Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA)
25 - 27 June 2013, Kuala Lumpur.

Interval-based Superstructure Synthesis of Heat and Mass Exchange Networks

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Abstract

This paper compares the approach and results of all the interval-based superstructure methods for the synthesis of optimal heat and mass exchange networks. Differences in approach are largely due to how the interval boundaries are defined. Approaches based on the stagewise superstructure simply define the number of intervals, whereas the interval-based superstructures define the interval boundaries by stream supply or target temperatures/compositions. Comparison of results over a range of heat and mass exchange network examples shows that not one of these approaches gives the solution with the lowest total annual cost for more than a few of the examples. Approaches that use more of the intervals generated tend to give better solutions. The non-linear sub-optimisation step of the heat exchanger network stagewise superstructure gives the largest number of best solutions.

Keywords: Heat exchanger network synthesis, Mass exchanger network synthesis, Superstructure, MINLP.

1. Introduction

The tasks of synthesizing cost effective heat exchanger networks (HENs) and mass exchanger networks (MENs) are key areas of process synthesis. Heat exchanger network synthesis (HENS) has received much attention over the years, stimulated by the development of the Pinch Approach by Linnhoff and Flower (1978). 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.

An important development in process synthesis has been the development of interval based superstructures for simultaneous optimization of all the competing costs in HENS (Yee and Grossman, 1990, Isafiade and Fraser, 2008a, Azeez *et al*., 2011 and 2012) and in MENS (Chen and Hung, 2005, Szitikai, *et al*., 2006, Comeaux, 2000, Isafiade and Fraser, 2008b, Azeez, *et al*., 2011 and 2012). Lewin (1998) adopted the genetic algorithm (GA) approach for simultaneous synthesis of heat exchanger networks while Krishna and Murty (2007) used a differential evolution (DE) technique.

Yee and Grossman (1990) developed the stagewise superstructure (SWS) for HENS, where the number of stages were determined by the maximum number of hot or cold streams present in the synthesis task. The MENS analogue of Yee and Grossmann's SWS (1990) was first presented by Chen and Hung (2005), using one more stage than Yee and Grossman did. Szitikai, *et al*. (2006) also used the key SWS idea of Yee and Grossman to develop a similar superstructure for MENS. Sztikai, *et al*., 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.

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. They also developed the mass exchange analogue of the IBMS for MENS (Isafiade and Fraser, 2008b). Subsequently, Azeez, *et al.* (2012) presented the Supply based Superstructure (SBS) approach for HENS and MENS, where the superstructure interval boundaries were defined using the supply temperatures of both the hot and the cold streams. They further developed this approach to both the Supply and Target-based Superstructure and the Target and the Supply-based Superstructure (T&SBS) (Azeez, *et al.*, 2011).

The purpose of this paper is to compare the methodology and results of all these interval-based mathematical programming techniques.

2. Methodology

Table 1 shows the differences between the various HENS superstructures as well as their similarities, in terms of their formulation and implementation, and Table 2 does the same for the various MENS superstructures. The major difference in the formulation of the superstructures is the way in which intervals have been defined. This leads to different ways of fixing the boundaries in each of the superstructures. The ways on which the boundaries are fixed also informs the intervals where the HEN/MEN streams will be present for heat/mass to be exchanged. Another important difference between the various approaches is the variation in the number of intervals created for heat/mass exchange.

3. Results, Discussion and Conclusions

The results of all the studies being compared in this paper are shown in Table 3, both for HENS examples (Examples 1 – 7) and for MENS examples (Examples 8 – 11). This table gives information about the structure of the solution (number of matches and number of stream splits), the usage of the intervals created (number and % used), and also the Total Annual Cost (TAC) of each of the solutions (with each being compared to the lowest TAC for that example).

What stands out in comparing the results for all the examples shown in Table 3 is that not one method consistently gives the solution with the lowest TAC. This is an important finding, in that it is clear that none of the methods developed so far achieves the global optimum solution for all the examples studied. Another finding to come out of this comparison is that in general, the better solutions in terms of TAC are those which use a greater proportion of the intervals created. When formulating the SBS, S&TBS and T&SBS approaches, we had thought that they might lead to better solutions because by providing more intervals they would enlarge the solution space. This now appears to not be the case, unless the intervals created can be fully utilised.

