWS of Yee and Grossmann (1990) is similar to a spaghetti design, but using a much smaller number of intervals: in spaghetti design the number of stages and enthalpy intervals are necessarily the same, but in SWS, the number of stages is usually the larger of the number of hot streams or cold streams. The present study incorporates a larger number of intervals than the SWS, which allows for more combinations of stream matches, as pointed out by Shenoy (1995).

The superstructures presented in this study offer the following advantages that also feature in the SWS, IBMS and SBS techniques:

- Different utilities in HENS at different temperature levels and costs as well as different external MSAs in MENS at different composition levels and costs are simultaneously considered in HEN and MEN superstructures respectively. This is especially significant because the pinch approach does not take minimum TACs into consideration for multiple utilities in HENS and multiple external MSAs in MENS.
- Simultaneous minimization of TAC in HENS and MENS.

5. S&TBS and T&SBS model equations for HENS

In this section the model equations for S&TBS and T&SBS are laid out. These include the balance equation, the objective function and stream existence conditionals.

5.1. Assignment of superstructure interval boundary temperatures in S&TBS and T&SBS

In Fig. 2, the interval boundary temperatures in S&TBS are respecified as follows (the lower case symbols represent opti-

misation variables):

$$k = 1; \quad T_{H1,1}^s \quad (1a)$$

$$k = 2; \quad T_{H2,2}^s, t_{H1,2} \quad (1b)$$

$$k = 3; \quad T_{C1,3}^t, t_{H1,3}, t_{H2,3} \quad (1c)$$

$$k = 4; \quad T_{C2,4}^t, t_{H1,4}, t_{H2,4}, t_{C1,4} \quad (1d)$$

$$k = 5; \quad T_{H1,5}^t, T_{H2,5}^t, T_{C1,5}^s, T_{C2,5}^s \quad (1e)$$

Similarly, in Fig. 3, the interval boundary temperatures in T&SBS are specified as follows:

$$k = 1; \quad T_{Hf,1}^s, T_{H1,1}^s, T_{H2,1}^s, T_{C1,1}^t, T_{C2,1}^t \quad (2a)$$

$$k = 2; \quad T_{H1,2}^t, t_{H2,2}, t_{C1,2}, t_{C2,2} \quad (2b)$$

$$k = 3; \quad T_{H2,3}^t, t_{C1,3}, t_{C2,3} \quad (2c)$$

$$k = 4; \quad T_{C1,4}^s, t_{C2,4} \quad (2d)$$

$$k = 5; \quad T_{C2,5}^s \quad (2e)$$

5.2. First set of stream existence conditionals in S&TBS

In order to select the set of intervals where each stream can exchange heat, the following set of conditionals should be used:

$$H_{i,k} \Phi(T_i^s \geq T_k) = 1 \quad (3a)$$

$$C_{j,k} \Phi(T_j^s \leq T_k) = 1 \quad (3b)$$

The superstructures with the above conditionals are labelled S&TBS Type 1. In S&TBS Type 2, the first conditional (for hot

streams) is the same as in Type 1 but the second conditional is stated as follows:

$$C_{j,k} \$(T_j^t \geq T_k) = 1 \quad (3c)$$

5.3. First set of stream existence conditionals in T&SBS

This superstructure works with the following stream existence conditionals: a hot stream should be considered for matching in an interval K (between the boundaries k and $k+1$) if its target temperature is less than or equal to the interval boundary that starts that interval (i.e. boundary k), while a cold stream is to be considered for matching in an interval K (between the boundaries k and $k+1$) if its supply temperature is less than or equal to the temperature interval boundary k that begins the interval.

$$H_{i,k} \$(T_i^t \leq T_k) = 1 \quad (4a)$$

$$C_{j,k} \$(T_j^s \leq T_k) = 1 \quad (4b)$$

5.4. Second set of stream existence conditionals in S&TBS and T&SBS

The second set are the stream existence conditionals for each type of superstructure, they consists of the stream supply temperature conditionals that identify the supply or target temperatures of the set of streams which define the interval boundaries in each type of the superstructure. They are mathematically stated as follows:

$$HS_{i,k} \$(T_i^s = T_k) = 1 \quad (5a)$$

$$HE_{i,k} \$(T_i^t = T_k) = 1 \quad (5b)$$

$$CS_{j,k} \$(T_j^s = T_k) = 1 \quad (5c)$$

$$CE_{j,k} \$(T_j^t = T_k) = 1 \quad (5d)$$

5.5. Overall stream heat balance equations in S&TBS and T&SBS

The sum of heat exchanged by each stream over all matches in the intervals where heat exchange takes place must equal the total heat load of that stream as shown in Eqs. (6) and (7) for hot stream i and cold stream j respectively.

$$(T_i^s - T_i^t)F_i = \sum_{j \in C} \sum_{k \in K} q_{ijk}, \quad i \in H \quad (6)$$

$$(T_j^t - T_j^s)F_j = \sum_{i \in H} \sum_{k \in K} q_{ijk}, \quad j \in C \quad (7)$$

The stream heat capacity flowrate F is modeled as a parameter for the process streams but as a variable in the case of utility streams.

5.6. Interval heat balance equations

The heat exchanged between hot stream i and cold stream j in interval K is calculated using the interval heat balance

equations for streams i and j respectively in Eqs. (8) and (9):

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

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

5.7. Temperature feasibility along the superstructures

Temperatures of hot streams decrease from left to right along the superstructure whereas cold stream temperatures increase from right to left. This is achieved using the feasibility constraints shown in Eqs. (10) and (11).

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

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

5.8. 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 . $Z_{i,j,k}$ has a value of '1' if match i,j exists in interval K and a value of '0' if otherwise. The thermal exchange between streams i and j is constrained to the smaller of the heat duties of the two streams involved in the match via the parameter Ω_H :

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

5.9. 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 the heat exchanger driving forces computations which are in turn used to calculate heat exchanger areas, as shown in Eqs. (13) and (14).

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

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

In order to avoid numerical errors that can arise due to negative temperature differences for matches that do not occur, the parameter Γ_H is put at the maximum of zero and the temperature differences between the hot and the cold streams involved in the match (Shenoy, 1995).

An exchanger minimum approach temperature (EMAT) is included in the model to avoid inclusion of exchangers of infinite areas in the model as shown in Eq. (15):

$$dt_{ijk} \geq \delta \quad (15)$$

where δ is a small positive number.

5.10. Objective function

As in other work, the objective function to be minimized in this study is the TAC of the network. The capital cost of each exchanger is the sum of a fixed cost and an area cost as shown

in the expression for TAC in Eq. (16).

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

Chen's first approximation is used (Chen, 1987) to avoid singularity problem when calculating the logarithmic mean temperature difference, LMTD, in Eq. (16) if the driving forces are equal.

$$LMTD_{ijk} = \left[\frac{(dt_{ijk})(dt_{ijk+1})(dt_{ijk} + dt_{ijk+1})}{2} \right]^{1/3} \quad (17)$$

This approximation has been used for comparison with other results which are based on it, rather than a more accurate approximation such as Chen's second approximation or that of Paterson (1984). The SBS of Azeez et al. (submitted for publication) compares the errors of the different log-mean approximations over a range of $\Delta T_2/\Delta T_1$ between 1.0 and 10.0 (Underwood, 1970; Paterson, 1984; Chen, 1987). Though Chen did not give errors for his two approximations, 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) noted that Chen's second approximation was somewhat less accurate than Underwood's at a ratio of 1.5, but much more accurate around 10.0, details are contained in Shenoy and Fraser (2003). Azeez et al. (submitted for publication) show that Chen's second approximation is not as good as Underwood's below a ratio of 5.0, but a bit better from 5.0 upwards. Chen's first approximation is worse than all the other approximations at ratios above 2.0.

5.11. Solution and initialisation

The S&TBS and T&SBS are modeled as MINLPs with the objective function being the minimum TAC. The models presented in this paper have 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, as done for the SBS. Solution times were of the order of seconds on a PC with a Pentium Dual CPU running at 1.73 GHz with 2 GB of memory.

The initialisation of the model is done through the use of the exchanger minimum approach temperature (EMAT) in HENS. Upper bounds are set for heat capacity flow rates of hot and cold utilities in HENS and external MSAs in MENS. The solutions obtained gave results which are reasonably close to those in the literature, as will be shown in the examples that follow.

