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Heat Exchanger Network Synthesis Including Detailed Exchanger Designs Using Mathematical Programming and Heuristics

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The synthesis of heat exchanger networks (HENs) has mainly been done through the use of approximate models for each of the individual heat exchangers that comprises the network. These approximate models do not adequately take into account key parameters such as the overall heat transfer co-efficient, TEMA standards, pressure drops, F_T correction factors, and multiple shells. These factors can significantly alter the cost of the network. This paper presents a new methodology for the synthesis of heat exchanger networks using detailed heat exchanger design models that takes into account the aforementioned design parameters. The newly developed method involves the following steps. First, a SYNHEAT (Yee and Grossmann, 1990) MINLP model is solved. The individual exchangers for the resulting network are then designed using heuristics, TEMA standards and the Bell-Delaware method. From the designs obtained for these individual exchangers, correction factors are inserted into the SYNHEAT model that account for changes in overall heat transfer coefficient, TEMA choices, pressure drops, Ft correction factors and the effect of multiple shell passes. The SYNEAT model is then re-run and individual exchangers re-designed and the procedure repeated until convergence is achieved. For each iteration the change in each correction factor is limited to avoid the omission of certain solutions. While the methodology cannot guarantee global optimality it can ensure that the synthesised processes are physically achievable and has also been shown to converge on physically meaningful parameters without the explicit formulation of complicated non-linear equations in the MINLP formulation.

1. Introduction

Heat Exchanger Network Synthesis (HENS) is one of the most well-known subjects in Process Integration as it can be used to decrease energy costs and environmental impact of a process through the utilisation of process heat rather than through the use of utilities. HENS has been attempted using a variety of methods, with most methods falling under either sequential approaches, like Pinch Technology, or simultaneous approaches. The simultaneous mathematical programming approach has received the most attention in recent years due to advances in solver capabilities and the ability to simultaneously consider multiple factors relating to the overall cost of the network using mixed-integer non-linear programming (MINLP).

The majority of mathematical programming approaches to HENS use a stage-wise superstructure-based model (SYNHEAT) first proposed by Yee and Grossmann (1990) that embeds a large number of possible stream matches into a superstructure that allows for stream splitting and isothermal mixing. This method is very good for considering potential networks, however the $\mathcal{NP}$ hard formulation makes it difficult to solve to global optimality with current solvers (Furman and Sahinidis, 2002). The formulation fails to consider details involved in heat exchanger design, such as changing heat transfer coefficients, pumping costs, number of baffles, tube passes, and number of shells, and cannot be extended to include these as the combinatorial nature of the problem combined with the increased non-linearity will result in non-optimal solutions. While the use of constant heat transfer coefficients and the simplifications of ignoring design

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decisions is convenient due to the solver limitations, the resulting heat exchanger network (HEN) can potentially be very far from the optimum once all design decisions are considered. Nevertheless a number of improvements and additions have been made to the original model, including recent work from Jongsuwat et al. (2014), where multiple matches are included in stream branches and that of Angsutorn et al. (2014) where solutions obtained from pinch technology are improved using mathematical approach.

Mizutani et al. (2003a) used a Generalised Disjunctive Programming (GDP) model to optimise individual exchangers using the Bell-Delaware method for shell-side calculations. Mizutani et al. (2003b) extended this model to include network optimisation. The model makes use of disjunctions in the topology selection and at the level of individual exchanger design. The model fails to take into account TEMA (Tubular Exchanger Manufacturers Association) standards and multiple shell and tube passes and makes use of an iterative procedure that ensures that the overall heat transfer coefficients for each exchanger are correct in the final design.

Ravagnani and Caballero (2007a) follow a similar procedure for the synthesis of individual exchangers, however the authors used a tube counting table to follow TEMA standards. They extended their model to include a bi-level decomposition where a SYNHEAT model is set up to do the network optimisation, followed by individual unit optimisation. The recalculated heat transfer coefficients are then substituted back into the SYNHEAT model and re-solved and global costs compared. This is done until 2 consecutives solutions are worse than the previous structure.