It is also clear from Table 3 that the SWS for heat exchanger network synthesis, with its non-linear sub-optimisation step does generally outperform all the other techniques. More work needs to be done to ensure a better comparison of the different approaches, with a view to developing a technique that will consistently give the best solution over a wide range of HENS and MENS problems.

Acknowledgements
This research was supported by the Department of Chemical Engineering and the Postgraduate Funding Office of the University of Cape Town, South Africa, the South African Water Research Commission, the National Research Foundation of South Africa and the Claude Leon Foundation.

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Table 1. Characteristics of the HENS superstructures

SWS of Yee and Grossman (1990)	IBMS of Isafiade and Fraser (2008a)	SBS of Azeez, et al. (2012)	S&TBS of Azeez, et al. (2011)	T&SBS of Azeez, et al. (2011)
Maximum of the number of hot streams or the number of cold stream determines the number of stages (intervals) in the superstructure.	The values of supply and target temperatures of either the hot streams or the cold streams determine the number of intervals in the superstructure (this normally gives more intervals than SWS).	The values of the supply temperatures of both the hot streams and the cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).	The values of the supply temperatures of hot streams and target temperatures of cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).	The values of the target temperatures of hot streams and supply temperatures of cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).
The fixed boundaries are the first and last: the first one being where the hot streams start and the cold streams end, while the last one is the hot streams end and cold streams start.	Interval boundaries are chosen based on the supply and target temperatures of either the hot streams or the cold streams.	Interval boundaries are chosen based on the supply temperatures of the hot streams and the cold streams.	Interval boundaries are chosen based on the supply temperatures of the hot streams and the target temperatures of the cold streams.	Interval boundaries are chosen based on the target temperatures of the hot streams and the supply temperatures of the cold streams.
Heat exchange between each hot stream and each cold stream is possible in all the stages of the superstructure.	Heat exchange by each hot stream is possible 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.	Heat exchange of streams is limited by needing to have positive temperature differences.	Same as IBMS.	Same as IBMS.
All streams exist in all the superstructure 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 in all the intervals. Converse applies in a cold-based superstructure.	The hot streams exist in all intervals defined by temperatures lower than their supply temperatures. The cold streams exist in all intervals defined by temperatures higher than their supply temperatures.	Hot streams existence in the intervals are as in SBS. Cold streams exist in all intervals at temperatures lower than their target values.	Hot streams exist across the intervals at temperature higher than the target values. Cold streams existence across intervals as in SBS.
MINLP model formulation but NLP sub optimisation step usually needed.	MINLP model formulation, NLP sub-optimisation not used.	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.
Utilities are placed at the ends of the superstructure	Utilities are treated as process streams in the superstructure	Same as IBMS	Same as IBMS	Same as IBMS

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. (2012)	S&TBS of Azeez, et al. (2011)	T&SBS of Azeez, et al. (2011)
The sum of the number of rich streams and the number of lean streams may determines the number of stages in the superstructure.	The values of the supply and target compositions of the rich streams and equilibrium equivalent of the lean streams determine the number of superstructure intervals.	The values of supply and target compositions of either the rich streams or the lean streams determines the number of superstructure intervals.	The values of supply compositions of both the rich streams and the lean streams determine the number of superstructure intervals.	The values of supply compositions of the rich streams and the target composition of the lean streams determine the number of superstructure intervals.	The values of the target compositions of rich streams and the supply composition of lean streams determine the number of superstructure intervals.
The fixed boundaries are the first and the last: the first is where the rich streams begin and the lean streams end, while the last is where the rich streams end and the lean streams begin.	Interval boundaries are chosen based on the supply and target compositions though the target is extended for the lean streams.	Interval boundaries are chosen based on the supply and compositions of either the rich streams or the lean streams.	Interval boundaries are chosen based on the supply compositions of the rich streams and the lean streams.	Interval boundaries are chosen based on the supply compositions of the rich streams and the target compositions of the lean streams.	Interval boundaries are chosen based on the target compositions of the rich streams and the supply compositions of the lean streams.
Mass exchange between rich and lean streams is possible in all the superstructure stages.	Extension of lean stream is adopted to ensure a match at least with each rich stream in the superstructure stages.	Mass exchange is limited by having to have positive composition differences.	Same as IMBS.	Same as IMBS.	Same as IMBS.
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 exist in all intervals at compositions lower than their supply composition. Lean streams exist in all intervals at compositions higher than their supply composition.	Rich streams exist in all intervals as in the SBS. Lean streams exist in all intervals at compositions lower than their target compositions	Rich streams exist in all intervals at compositions higher than their target composition. Lean streams exist in all intervals as in SBS.
The target compositions of rich streams are fixed at the last interval location while those of lean streams are fixed at the first interval location.	The target composition of each rich stream is set at the interval defined by its target value while the target of each lean 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
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 used.	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 streams.	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.
Process and external lean streams are equally treated in the superstructure	Same as in SWS	Same as in SWS	Same as in SWS	Same as in SWS	Same as in SWS