6. HENS examples

6.1. Example 1 (4SP1)

This is the 4SP1 problem with two hot streams, two cold streams, one hot utility (steam) and one cold utility (water) taken from Lee et al. (1970). The stream and cost data are shown in Table 3. The workers that have solved this problem, the methods adopted, network costs and characteristics are

Table 3 – Stream and capital cost data for Example 1, from Lee et al. (1970).

Stream	T^s (°F)	T^t (°F)	F (Btu/(h °F))
H1	320	200	16,666.8
H2	480	280	20,000
C1	140	320	14,450.1
C2	240	500	11,530
S1	540	540	–
W1	100	180	–

Hot utility (S1) cost = 12.76 (\$/year)/(kBtu/h), cold utility (W1) cost = 5.24 (\$/yr)/(kBtu/h), heat exchanger annual cost = \$35(A)^{0.6} (A in ft²), U = 150 Btu/(h ft² °F) for all matches apart from those involving steam where U = 200 Btu/(h ft² °F).

shown in Table 4. The supply and target based superstructure (S&TBS) and the target and supply based superstructure (T&SBS) were applied to this problem and the results compared well with those of previous workers as shown in Table 4 where all the methods generated solutions involving five units each. Note that Table 4 and all subsequent results tables are arranged in descending order of TAC for ease of comparison.

The network structure obtained for S&TBS Type 1 is shown in Fig. 5 (for each example only the best network is shown). The two S&TBS networks, in a manner similar to SBS, have five intervals with a split of one of the hot streams (H1 for Type 1 and H2 for Type 2), while the T&SBS network has six intervals with splits of both hot streams.

6.2. Example 2 (Shenoy, 1995)

This problem where the heat transfer coefficients are equal for all streams is the 4S1 Example of Shenoy (1995). It involves two hot streams, two cold streams, a hot and a cold utility. The SWS of Yee and Grossmann (1990) with the Paterson (1984) approximation for LMTD was employed by Shenoy (1995) to solve the problem for minimum TAC. The stream and cost data are shown in Table 5.

The network characteristics of the solutions as presented by various workers and the present studies are as presented in Table 6. The splits occur in H2 and C2 in SBS and SWS, while in IBMS, it occurs in H2 and C1 in the hot base and in H2, C1 and C2 in the cold base. The Type 1 and Type 2 of S&TBS have basically the same structure as shown in Fig. 6 with TAC of 235,781\$/year each, while the T&SBS has a TAC of 235,781\$/year. The S&TBS is split in two ways i.e. H2 and C2 while T&SBS is split in three ways, i.e. H2, C1 and C2. The splits in H2 in all the superstructures is due to its largest heat content, while the largest energy demand stream C1 exchanges heat with hot utility and H2 in all the superstructures.

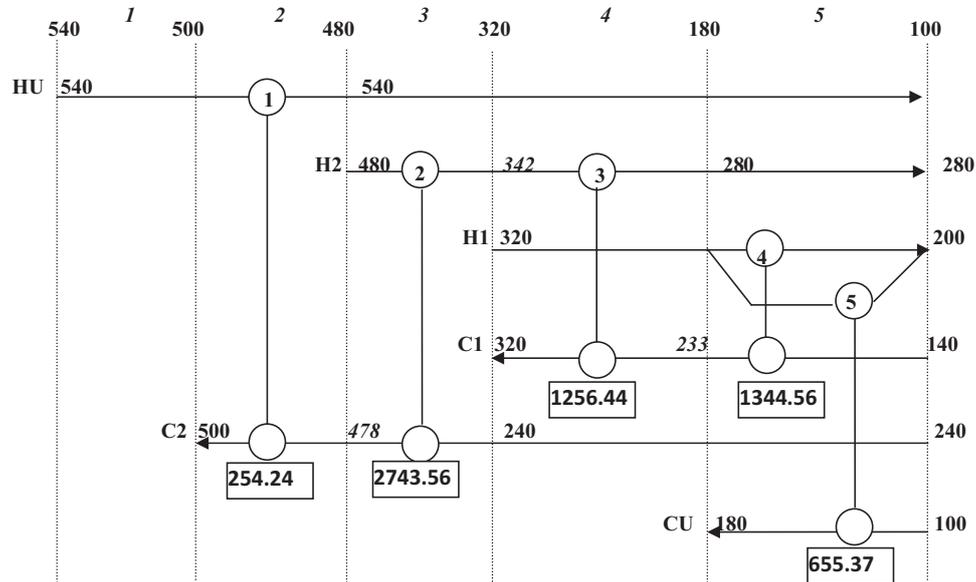
6.3. Example 3 (Linnhoff et al., 1982)

This an example of Linnhoff et al. (1982) that involves two hot streams, two cold streams, along with steam and cooling water as utilities. The stream and cost data are shown in Table 7. The SWS of Yee and Grossmann (1990) fixed two stages for this problem to obtain a TAC of \$80,274/year using DICOPT++ in GAMS (Brooke et al., 1988). The TAC as obtained by different sets of workers are as shown in Table 8. The T&SBS network structure obtained by the present study is shown in Fig. 7. Note that Yee and Grossmann used a subsequent non-linear optimisation step to obtain their solution.

Table 4 – Comparison of results for Example 1.

Method	ΔT_{\min} ($^{\circ}\text{F}$)	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
Tree structure technique of Ponto and Donaldson (1974)	–	–	–	13,534	27.92
Branch and bound method of Lee et al. (1970)	18	0	5	13,481	27.42
T&SBS	0.5	2	5	11,204	5.90
S&TBS (Type 2)	1.6	1	5	10,795	2.03
SBS of Azeez et al. (submitted for publication)	1.9	1	5	10,794	2.02
S&TBS (Type 1)	0.9	1	5	10,786	1.95
DEM of Krishna and Murty (2007)	2.1	0	5	10,782	1.91
Mathematical optimisation 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 that this TAC was calculated by Bagajewicz et al. (1998).

**Fig. 5 – The S&TBS (Type 1) network structure for Example 1 featuring five units with a TAC of \$10,786.****Table 5 – Stream and cost data for Example 2 (Shenoy, 1995).**

Stream	T^s ($^{\circ}\text{C}$)	T^t ($^{\circ}\text{C}$)	F ($\text{kW}^{\circ}\text{C}^{-1}$)	h ($\text{kW m}^{-2} \text{ }^{\circ}\text{C}^{-1}$)	Cost ($\text{\$ kW}^{-1} \text{ year}^{-1}$)
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

Annualisation factor = 0.322.

Capital cost = $\text{\$}30,000 + 750(A)^{0.81}$ for all exchangers (A in m^2).

Table 6 – Cost comparison for Example 2.

Method	Stream splits	No. of intervals	No. of units	TAC(\$/year)	Difference (%)
T&SBS	3	6	6	240,253	2.06
Cold stream based IBMS of Isafiade and Fraser (2008b)	3	5	6	239,332	1.67
Hot stream based IBMS of Isafiade and Fraser (2008b)	2	5	6	237,800	1.02
SBS of Azeez et al. (submitted for publication)	2	5	6	235,931	0.20
S&TBS (Type 1)	2	6	6	235,781	0.16
S&TBS (Type 2)	2	6	6	235,781	0.16
SWS of Yee and Grossmann (1990)	2	2	6	235,400	0.00

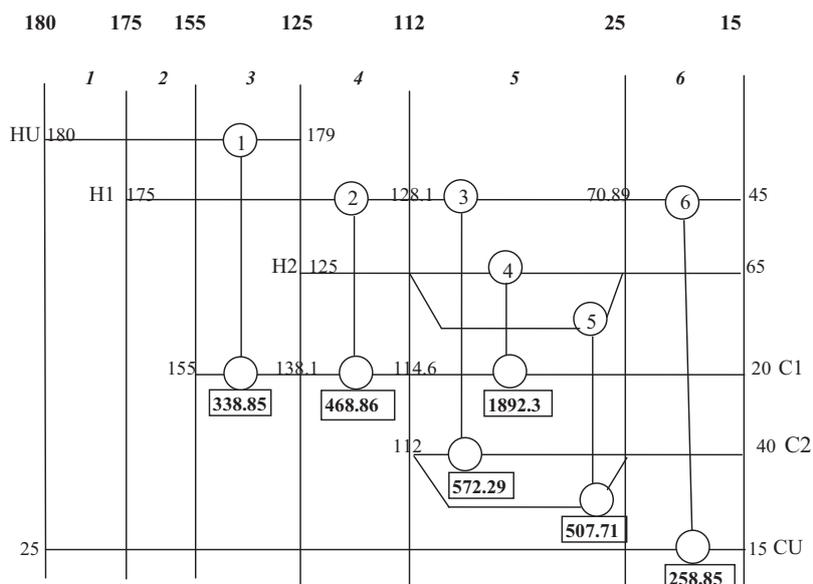


Fig. 6 – Network structure of S&TBS (Types 1 and 2) for Example 2 featuring six units with TAC of \$235,781.

