CHEMICAL ENGINEERING TRANSACTIONS

VOL. 52, 2016

A publication of AIDIC

The Italian Association
of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Petar Sabev Varbanov, Peng-Yen Liew, Jun-Yow Yong, Jiří Jaromír Klemeš, Hon Loong Lam

ISBN 978-88-95608-42-6; **ISSN** 2283-9216

DOI: 10.3303/CET1652133

A Systematic Comparison of Stagewise/Interval-Based Superstructure Approaches for the Optimal Synthesis of Heat Exchange Networks

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This article describes a study in which the various stagewise and interval-based superstructures for the mixed integer non-linear programming (MINLP) optimisation of heat exchanger networks were systematically compared, using exactly the same basis. The effect of using different logarithmic mean temperature difference (LMTD) approximations on the Total Annual Cost of the network and the network structure were examined. The accuracy of the approximations was also analyzed over a wide range of temperature difference ratios. It is concluded that the best approximation, which is the Underwood-Chen approximation, should be used in future mathematical optimisation of Heat Exchanger Network Synthesis problems.

1. Introduction

The task of synthesizing cost effective heat exchanger networks (HENs) is a key area of process synthesis. The solution procedure employed so far have been both sequential and simultaneous in nature. Chief among the sequential approach is the popular Pinch Technology (Linnhoff et al., 1982), while examples of the simultaneous approach are the methods presented by Yee and Grossmann (1990) where the stage-wise superstructure approach was used, and that of Isafiade and Fraser (2008) where the interval based MINLP superstructure (IBMS) approach was used. A significant number of the structures used in the simultaneous approaches have been largely based on insights from the sequential approaches. Some methods have even involved combination of both sequential and simultaneous approaches in what is known as hybrid methods. These methods combine the benefits of both approaches. In some cases, the hybrid methods use the solutions obtained from the sequential methods to give initial conditions to the non-linear program solver responsible for solving the simultaneous synthesis aspect of the structure. For the simultaneous approaches that are Interval/stage-wise based in the context of heat exchange networks, the superstructure definition method entails partitioning the HENS problem to be optimised using temperatures of the streams participating in the problem. The nature of such partitioning is such that hot streams are made to run from left to right, i.e. their temperatures decrease in that order, while cold streams are positioned in the opposite direction. Depending on the approach being used, the utilities may be included as part of the streams to define the partitioned HENS structure, or they may be appended after some information may have been obtained in a previous step. The superstructures of these simultaneous methods are believed to embed all potentially optimal/near optimal network structures. They are usually represented as mixed integer non-linear program (MINLP), and they simultaneously establish trade-offs among competing variables in heat exchanger network synthesis problems.

This study focuses on a systematic comparison of the stage-wise/interval-based MINLP superstructure approaches for HENS where the approximated logarithmic mean temperature differences (LMTD) have been used. It should be known that even though the pinch technology approach has shortcomings such as tediousness and a lack of adequate simultaneous trade-offs among competing variables (due to the two-stage design approach), it does not require the use of approximated LMTDs since the designer makes choices as to what temperatures to use when determining the required heat exchange area. This is unlike the mathematical

Please cite this article as: Fraser D. M., Short M., Crimes J., Azeez O. S., Isafiade A. J., 2016, A systematic comparison of stagewise/interval-based superstructure approaches for the optimal synthesis of heat exchange networks, Chemical Engineering Transactions, 52, 793-798 DOI:10.3303/CET1652133

based approaches (e.g. the stage-wise and interval based methods), where solvers could encounter the problem of singularities in determining the required heat exchange area, hence an approximated version of LMTD is used.

Yee and Grossman (1990) developed the Stage-Wise Superstructure (SWS) for HENS, where the number of stages was determined by the maximum number of hot or cold streams present in the synthesis task. There have been a number of variations of the SWS approach, but possibly the most significant from a structural point of view was that by Ponce-Ortega et al. (2010) who incorporated utilities at each stage in the superstructure, rather than at the extremes. Short et al. (2015) extended the SWS model through the use of correction factor approach to synthesise networks that take into consideration more detailed exchanger designs, while Kang et al. (2015) applied the SWS model to multi-period HENS. Isafiade and Fraser (2008) developed the Interval Based MINLP Superstructure (IBMS) for HENS using either the supply and target temperatures of hot streams to define the interval boundaries in a hot-based superstructure or the supply and target temperatures of cold streams in a cold-based superstructure. Note that in these IBMS superstructures, the utility streams are also included as streams, and will therefore define intervals as well. Note also that where streams re-combine in an interval after being split and exchanging heat, they are assumed to mix at the same temperature. Subsequently, Azeez, et al. (2013) presented the Supply-Based Superstructure (SBS) approach for HENS, 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 (S&TBS) and the Target and Supply-Based Superstructure (T&SBS) (Azeez et al., 2012).