Table 3. Comparison of results using different methods.

Example	Method	No of units	Stream Splits	No of intervals created	No of intervals used.	% intervals used	TAC	Percent Difference (%)
1. 4SP1 (Lee *et al.*, 1970)	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. 4S1 (Shenoy, 1995)	T&SBS	6	3	6	3	50	240,253	2.06
	IBMS (Cold based)	6	3	5	3	60	239,332	1.67
	IBMS (Hot based)	6	2	5	4	80	237,800	1.02
	SBS	6	2	5	4	80	235,931	0.2
	S&TBS (Both Types)	6	2	6	4	67	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 (Yee and Grossmann, 1990)	Cold based (IBMS)	7	1	3	3	100	595,064	3.81
	T&SBS	7	1	6	4	67	581,954	1.53
	Hot based (IBMS)	7	1	7	3	43	581,942	1.52
	S&TBS (Type 1)	7	1	7	3	43	581,942	1.52
	SBS	8	1	6	4	67	580,023	1.19
	S&TBS (Type 2)	10	1	7	5	71	577,602	0.77
	SWS	7	1	5	-	-	576,640	0.6
5. Aromatic Plant (Linnhoff & Ahmad, 1990)	S&TBS (Type 1)	13	3	9	5	56	2,979,000	2.55
	SBS	14	6	9	5	56	2,976,000	2.44
	S&TBS (Type 2)	11	1	9	5	56	2,940,000	1.21
	T&SBS	17	7	10	6	60	2,922,000	0.59
6. Multiple Utility I (Shenoy, *et al.*, 1998)	T&SBS	7	1	6	5	83	101,893	4.96
	S&TBS	6	2	5	4	80	101,889	4.95
	SBS	6	2	5	4	80	101,889	4.95
	IBMS	9	-	-	-	-	97,211	0.14
	SWS	7	-	-	-	-	97,079	0.00

Example	Method	No of units	Stream Splits	No of intervals created	No of intervals used.	% intervals used	TAC	Percent Difference (%)
7. Multiple Utility 2 (Shenoy, *et al.*, 1998)	T&SBS	8	3	8	4	50	1,226,806	9.40
	IBMS	7	2	7	5	71	1,150,460	2.61
	S&TBS	7	1	8	4	50	1,150,436	2.60
	SBS	8	2	8	5	63	1,125,417	0.38
	SWS	8	-	-	-	-	1,121,175	0.00
8. Ammonia removal (Hallale, 1998)	SWS	8	1	-	-	-	134,000	3.16
	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	129,901	0.00
9. Dephenolization of aqueous waste (El-Halwagi, 1997)	S&TBS (Type 2)	5	1	4	3	75	421,147	26.85
	Lean based 1 (IBMS)	5	0	-	-	-	358,292	7.92
	SBS	6	0	4	4	100	339,579	2.28
	Lean based 2 (IBMS)	6	0	5	5	100	338,168	1.86
	NLP Option 1	7	2	-	-	-	333,300	0.39
	NLP Option 2	8	2	-	-	-	332,000	0.00
10.Coke oven gas (El-Halwagi and Manousiouthakis, 1989)	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	67	446,840	3.99
	SWS	4	2	-	-	-	429,700	0.00
11. Dephenolization of coal conversion waste (Papalexandri, *et al.*, 1994)	SWS	NA	1	-	-	-	720,000	4.66
	SWS	7	1	-	-	-	694,000	0.87
	SBS	8	1	5	4	80	693,976	0.86
	IBMS	8	1	6	4	67	689,300	0.19