Table 7 – Stream and cost data for Example 3 (Yee and Grossmann, 1990).

Stream	T^s (K)	T^t (K)	F (kW K ⁻¹)	Cost (\$kW ⁻¹ year ⁻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

$U = 0.8 \text{ kW m}^{-2} \text{ K}^{-1}$ for all matches except those involving steam.

$U = 1.2 \text{ kW m}^{-2} \text{ K}^{-1}$ for matches involving steam.

Heat exchanger annual cost = \$1000(A)^{0.6} (A in m²).

Table 8 – Cost comparison for Example 3.

Method	Stream splits	No. of units	TAC (\$/year)	Difference (%)
S&TBS (Type 1)	1	5	93,391	16.34
S&TBS (Type 2)	1	5	90,672	12.95
SBS of Azeez et al. (submitted for publication)	2	7	90,521	12.77
Magnets Solution of Grossman (1985)		6	89,832	11.91
Pinch technique of Linnhoff et al. (1982)		7	89,832	11.91
T&SBS	2	6	87,611	9.13
SWS of Yee and Grossmann (1990)	2	5	80,274	0.00

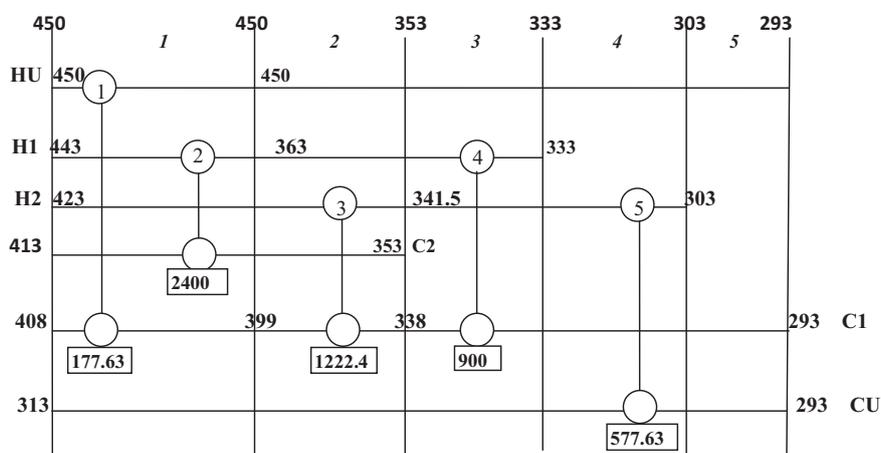


Fig. 7 – T&SBS network structure for Example 3 featuring five units with TAC of 87,611\$/year.

Table 9 – Stream data for Example 4, from Yee and Grossmann (1990).

Stream	T^s (K)	T^t (K)	F (kW K^{-1})	Cost ($\text{\$ kW}^{-1} \text{ year}^{-1}$)
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 ($\text{kW m}^{-2} \text{ K}^{-1}$) = 1 for all matches, heat exchanger annual cost = $\$1200(A)^{0.6}$ for all exchangers (A in m^2).

Table 10 – Comparison of results for Example 4.

Method	No. of intervals	Stream splits	No. of units	Cost ($\text{\$/year}$)	Difference (%)
Cold stream based IBMS of (2008)	3	1	7	595,064	3.81
T&SBS of this study	6	1	7	581,954	1.53
Hot stream based IBMS of Isafiade and Fraser (2008b)	7	1	7	581,942	1.52
S&TBS (Type 1)	7	1	7	581,942	1.52
SBS of Azeez et al. (submitted for publication)	6	1	8	580,023	1.19
S&TBS (Type 2)	7	1	10	577,602	0.77
SWS of Yee and Grossmann (1990)	5	1	7	576,640	0.60
GA of Lewin (1998)	–	2	9	573,205	0.00

6.4. Example 4 (magnets problem)

This example was taken from the Magnets User Manual and used for the analysis of the SWS method by Yee and Grossmann (1990) for cases that required stream splits. It involves five hot streams, one large cold stream, one hot utility (steam) and one cold utility (cooling water). The stream and cost data are shown in Table 9. The problem was solved in anticipation of many splits which is reflected in the solutions as solved by different sets of workers (Yee and Grossmann, 1990; Isafiade and Fraser, 2008a; Azeez et al., submitted for publication). The present techniques are applied to this problem and the results compare well with those of previous workers, as shown in Table 10. S&TBS Type 2 has the lowest cost out of all the interval-based superstructures, apart from Yee and Grossmann's five stage SWS superstructure (equal to the number of hot streams). They used an NLP sub optimisation step to obtain a TAC of $\$576,640$ which is 0.2% lower than the TAC of $\$577,602$ obtained by S&TBS Type 2. The network structure of the S&TBS Type 2 is shown in Fig. 8.

6.5. Example 5 (aromatic plant)

This is the aromatic plant problem that involves the determination of a cost optimal network of heat exchangers for four hot streams and five cold streams having significantly different heat transfer coefficients (Linnhoff and Ahmad, 1990; Lewin, 1998; Krishna and Murty, 2007). The stream and cost data are shown in Table 11 and a comparison of costs with previous works in Table 12. The cost comparison shows that the new S&TBS and T&SBS methods are able to solve problems with different heat transfer coefficients (Fig. 9). The method of Pettersson (2005) and the T&SBS have seventeen units and seven streams splits each and they feature the lowest TAC in Table 12 though Pettersson is 0.6% lower than T&SBS.

Note that in these five HENS problems, a different technique has the lowest TAC – no one of them is consistently better or worse than the others.

7. S&TBS and T&SBS model equations for MENS

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

7.1. Assignment of superstructure interval boundary compositions for S&TBS

The model equations are presented below.

$$k = 1; Y_{R1,1}^s \quad (18a)$$

$$k = 2; Y_{R2,2}^s, Y_{R1,2} \quad (18b)$$

$$k = 3; Y_{S1,3}^{t*}, Y_{R1,3}, Y_{R2,3} \quad (18c)$$

$$k = 4; Y_{S2,4}^{t*}, Y_{R1,4}, Y_{R2,4}, Y_{S1,4}^* \quad (18d)$$

$$k = 5; Y_{R1,5}^t, Y_{R2,5}^t, Y_{S1,5}^{s*}, Y_{S2,5}^{s*} \quad (18e)$$

7.2. Assignment of superstructure interval boundary compositions for T&SBS

The model equations are presented below.