The comparison of these stage-wise/interval based superstructure techniques done by Azeez, et al. (2013) showed that no one approach consistently gave the lowest Total Annual Cost (TAC). This comparison also raised some questions, particularly with regard to whether exactly the same detailed sizing and costing equations had been used, especially with respect to the LMTD approximations used. The primary purpose of this paper is therefore to compare all these interval based/stage-wise approaches using exactly the same set of equations. In order to do this, it was necessary to investigate the effect of using different LMTD approximations, owing to the fact that most of the superstructure-based studies concerned did not use the most accurate of these approximations and most of them also did not check the accuracy of the approximation used.

1.1 LMTD approximations

Most of the approaches have used Chen's first approximation (more aptly named the Paterson-Chen approximation by Huang, et al. (2012), see Equation 3) for determination of the LMTD (Chen, 1987). Yee et al. (1990) made this choice because neither the Paterson approximation Eq(2) nor Chen's second approximation (called the Underwood-Chen approximation by Huang et al. (2012), Eq(4) approximated the LMTD as zero when either of the exchanger approach temperatures was equal to zero.

Underwood (1970) proposed the following form for calculating the LMTD, where the individual temperature differences are ΔT_1 and ΔT_2:

$$\Delta T_{LMTD,Underwood} = \left[\frac{1}{2}\left(\Delta T_1^{1/3} + \Delta T_2^{1/3}\right)\right]^3 \tag{1}$$

Underwood (1970) pointed out that this approximation is accurate to about 1% even when the ratio $\Delta T_1/\Delta T_2$ is as large as 27. Paterson's (1984) LMTD approximation has the following form:

$$\Delta T_{LMTD,Paterson} = \frac{1}{3}\Delta T_{AM} + \frac{2}{3}\Delta T_{GM} \tag{2}$$

where ΔT_{AM} and ΔT_{GM} are respectively the arithmetic and geometric means of ΔT_1 and ΔT_2. Paterson indicated that the accuracy of this approximation was within 1% for a ratio of $\Delta T_1/\Delta T_2$ equal to 10 (which he considered a large ratio for temperature differences in a heat exchanger). Chen (1987) proposed first:

$$\Delta T_{Paterson-Chen} = \Delta T_{AM}^{1/3} \cdot \Delta T_{GM}^{2/3} \tag{3}$$

and then a modification of the indices in the Underwood approximation:

$$\Delta T_{Underwood-Chen} = \left[\frac{1}{2}\left(\Delta T_1^{0.3275} + \Delta T_2^{0.3275}\right)\right]^{1/0.3275} \tag{4}$$

Chen did not calculate accuracies for these two methods, but showed that his Underwood-Chen method was more accurate than Paterson's over a range of $\Delta T_1/\Delta T_2$ from 1.5 to 10. This inaccuracy was avoided by choosing Chen's first approximation, which is unfortunate, because Chen (1987) indicated that this is the least accurate of the available approximations. Yee, et al. (1990) noted that the Paterson-Chen approximation tends to underestimate the driving force (and it therefore overestimates the area and thus the capital cost). Most subsequent authors have followed the approach of Yee, et al. (1990) in using the Paterson-Chen approximation, although Björk and Westerlund (2002) used the Paterson approximation, noting that it tends to overestimate the driving force and hence underestimate the area (and capital cost). The Underwood-Chen approximation (Equation 4), which is based on Underwood's insightful approximation (Underwood, 1970), has been shown to be most accurate approximation (Chen, 1987), and in this study we argue that it is preferable to use the best possible approximation in the optimisation of HENs. Both approximations were applied for all the approaches to investigate the effect of improving the LMTD approximation on the optima found. It was pointed out by Shenoy and Fraser (2003) that neither Paterson (1984) which presented the approximated LMTD in Equation 2 nor Chen (1987) which presented the approximated LMTD in Equations 3 and 4, considered temperature difference ratios greater than 10 to be important to consider for heat exchanger design. Both of these authors presented numerical results for temperature difference ratios between 1.5 and 10, but neither of them presented the errors for the approximations. However, Paterson (1984) did state that his approximation was accurate to less than 1% up to a temperature difference ratio of 10, Chen (1987) pointed out that Underwood-Chen approximation was the most accurate of the four approximations, and Paterson (1987) conceded that while the Underwood-Chen approximation was less accurate than his approximation at a temperature difference ratio of 1.5 (where the errors were very small), it was more accurate at a ratio of 10 (where the errors were much larger). What neither of these authors pointed out was the much more significant errors of the Paterson-Chen approximation although it was clear to observe in the data Chen presented.