$$k = 1; Y_{R1,1}^s, Y_{R2,1}^s, Y_{S1,1}^{t*}, Y_{S2,1}^{t*} \quad (19a)$$

$$k = 2; Y_{R1,2}^t, Y_{R2,2}^t, Y_{S1,2}^{s*}, Y_{S2,2}^{s*} \quad (19b)$$

$$k = 3; Y_{R2,3}^t, Y_{S1,3}^{s*}, Y_{S2,3}^{s*} \quad (19c)$$

$$k = 4; Y_{S1,4}^{s*}, Y_{S2,4}^{s*} \quad (19d)$$

$$k = 5; Y_{S2,5}^{s*} \quad (19e)$$

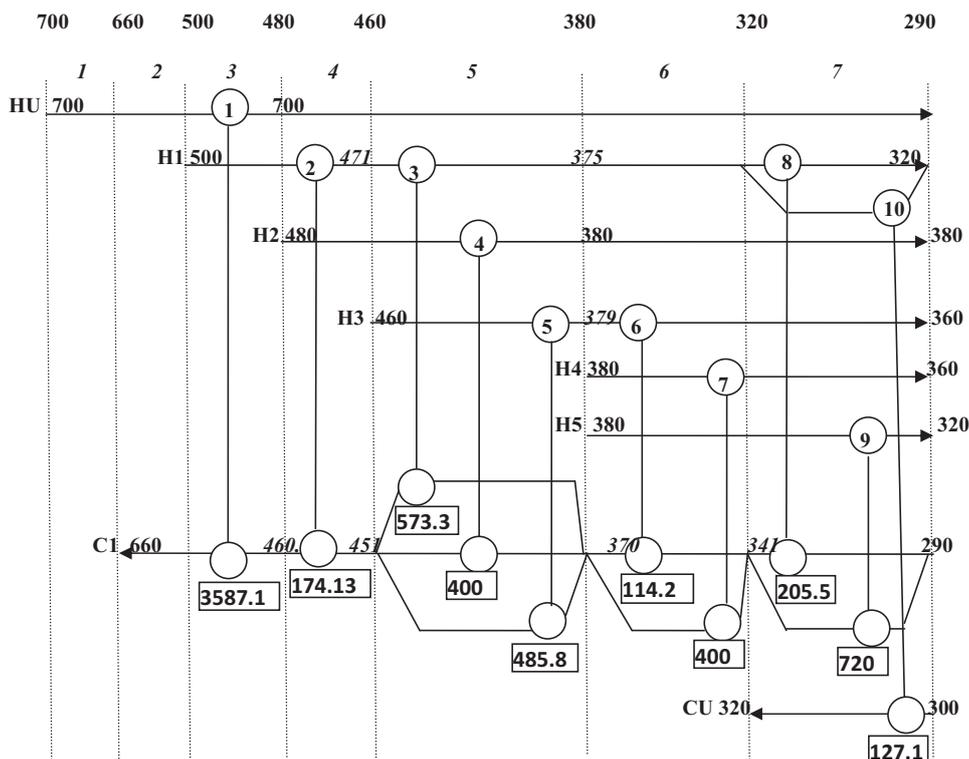


Fig. 8 – The S&TBS (Type 2) network structure for Example 4 featuring ten units with multiple split of the cold stream with a TAC of \$577,602.

Table 11 – Stream data for Example 5 from Krishna and Murty (2007).

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 = 5 years; rate of interest = 0%; exchanger cost = \$10,000 + 350(A) (A in m²); hot oil cost = 60 (\$/year)/kW; water cost = 6 (\$/year)/kW.

Table 12 – 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 et al. (1995)	0	10	2.980	2.58
S&TBS (Type 1)	3	13	2.979	2.55
SBS of Azeez et al. (submitted for publication)	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
S&TBS (Type 2)	1	11	2.940	1.21
GA of Lewin (1998)	2	12	2.936	1.07
T&SBS	7	17	2.922	0.59
Sequential match reduction approach of Pettersson (2005)	7	17	2.905	0.00

7.3. First set of stream existence conditionals for MENS

In a similar manner to HENS, the type A of S&TBS uses stream existence conditionals 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:

$$R_{r,k} \$(Y_r^s \geq Y_k) = 1 \tag{20a}$$

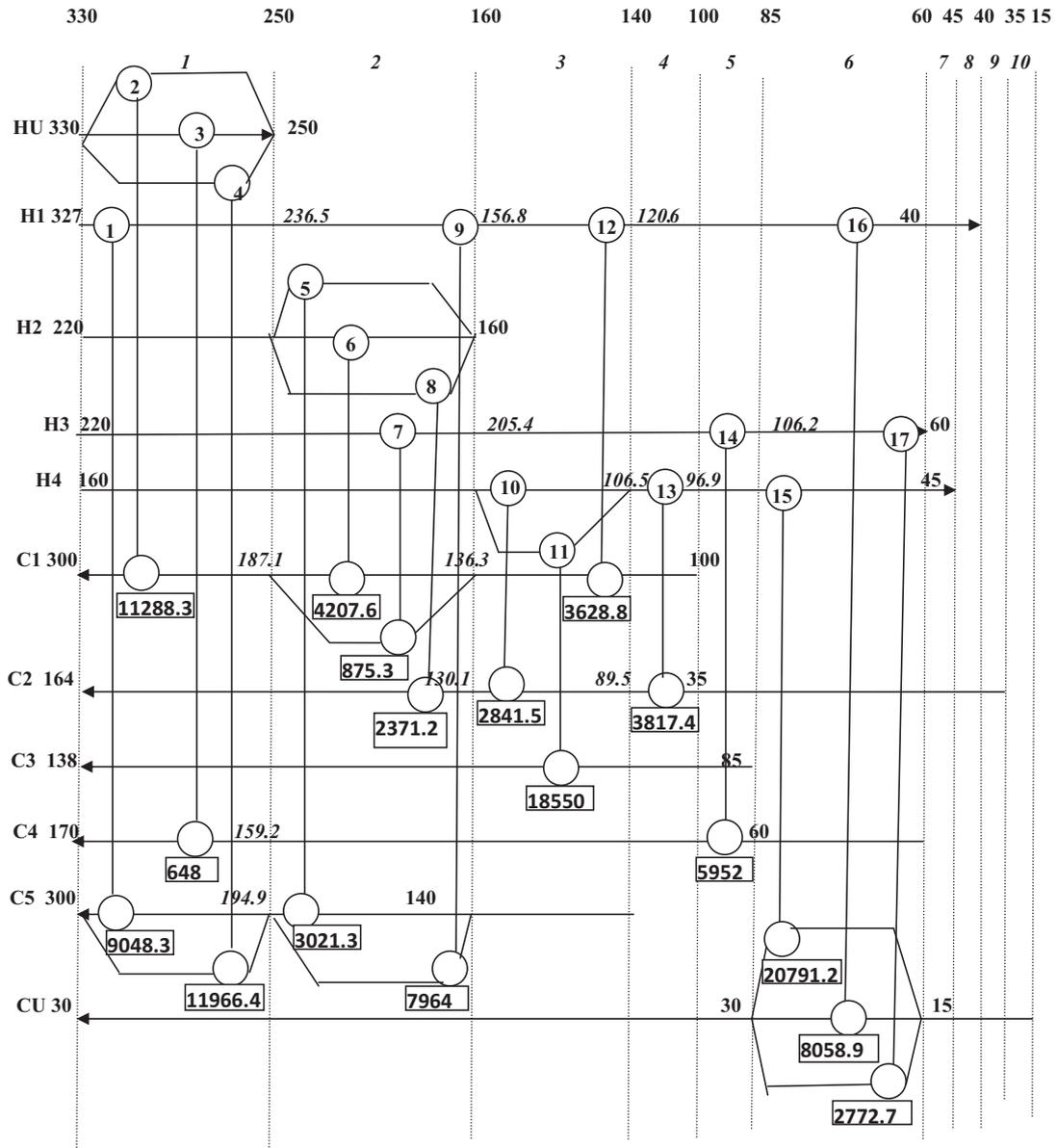


Fig. 9 – The T&SBS network structure of Example 5 featuring seventeen units with a TAC of M\$2.922.

$$S_{l,k} \$(Y_l^{*s} \leq Y_k) = 1 \tag{20b}$$

$$SST_{l,k} \$(Y_l^{*s} = Y_k) = 1 \tag{21c}$$

The conditional in Type 2 of S&TBS are the same for Type 1 but the second conditional is as shown in Eq. (20c).

$$SED_{l,k} \$(Y_r^t = Y_k) = 1 \tag{21d}$$

$$S_{l,k} \$(Y_l^{*t} \geq Y_k) = 1 \tag{20c}$$

7.5. Overall stream mass balance equations

In T&SBS, these conditionals are stated as follows:

The total mass change of each stream must equal the overall mass exchanged by each stream over all matches across all intervals, as represented by Eqs. (22) and (23) for rich stream *i* and lean stream *j* respectively.

$$R_{r,k} \$(Y_r^t \leq Y_k) = 1 \tag{20d}$$

$$(Y_r^s - Y_r^t)G_r = \sum_{k \in K} \sum_{j \in S} M_{rjk}, \quad r \in R \tag{22}$$

$$S_{l,k} \$(Y_l^{*s} \leq Y_k) = 1 \tag{20e}$$

7.4. Second set of stream existence conditionals

$$(Y_l^{*t} - Y_l^{*s})L_l = \sum_{k \in K} \sum_{r \in R} M_{rjk}, \quad l \in S \tag{23}$$

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

$$RST_{r,k} \$(Y_r^s = Y_k) = 1 \tag{21a}$$

While the rich stream flowrate *G_r* is modeled as a parameter in Eq. (22), the lean stream flowrate *L_l* in Eq. (23) is modeled as a variable.

$$RED_{r,k} \$(Y_r^t = Y_k) = 1 \tag{21b}$$

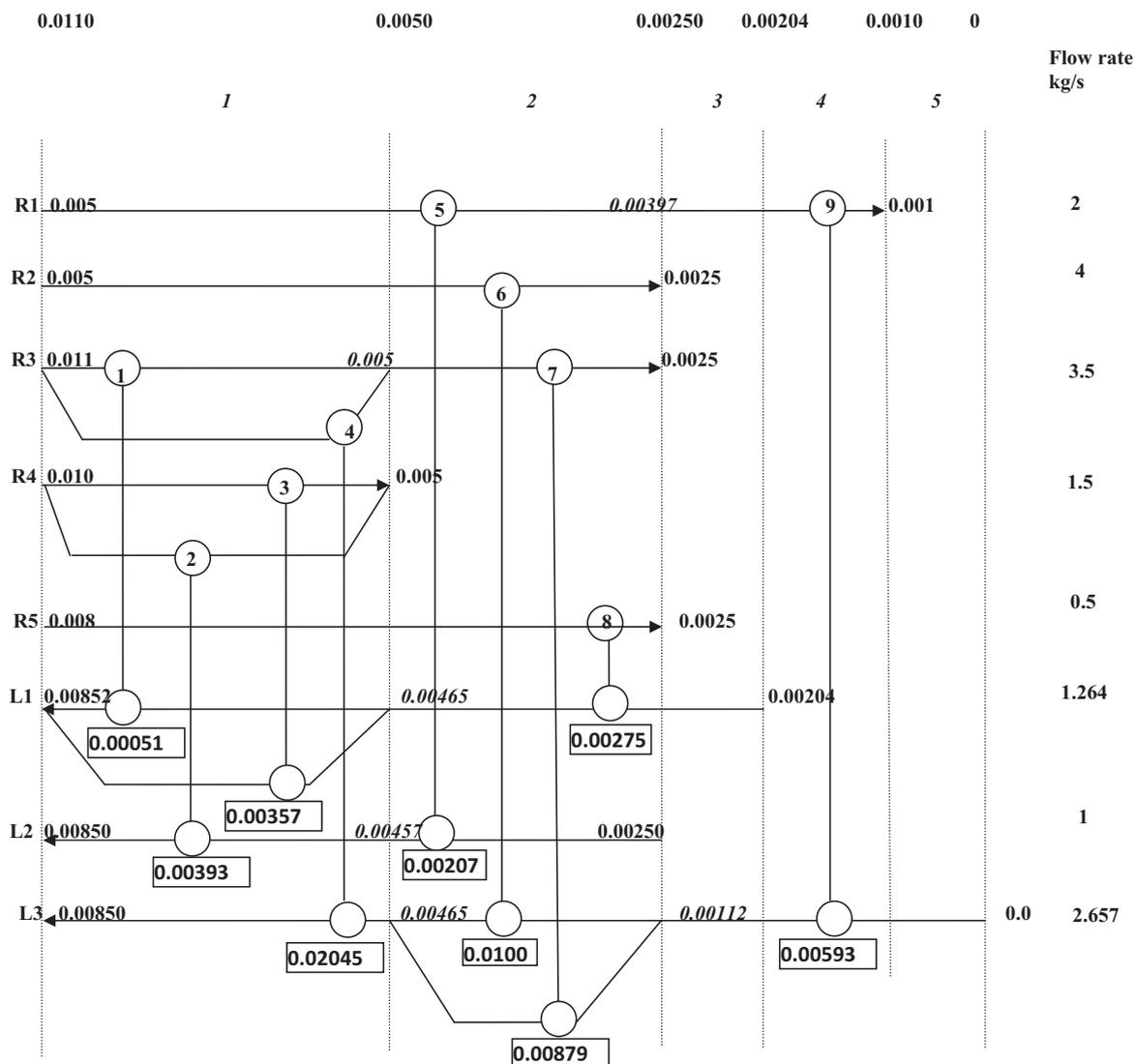


Fig. 10 – The T&SBS network structure of Example 6 featuring nine units with a TAC of \$131,524.

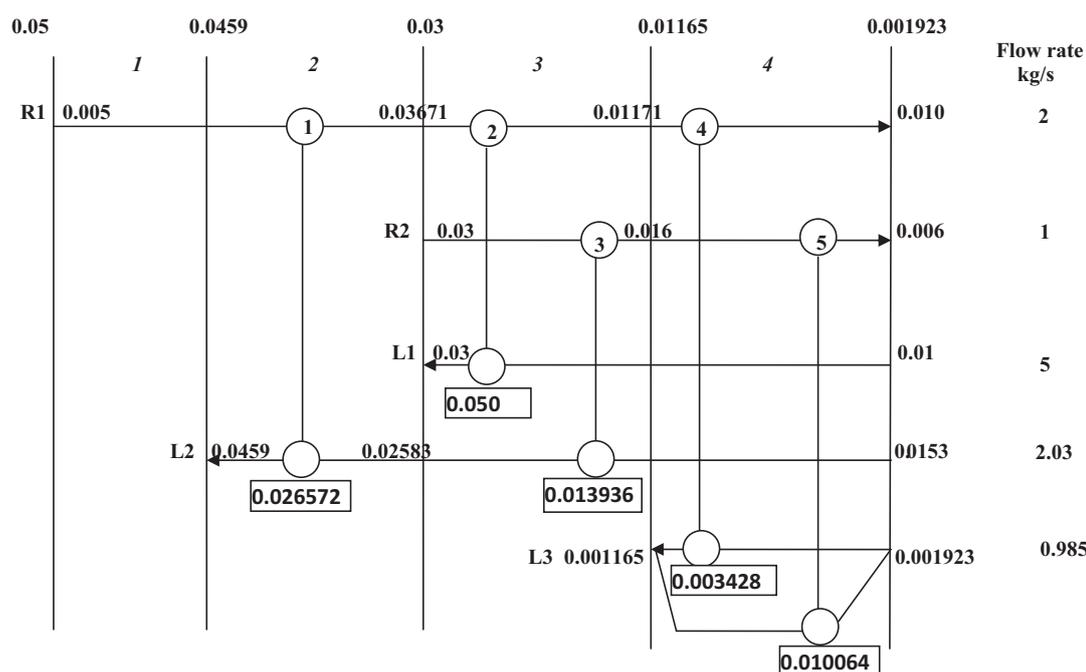


Fig. 11 – The S&TBS network structure of Example 7 featuring five units with a TAC of \$421,147.

7.6. Interval mass balances

The mass exchanged by each stream in an interval is determined using the interval mass balance equations for rich and lean streams which are presented in Eqs. (24) and (25).

$$(y_{r,k} - y_{r,k+1})G_r = \sum_{l \in S} M_{rlk}, \quad k \in K \quad (24)$$

$$(y_{l,k}^* - y_{l,k+1}^*)L_l = \sum_{r \in R} M_{rlk}, \quad k \in K \quad (25)$$

7.7. Composition feasibility along the superstructure

Constraints are used to achieve monotonic decrease of composition from the first composition location to the last composition location in the two superstructures, this implies a decrease in composition from supply to target for rich streams and target to supply for lean streams.

$$y_{r,k} \geq y_{r,k+1}, \quad k \in K, r \in R \quad (26)$$

$$y_{l,k}^* \geq y_{l,k+1}^*, \quad k \in K, l \in S \quad (27)$$

7.8. 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 '0' if otherwise. 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.

$$M_{rlk} - \Omega Z_{rlk} \leq 0, \quad r \in R, l \in S, k \in K \quad (28)$$

7.9. 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). This is done so as to avoid numerical errors due to negative composition differences for matches that do not exist.

$$dy_{rlk} \leq y_{r,k} - y_{l,k}^* + \Gamma_M(1 - Z_{rlk}), \quad k \in K, r \in R, l \in S \quad (29)$$

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

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

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

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:

$$dy_{rlk} \geq \epsilon \quad (33)$$

where ϵ is a small positive value.