Huang, et al. (2012) compared the effect of using six different LMTD approximations on the solutions of five different examples (mostly from Björk and Westerlund (2002)) using their approach, which was based on the SWS model of Yee and Grossmann (1990), but with fully non-isothermal mixing. The six approximations were the four already discussed, plus the use of LMTD constraints and an ε-LMTD method. They found that Paterson's approximation gave the lowest optima (in terms of TAC). They did, however, recognise that this approximation underestimates the heat transfer area, which indicates that this approach will also underestimate the TAC. They supplemented their approach by adding a step using the actual LMTD to calculate a more accurate TAC for the Paterson approximation. It would have been instructive had they done this with the other approximations as well.

2. Methodology

2.1 General model formulation

The major difference in the formulation of the interval based/stage-wise 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 way in which the boundaries are fixed also defines the intervals in which process streams can exchange heat. Another important difference between the various approaches is the variation in the number of intervals created for heat exchange.

2.2 Programming of models

Each of the stage-wise/interval based approaches covered in the Introduction was then programmed in the same framework and using the same sizing and costing equations (including both sets of LMTD approximations). All examples were modelled as MINLP with the objective being the minimisation of the TAC. All the models were solved in the General Algebraic Modelling System (GAMS) environment (Rosenthal, 2007) version 22.3 using the solver DICOPT++ for the solution of the MINLP, which uses CPLEX for MILP and CONOPT for NLP sub-problems. Solution times were generally reasonable (1 – 90 s) on a PC with an Intel ® Core ™ i7-4700MQ CPU at 2.4 GHz with 16 GB RAM. A comprehensive list of model equations can be found in Yee and Grossman (1990).

3. Results and discussions

3.1 Comparison with previous techniques

The first step undertaken for each example was to find the best possible solution (by choosing different initial conditions for the optimisation) and compare it with the best solution previously obtained for that example, using the Paterson-Chen LMTD approximation. Four examples (Linnhoff problem (Linnhoff et al., 1982), Lee problem (Linnhoff et al., 1982), magnets (Yee and Grossmann, 1990) and Shenoy problem (Shenoy et al., 1998)) were studied and it was found that in most of the cases the solutions obtained were close to the solutions reported in literature. The results obtained in this way were then used as the basis for the other comparison that was done. It was also found that bounds, initialisations, formulation of gamma, exchanger minimum approach temperature (EMAT) can lead to different solutions.

3.2 Comparison with Underwood-Chen LMTD Approximation

The second step undertaken was to compare the best results obtained in the first step with those that were obtained using the Underwood-Chen LMTD approximation in place of the Paterson-Chen approximation.

These comparisons are shown in Table 1, where it will be noted that in most cases the optimum TAC is slightly lower than that obtained using the Paterson-Chen approximation. In some cases the optimum TAC is slightly higher, and in a few cases it is significantly higher. In Table 1, HU and CU represent hot and cold utilities.

Table 1: Comparison of results for the Underwood-Chen LMTD approximation to the Paterson-Chen approximation.