The integer infeasible path MINLP (IIP-MINLP) formulation of Sorsak and Kravanja (2002) which enables the solver to

search for feasible solution through an infeasible path (as used by Sztikai et al., 2006) is used in SBS model. The equation for this is:

$$w_{r,l,k} = dw_{r,l,k} + ew_{r,l,k} - fw_{r,l,k}, \quad r \in R, l \in S, k \in K \quad (34)$$

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.

7.10. Objective function

The objective function, i.e. TAC, is as shown in Eqs. (35) and (36) where the exchanger mass based calculation method of Hallale (1998) is used for continuous contact columns and 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:

$$\min \left(\sum_{l \in S} (AC_l)(L_l) + \sum_{r \in R} \sum_{l \in S} \sum_{k \in K} CB_{rl} Z_{rlk} + \sum_{r \in R} \sum_{l \in S} \sum_{k \in K} ACH_{rl} \left[\frac{M_{rlk}}{K_w(LMCD_{rlk})} \right]^{D_{rl}} + VT \right) \quad (35)$$

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 objective function is:

$$\min \left(\sum_{l \in S} (AC_l)(L_l) + \sum_{r \in R} \sum_{l \in S} \sum_{k \in K} CB_{rl} Z_{rlk} + \sum_{r \in R} \sum_{l \in S} \sum_{k \in K} ACT_{rlk}(N_{rlk}) \right) \quad (36)$$

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

To avoid the problem of singularities associated with using the LMCD for mass exchanger sizing the first approximation of Chen (1987) is used, as was done for LMTD in HENS. The comparison of the different log-mean approximations and the errors associated with them is given in Azeez et al. (submitted for publication).

$$LMCD_{rlk} = \left[\frac{(dy_{rlk})(dy_{rlk+1})(dy_{rlk} + dy_{rlk+1})}{2} \right]^{1/3} \quad (37)$$

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

$$N_{rlk} = \left(\frac{\Delta y^n + \Delta y^{*n}}{\Delta y_1^n + \Delta y_2^n} \right)^{1/n} \quad (38)$$

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) for calculating the number of stages was obtained from the logarithmic mean approximations of

Table 13 – Stream and cost data for Example 6 from Hallale (1998).

Rich stream		R (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 (kg/s)	X ^s	X ^t	m	b	Cost (\$/kg)
L1		1.8	0.0017	0.0071	1.2	0	0
L2		1	0.0025	0.0085	1	0	0
L3		α	0.00	0.0017	0.5	0	0.001

$K_w = 0.02 \text{ kg NH}_3/(\text{s kg})$; annualisation factor = 0.225; annual operating time = 8150 h.

Table 14 – Comparison of costs with previous workers.

Method	Splits: rich/lean	No. of units	TAC (\$/year)	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	2.65
S&TBS (Type 1)	2/1	9	132,372	1.90
S&TBS (Type 2)	2/1	9	132,331	1.87
T&SBS	2/1	9	131,524	1.25
SBS of Azeez et al. (submitted for publication)	1/2	9	129,901	0.00

Underwood (1970) and the second approximation of Chen (1987). The error in using Eq. (38) for calculating the number of stages is a function of the ratio of the driving forces ($\Delta y_1/\Delta y_2$). 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 and Fraser, 2003). Fraser and Shenoy (2004) presented a detailed analysis of errors in terms of the absorption and effectiveness factors.

8. MENS examples

8.1. Example 6 (ammonia removal)

This example is taken from Hallale (1998). It has also been solved by other sets of workers (Szitkai et al., 2006; Emhamed et al., 2007; Isafiade and Fraser, 2008b; Azeez et al., submitted for publication). In this problem, ammonia is to be removed from five gaseous streams (mainly air). Two process MSAs and one external MSA, L1, L2 and L3 respectively, are available for ammonia removal. Packed column mass exchangers are to be used; stream and cost data for the problem are as shown in Table 13. The exchanger cost based on mass of Hallale (1998) is adopted in this study for comparison with previous workers. Table 14 compares the results of this study with those of previous workers. The SBS method features the lowest TAC

(1.2% lower than the next lowest one, which is T&SBS), while the methods of S&TBS and T&SBS (Fig. 10) give TACs that are within 0.7% of each other.

8.2. Example 7 (dephenolisation of aqueous wastes)

This example is taken from El-Halwagi (1997). In this problem, phenol is to be absorbed by solvent extraction from two aqueous streams, R1 and R2. Two process MSAs, namely gas oil (L1) and lube oil (L2), and one external MSA, light oil (L3) are available for the absorption. The problem specification is that the entire gas oil stream should be used. The mass exchangers are sieve tray columns. The capital cost data of Papalexandri et al. (1994) with the specification of \$4552 per equilibrium stage per year was used. Stream data for the problem can be found in Table 15, while the cost comparison with previous workers can be found in Table 16. Figure 11 illustrates the S&TBS Type 2 structure. The S&TBS (Type 1) and T&SBS have no solution for this problem (Table 18).

8.3. Example 8 (coke oven gas problem)

This example was taken from El-Halwagi and Manousiouthakis (1989). It has been solved by the following sets of workers: Hallale and Fraser (2000a), Isafiade (2008), and Azeez et al. (submitted for publication). Hallale and Fraser used pinch technology while Isafiade used the

Table 15 – Stream and cost data for Example 7, from 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)
L1		5	0.005	0.015	2.00	0	0
L2		3	0.01	0.030	1.53	0	0
L3		∞	0.0013	0.015	0.71	0.001	0.01

Table 16 – Summary and comparison of TAC for Example 7.

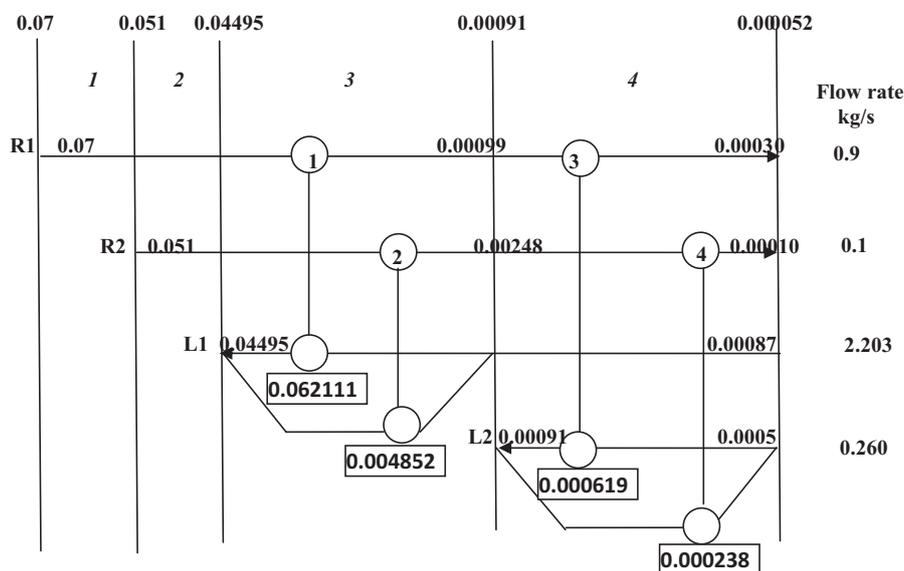
Method	Splits: rich/lean	No. of units	Total cost (\$/year)	Difference (%)
S&TBS (Type 2)	0/1	5	421,147	26.85
Lean based IBMS of Isafiade and Fraser (2008b)	0/0	5	358,292	7.92
Pinch technique of Hallale and Fraser (2000a)	0/2	7	345,416	4.04
SBS of Azeez et al. (submitted for publication)	0/0	6	339,579	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

Table 17 – Stream and cost data for Example 8 (El-Halwagi and 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 (\$/year)/(kg/s)
L1	2.3	0.0006	0.031	1.45	0	117,360
L2	∞	0.0002	0.0035	0.26	0	176,040

Table 18 – Summary and comparison of TAC for Example 8.

Method	Splits: rich/lean	No. of units	Total cost (\$/year)	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
T&SBS	0/2	4	526,471	22.52
S&TBS (Type 1)	0/2	4	524,244	22.00
S&TBS (Type 2)	0/2	4	524,244	22.00
SBS of Azeez et al. (submitted for publication)	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

**Fig. 12 – The S&TBS (Type 1) network structure for Example 8 featuring four units with TAC of \$524,244.**

IBMS method. The problem involves the removal of hydrogen sulphide 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. The stream and cost data are shown in Table 17. The stream flowrates are assumed to be constant (El-Halwagi and Manousiouthakis, 1989). The columns used are stagewise columns and the cost per stage per year of Papalexandri et al. (1994) is used in the column

costing (\$4552). The networks for the solutions as shown in Fig. 12 are all the same, even though the TAC for T&SBS is slightly higher than those for S&TBS. Table 18 compares the TAC obtained by different workers.

9. Discussion

Table 19 compares the performance of the various interval based approaches in terms of the number of intervals created

Table 19 – Comparison of interval based results for all examples.

Example	Method	Number of units	Stream split	No. of intervals created	No. of intervals used	Intervals used (%)	TAC	Difference (%)
1. 4SP1	T&SBS	5	2	6	3	50	11,204	5.90
	S&TBS (Type 2)	5	1	5	3	60	10,795	2.03
	SBS	5	1	5	3	60	10,794	2.02
	S&TBS (Type 1)	5	1	5	4	80	10,786	1.95
2. Shenoy (1995)	T&SBS	6	3	6	3	50	240,253	2.06
	Cold based IBMS	6	3	5	3	60	239,332	1.67
	Hot based IBMS	6	2	5	4	80	237,800	1.02
	SBS	6	2	5	4	80	235,931	0.2
	S&TBS (Type 1 & Type 2)	6	2	6	4	66.7	235,781	0.16
	SWS	6	2	2	2	100	235,400	0.00
3. Linnhoff et al. (1982)	S&TBS (Type 1)	5	1	6	3	50	93,391	16.34
	S&TBS (Type 2)	5	1	6	3	50	90,672	12.95
	SBS	7	3	4	3	75	90,521	12.77
	T&SBS	5	0	5	4	80	87,611	9.13
	SWS	5	2	2	2	100	80,274	0.00
4. Magnets problem	Cold based IBMS	7	1	3	3	100	595,064	3.81
	T&SBS	7	1	6	4	66.7	581,954	1.53
	Hot based IBMS	7	1	7	3	42.9	581,942	1.52
	S&TBS (Type 1)	7	1	7	3	42.9	581,942	1.52
	SBS	8	1	6	4	66.7	580,023	1.19
	S&TBS (Type 2)	10	1	7	5	71.4	577,602	0.77
	SWS	7	1	5	–	–	576,640	0.6
5. Aromatic plant	S&TBS (Type 1)	13	3	9	5	55.6	2,979,000	2.55
	SBS	14	6	9	5	55.6	2,976,000	2.44
	S&TBS (Type B)	11	1	9	5	55.6	2,940,000	1.21
	T&SBS	17	7	10	6	60	2,922,000	0.59
6. Ammonia removal	'SWS'	8	1	–	–	–	134,000	3.16
	Lean based IBMS	7	2	5	3	60	133,323	2.65
	S&TBS (Type 1)	9	3	6	3	50	132,372	1.90
	S&TBS (Type 2)	9	3	6	3	50	132,331	1.87
	T&SBS	9	3	5	3	60	131,524	1.25
	SBS	9	3	6	5	83.3	129,901	0.00
7. Dephenolisation of aqueous waste	S&TBS (Type 2)	5	1	4	3	75	421,147	26.85
	Lean based IBMS #1	5	0	–	–	–	358,292	7.92
	SBS	6	0	4	4	100	339,579	2.28
	Lean based IBMS #2	6	0	5	5	100	338,168	1.86
8. Coke oven gas	Rich based IBMS	4	0	3	3	100	530,471	23.45
	T&SBS	4	2	4	2	50	526,471	22.52
	S&TBS (Type 1)	4	2	4	2	50	524,244	22.00
	S&TBS (Type 2)	4	2	4	2	50	524,244	22.00
	SBS	5	0	3	3	100	469,968	9.37
	Lean based IBMS	4	2	3	2	66.7	446,840	3.99
	'SWS'	4	2	–	–	–	429,700	0.00

and the percentage of the intervals used out of those created and the effect on TAC of HENS and MENS. Note that the difference column reflects the differences relative to the lowest TAC, as given in the tables for each individual problem.

As indicated in the motivation, one of the goals of this study was to develop a partitioning system for HENS and MENS problems that would give better solutions than other partitioning systems. At this stage, Table 19 shows that there is no single partitioning technique that consistently provides the most optimum solutions (nor does any other technique for that matter, although all of them have not been applied to all of the problems). The SWS technique for HENS still appears to outperform the other partitioning techniques, but then it incorporates a second stage of non-linear optimisation, which no doubt accounts for this.

In general it seems from Table 19 that a system that is able to use most of the intervals created gives a lower TAC (where

the number of intervals has been reported). This is clearly the case for half of the problems studied. In Examples 1, 3, 5, and 7 the % of intervals used increases monotonically as the TAC decreases. Example 2 also largely conforms to this trend, while for Examples 4, 6 and 8 there is no clear trend of % of intervals used versus TAC. In comparing the problems in Table 19, it is clear that although using all the intervals created often gives the lowest TAC, this is not always the case.

It should be noted that, as expected, the S&TBS and T&SBS techniques mostly generate more intervals than the other partitioning techniques for the problems studied. This was one of the main motivations behind exploring these techniques. What Table 19 shows is that increasing the number of intervals does not necessarily lead to better solutions, unless a high proportion of those intervals can all be utilised in the solution.

It should be noted that using stream temperatures as a basis for the partitioning, are not well suited to incorporation

into the optimisation of wider flowsheeting problems, unless a way can be found to automate the assignment of the partition temperatures and thus allow them to be varied as part of the optimisation. This would only be possible using a system such as Mipsyn (Kravanja, 2010).

10. Conclusions

The present study explored different ways of using key parameters such as supply temperatures/compositions of hot/rich streams and target temperatures/compositions of cold/lean streams for defining the interval boundaries of superstructures in the synthesis of HENs and MENs. The results obtained in this study compare well with other literature problems.

This study demonstrates that, so far, the outcome of various techniques presented in the literature have been problem specific, since there is no particular technique that globally or conclusively obtains the lowest TAC for all the HEN and MEN problems presented in this study. The results shown in Table 19 suggest that it might be an advantage for a technique to create as many intervals as possible. It does seem to be generally better for any method to use a high percentage of the intervals created to minimize the TAC of the network. The study also demonstrated that the optimum number of intervals appears to be problem specific, and not general for all HENS/MENS tasks.

As far as solution techniques are concerned, it does seem that inclusion of non-linearities such as the equations for the determination of number of stages for stagewise mass transfer does make it more difficult for GAMS with DICOPT++ to obtain a solution. Increasing the number of variable streams (such as utilities), on the other hand, does not appear to provide the kind of non-linearity that this system struggles to solve.