Problem	Approach	Our models Paterson-Chen		Our Models, Underwood-Chen			
		Splits	Units	Splits	Units	TAC	% diff. from Paterson-Chen
Linnhoff	IBMS	1	6			no soln	
	SBS	2	6	1	5	96,123	-0.08 %
	S&TBS	1	5	1	5	90,329	-0.09%
	T&SBS	1	5	0	5	90,310	4.87%
	SWS	2	5	3	6	87,030	-1.43%
Lee	IBMS	2	5	1	5	11,145	-1.64%
	SBS	1	5	1	5	10,570	-1.97%
	S&TBS	1	5	2	5	10,620	0.39%
	T&SBS	2	5	1	5	11,384	-0.80%
	SWS	1	5	1	9	10,760	1.41%
Magnets	IBMS	3	6	3	7	628,684	-1.03%
	SBS	3	7	5	10	594,984	-0.02%
	S&TBS	5	10	4	8	577,501	-0.04%
	T&SBS	4	8	2	8	587,087	-0.02%
	SWS	2	8	2	5	589,681	-0.54%
Shenoy	IBMS (3HU, 2CU)	2	9	1	9	1,151,864	1.41%
	IBMS (2HU, 1CU)	1	7	1	7	1,149,266	-0.25%
	SBS	0	8	1	9	1,255,769	1.55%
	S&TBS	1	10	0	9	1,169,983	-2.09%
	T&SBS	1	9			no soln	
	SWS	1	9	1	9	1253167	1.84%

There are some different ways in which these results can be interpreted. Huang et al. (2012) argued that the approximation that gives the best optimum should be used. What they, in effect, did was to use the approximation that gave the lowest TAC, and then add a step which recalculated the LMTDs and then further optimised the solution on that basis. An even more important insight is gained if you examine the structures of the optimum networks, as indicated by the numbers of splits and units for each particular problem and each particular solution methodology in Table 1. From this comparison (only three out of nineteen solutions have the same structure) it is clear that the optimal structures are almost always different for the two different approximations. This underscores the importance of using the best possible approximation in obtaining such solutions, particularly where the structure is then fixed in a subsequent non-linear optimisation step.
Another way of examining this issue is to compare the results of a solution using an LMTD approximation with the solution obtained when using the actual LMTD for each exchanger (without further optimisation). The results of this comparison are shown in Table 2 for one of the examples studied, using both sets of approximations. This shows that in most cases the differences between the approximation and the actual LMTD are very small. There are, however, a few cases where there are significant differences.
Looking first at the Shenoy Example, shown in Table 2, it is noted that the magnitude of the error is small when the approximate LMTD values are compared to the actual LMTD values. In this example, all the errors for the Underwood-Chen Approximation are less than 0.1 %, whereas for the Paterson-Chen Approximation only three of the nine errors are less than 0.1 % and the largest error is 2.65 %. The Lee example was also studied, but the detailed results are not shown here. In this example, there are some very large errors in the approximations. Examination of the temperature differences at each end of the exchangers reveals that these large errors in the approximations occur when the ratio of the two temperature differences is large, higher than 10. Values of around 30, 50 and 60 were seen for the Lee example. In these cases it was observed that the approximation errors are much lower for Underwood-Chen than for Paterson-Chen, with a highest value of -2.07% compared to 15.6%. The sign of these errors indicates that the underestimation of LMTDs for Paterson-

Chen in such cases is much larger than the overestimation for Underwood-Chen. Thus, although Underwood-Chen overestimates the LMTD and therefore underestimates the area and cost, LMTD and overestimation of area and cost by Paterson-Chen, which leads to more unrealistic results. Shenoy and Fraser (2003) highlighted that, with the Paterson-Chen approximation, such large errors are to be expected at such large ratios of the temperature differences. Figures 1 and 2 examines this more closely: Figure 1 shows the errors for the four approximations discussed earlier over the temperature difference range from 1.0 to 10.0, whereas Figure 2 shows the errors over a range up to 100.0. The Lee problem has shown clearly that temperature difference ratios well over 10.0 may be encountered in HENS problems. In the light of this, it is even more important not to use the Paterson-Chen approximation, due to the large errors associated with it at high temperature difference ratios.

Table 2: Shenoy Example, IBMS (3HU, 2CU)