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References

- Azeez, O.S., Isafiade, A.J., Fraser, D.M. Supplied based superstructure synthesis of heat and mass exchanger network. *Comput. Chem. Eng.*, submitted for publication.
- Bagajewicz, M.J., Pham, R., Manousiouthakis, V., 1998. On the state space approach to mass/heat exchanger network design. *Chem. Eng. Sci.* 53 (14), 2595–2621.
- Brooke, A., Kendrick, D., Meeraus, A., 1988. *GAMS: A Users's Guide*. Scientific Press, Palo Alto, CA.
- Cerda, J., Westerbag, A.W., Mason, D., Linnhoff, B., 1983. Minimum utility usage in heat exchanger network synthesis—a transportation problem. *Chem. Eng. Sci.* 38, 373–387.
- Chen, J.J., 1987. Letter to the editor: comments on improvement on a replacement for the logarithmic mean. *Chem. Eng. Sci.* 42, 2488–2489.
- Chen, C.L., Huang, P.S., 2005. Simultaneous synthesis of mass exchange networks for waste minimization. *Comput. Chem. Eng.* 29, 1561–1576.
- Ciric, A.R., Floudas, C.A., 1990. Application of the simultaneous match-network optimisation approach to the pseudo-pinch problem. *Comput. Chem. Eng.* 14, 241–250.
- Ciric, A.R., Floudas, C.A., 1991. Heat exchanger network synthesis without decomposition. *Comput. Chem. Eng.* 15, 385–396.
- Colberg, R.D., Morari, M., 1990. Area and capital cost targets for heat exchanger network synthesis with constrained matches and unequal heat transfer coefficients. *Comput. Chem. Eng.* 14, 1–22.
- Comeaux, R.G., 2000. Synthesis of mass exchange networks with minimum total cost. MPhil Thesis. UMIST, Manchester.
- El-Halwagi, M.M., 1997. *Pollution Prevention through Process Integration: Systematic Design Tools*. Academic Press, San Diego, CA.
- El-Halwagi, M.M., Manousiouthakis, V., 1989. Synthesis of Mass Exchange Networks. *AIChE J.* 35 (8), 1233–1244.
- Emhamed, A.M., Lelkes, Z., Rev, E., Farkas, T., Fonyo, Z., Fraser, D.M., 2007. New hybrid method for mass exchange network optimization. *Chem. Eng. Commun.* 194 (12), 1688–1701.
- Floudas, C.A., Ciric, A.R., Grossman, I.E., 1986. Automatic synthesis of optimum heat exchanger network configurations. *AIChE J.* 32 (2), 276–290.
- Fraser, D.M., Shenoy, U.V., 2004. A new method for sizing mass exchange units without the singularity of the Kremser equation. *Comput. Chem. Eng.* 28, 2331–2335.
- Grossman, I.E., 1985. *Magnets User's Guide*. Carnegie Mellon University, Pittsburgh.
- Grossmann, I.E., Sargent, R.W., 1978. Optimum design of heat exchanger networks. *Comput. Chem. Eng.* 2, 1–7.
- Hallale, N., 1998. Capital cost targets for the optimum synthesis of mass exchange networks. PhD Thesis. Department of Chemical Engineering, University of Cape-Town, Cape-Town, South Africa.
- Hallale, N., Fraser, D.M., 2000a. Capital and total cost targets for mass exchange networks. Part 1: simple capital cost models. *Comput. Chem. Eng.* 23, 1661–1679.
- Hallale, N., Fraser, D.M., 2000b. Capital and total cost targets for mass exchange networks. Part 2: detailed capital cost models. *Comput. Chem. Eng.* 23, 1681–1699.
- Isafiade, A.J., Fraser, D.M., 2008a. Interval based MINLP superstructure synthesis of heat exchange networks. *Chem. Eng. Res. Des.* 86 (3), 245–257.
- Isafiade, A.J., Fraser, D.M., 2008b. Interval based MINLP superstructure synthesis of mass exchange networks. *Chem. Eng. Res. Des.* 86 (8), 909–924.
- Isafiade, A.J., 2008. Interval based MINLP superstructure synthesis of heat and mass exchange networks. PhD Thesis. University of Cape Town.
- Kravanja, Z., 2010. Challenges in sustainable integrated process synthesis and the capabilities of an MINLP process synthesizer MIPSYN. *Comput. Chem. Eng.* 34, 1831–1848.
- Krishna, M.Y., Murty, C.V.S., 2007. Synthesis of cost-optimal heat exchanger networks using differential evolution. *Comput. Chem. Eng.* 32, 1861–1876.
- Lawler, E.L., Wood, D.E., 1966. *Oper. Res.* 11 (4), 699–719.
- Lee, K.F., Masso, A.H., Rudd, D.F., 1970. Branch and bound synthesis of integrated process designs. *Ind. Eng. Chem. Fundam.* 9 (1), 48–58.
- Lewin, D.R., 1998. A generalized method for HEN synthesis using stochastic optimization. II. The synthesis of cost-optimal networks. *Comput. Chem. Eng.* 22 (10), 1387–1405.
- Linnhoff, B., Mason, D.R., Wardle, I., 1979. *Comput. Chem. Eng.* 3, 295.
- Linnhoff, B., Ahmad, S., 1990. Cost optimum heat exchanger networks (part I). *Comput. Chem. Eng.* 14 (7), 729–750.
- Linnhoff, B., Flower, J.R., 1978. Synthesis of heat exchanger networks, I. Systematic generation of energy optimal networks. *AIChE J.* 24 (4), 633–642.
- Linnhoff, B., Hindmarsh, E., 1983. The pinch design method for heat exchanger networks. *Chem. Eng. Sci.* 38, 745–763.
- Linnhoff, B., Townsend, D.W., Boland, D., Hewitt, G.F., Thomas, B.E.A., Guy, A.R., Marsland, R.H., 1982. *A User Guide on Process Integration for the Efficient Use of Energy*. The Institute of Chemical Engineering, UK.
- Martin, L.L., Manousiouthakis, V.I., 2001. Total annualized cost optimality properties of state space models for mass and heat exchanger networks. *Chem. Eng. Sci.* 56, 5835–5851.

- Nishida, N., Liu, Y.A., Lapidus, L., 1977. Studies in chemical process design and synthesis: III. A simple and practical approach to the optimal synthesis of heat exchanger networks. *AIChE J.* 23 (1), 77–93.
- Papalexandri, K.P., Pistikopoulos, E.N., Floudas, C.A., 1994. Mass exchange networks for waste minimization. *Trans. IChemE* 72, 279–294.
- Papoulias, S.A., Grossmann, I.E., 1983. A structural optimization approach in process synthesis—II. Heat recovery networks. *Comput. Chem. Eng.* 7, 707.
- Paterson, W.R., 1984. A replacement for the logarithmic mean. *Chem. Eng. Sci.* 39, 1635–1636.
- Paterson, W.R., 1987. Author's reply to comments by J.J.J. Chen. *Chem. Eng. Sci.* 42, 2490–2491.
- Pettersson, F., 2005. Synthesis of large-scale heat exchanger networks using a sequential match reduction approach. *Comput. Chem. Eng.* 29 (5), 993–1007.
- Pho, T., Lapidus, L., 1973. Synthesis of optimal heat exchanger networks by tree searching algorithms. *AIChE J.* 19, 1182.
- Ponto, J.W., Donaldson, R.A.B., 1974. A fast method for the synthesis of optimal heat exchanger networks. *Chem. Eng. Sci.* 29, 2375–2377.
- Price, K., Storn, R., 1997. Differential evolution. *Dr. Dobb's J.*, 18–24.
- Rathore, R.N.S., Power, G.J., 1975. A forward branching scheme for the synthesis of energy recovery systems. *Ind. Eng. Chem. Process Des. Dev.* 14, 175.
- Rosenthal, R.E., 2007. *GAMS – A User's Guide*. GAMS Development Corporation, Washington, DC, USA.
- Shenoy, U.V., 1995. *Heat Exchange Network Synthesis. Process Optimisation by Energy and Resource Analysis*. Gulf Publishing Company, Houston, TX.
- Shenoy, U.V., Fraser, D.M., 2003. A new formulation of the Kremser equation for sizing mass exchangers. *Chem. Eng. Sci.* 58, 5121–5124.
- Sorsak, A., Kravanja, Z., 2002. Simultaneous MINLP synthesis of heat exchanger networks comprising different exchanger types. *Comput. Chem. Eng.* 26, 599–615.
- Szitkai, Z., Farkas, T., Lelkes, Z., Fonyo, Z., Kravanja, Z., 2006. Fairly linear mixed integer nonlinear programming model for the synthesis of mass exchange networks. *Ind. Eng. Chem. Res.* 45, 236–244.
- Umeda, T., Niida, K., Shiroko, K., 1979. A thermodynamic approach to heat integration in distillation systems. *AIChE J.* 25 (3), 423–429.
- Underwood, A.J.W., 1970. Simple formula to calculate mean temperature difference. *Chem. Eng.* 77 (June), 192.
- Yee, T.F., Grossmann, I.E., 1990. Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis. *Comput. Chem. Eng.* 14 (10), 1165–1184.
- Zhu, X.X., O'Neill, B.K., Roach, J.R., Wood, R.M., 1995. A method for automated heat exchanger network synthesis using block decomposition and non-linear optimization. *Trans. IChemE Part A* 73 (11), 919–930.