Paterson-Chen							Underwood-Chen						
Match	LMTD	Approx. LMTD	% diff.	ΔT1	ΔT2	ΔT ratio	Match	LMTD	Approx. LMTD	% diff.	ΔT1	ΔT2	ΔT ratio
1.2.7	20.84	20.79	0.25	11.1	35.0	3.14	1.2.6	20.84	20.81	0.08	9.9	37.8	3.82
1.3.7	19.03	19.02	0.04	14.1	25.0	1.77	1.3.6	19.03	20.22	0.03	14.2	27.8	1.96
1.5.7	64.92	64.87	0.07	90.0	45.0	0.50	1.5.8	64.92	32.64	0.03	22.8	45.0	1.97
2.1.3	24.22	23.98	1.01	50.7	9.10	0.18	2.1.6	24.22	20.20	0.08	41.1	8.00	0.19
2.4.8	34.80	34.06	2.11	84.1	10.0	0.12	2.2.4	34.80	55.93	0.00	50.0	62.3	1.25
3.1.1	58.60	58.57	0.05	45.0	74.7	1.66	2.4.9	58.60	34.48	0.03	83.0	10.0	0.12
4.2.4	40.03	39.98	0.12	25.0	60.1	2.41	3.1.1	40.03	63.99	0.03	45.0	87.7	1.95
4.3.4	44.52	44.48	0.11	30.0	63.1	2.10	4.3.4	44.52	44.53	0.04	30.0	63.2	2.11
5.3.7	35.04	34.11	2.65	9.10	89.0	9.78	5.2.7	35.04	99.50	0.00	100	99.0	0.99

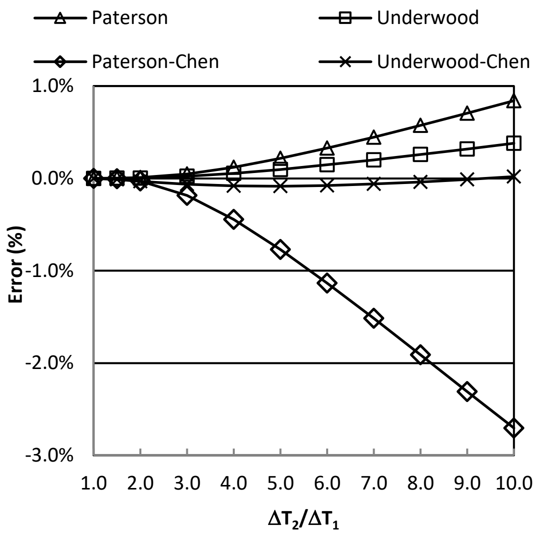

Figure 1: Temperature difference approximation errors, ratios up to 10.

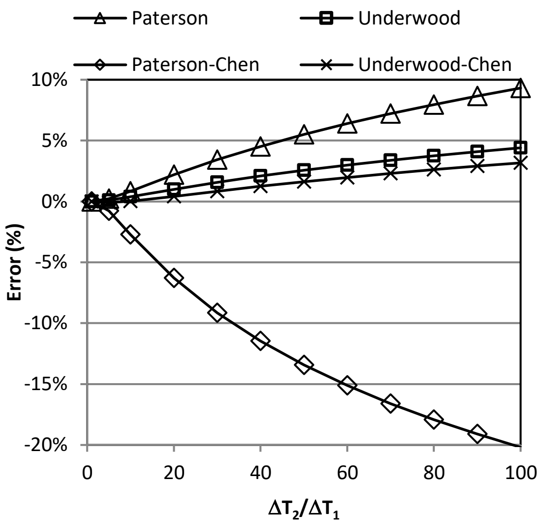

Figure 2: Temperature difference approximation errors, ratios up to 100.

4. Conclusions

Comparing the results of all the different stagewise/interval-based superstructures on the same basis, in terms of detailed equations for sizing and costing, it was found that the differences in terms of structure and optimum TAC obtained was as previously noted: no one approach consistently gives the best optimum value over a range of problems. When the effect of using a different LMTD approximation was examined, it was found that this does affect not only the optimum value of the TAC obtained, but also the structure of the optimum heat exchange network. This study has shown that the accuracy of the approximations is a strong function of the ratio of temperature differences – where this is large the Paterson-Chen approximation seriously underestimates the value of the LMTD, and gives much larger errors than any of the other approximations.

There is no way of knowing a priori what sort of temperature difference ratios will be encountered in a particular problem. Therefore, because the Underwood-Chen approximation gives LMTD values much closer to the actual LMTD, it is recommended that in future this approximation should be used in MINLP optimisations of heat exchanger networks, instead of the Paterson-Chen Approximation, especially because of the very large approximation errors when the temperature difference ratio is high, as has been shown to be the case for the Lee problem. It is planned to repeat this comparison for mass exchange networks to see if the same results apply for mass exchange problems.

Acknowledgements

This study was partly supported by the National Research Foundation of South Africa, and the Research Office of the University of Cape Town, South Africa.

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