The synthesis procedure presented in this paper makes use of a similar procedure to that of Ravagnani and Caballero (2007b) in that there is a bi-level optimisation in which on one level network synthesis is done and on the other detailed individual exchanger designs. The network synthesis makes use of simplified models (as used in the Yee and Grossmann SWS model) for exchangers in order to address the complexities involved with the simultaneous optimisation of the network. These are discussed in detail in Yee and Grossmann (1990b). However a key difference lies in the formulation of the objective function which is discussed in Section 2. The objective function of network synthesis model presented in this study is modified through the use of detailed designs in order to provide it with more information regarding non-ideal behaviour of the actual individual exchanger designs. In this way it is possible to exclude networks that will no longer be optimal once all of the non-ideal considerations are taken into account and keep the MINLP model simple enough to consider large problems. The method is detailed below while section 3 presents two examples.

2. Methodology

The methodology for the topology optimisation is the same as that of the SYNHEAT method presented by Yee and Grossmann (1990) with small adjustments, so only the additions will be presented in this paper and the reader is encouraged to refer to the original paper for the full formulation. The main difference in the formulation of this paper and the original SYNHEAT model is the inclusion of correction factors in the objective function that allow for it to converge to the same total annual cost (TAC) as the network that is obtained through a rigorously designed individual heat exchangers after the optimisation.

$$\begin{aligned}\min\ & \sum_{i\in H} CUC.qc_i + \sum_{j\in C} HUC.qh_j + CF\Big(\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} z_{i,j,k} NSP_{i,j,k} + \sum_{i\in H} zcu_i + \sum_{j\in C} zhu_j\Big) \\ & + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} NSP_{i,j,k} AC\big[\, CorF_{i,j,k} q_{i,j,k} / NSP_{i,j,k} U_{i,j,k} (LMTD_{i,j,k})\big]^{AE} + \sum_{i\in H} AC\big[\, qc_i / U_i (LMTD_i)\big]^{AE} \\ & + \sum_{j\in C} AC\big[\, qh_j / U_j (LMTD_j)\big]^{AE} + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} NSP_{i,j,k} PC.z_{i,j,k}\big[\, delPc_{j,k} VolFc_j + delPh_{i,k} VolFh_j\big]\end{aligned} \tag{1}$$

Where CUC and HUC are the costs of the cold and hot utilities per kW, $q_{i,j,k}$ is the energy transferred between hot process stream i with cold process stream j in interval k, qh_j and qc_i is the energy transferred from hot utility to cold stream j and from cold utility to hot stream i. $z_{i,j,k}$ is the binary variable representing a process stream match between hot process stream i with cold process stream j in interval k. zcu_i and zhu_j is the binary variable representing a stream match between a cold process stream and a hot utility and a hot utility and a cold process stream. CF is the fixed cost associated with an exchanger, AC is a variable cost factor based on the area, AE is the area cost index, and PC is the cost associated with pumping. $NSP_{i,j,k}$ is a correction factor that accounts for the number of shell passes, discussed below. $delPc_{j,k}$ and $delPh_{i,k}$ are the pressure drops per shell pass of the cold and hot streams in interval k. $VolFc_j$ and $VolFh_i$ are the volumetric flowrates of the cold and hot streams. $U_{i,j,k}$ are the overall heat transfer coefficients that are match dependent and corrected for in each iteration. $CorF_{i,j,k}$ are match-specific correction factors that are applied to the areas to make them converge on an area that can be rigorously designed outside of the MINLP formulation. These factors correct for the unapproximated LMTD, the F_T correction factor, and

TEMA decision. This new objective function aims to encompass all of the cost features of a network generated in a rigorous way. The cost features that are not possible to model in the

MINLP network formulation, due to the non-linearities involved in the calculation of these factors, are lumped and added into the objective function.

The differences between this new formulation and the objective function used in the original SWS and the models of Mizutani et al. (2003b), which used GDP and Bell-Delaware method, and that of Ravagnani and Caballero (2007b), which used tube counting tables to follow TEMA standards, are outlined below. Firstly, the pressure drop is now included as an implicitly calculated factor. This means that the model can choose to exclude matches with excessive pressure drops, but has the weakness of not being able to design individual exchangers that can mitigate this pressure drop and also that stream splits can no longer be included, unless the flow splits can be explicitly calculated in the model and included in the objective function. Notice also that the pressure drops are associated with a stream and not the shell- or tube-side.

The fixed cost is now multiplied by the number of shells that are required for each match as the fixed cost would require the purchasing of multiple identical shells. This is also added into the variable area cost term by dividing the area by the number of shells that would be required for the individual exchangers and multiplying that area by the number of shells that would be needed in the series shell exchangers. Note that this gives a network with realistic individual exchangers. However it would also add to the overall cost of the model and will therefore make the solutions obtained in this methodology have a higher TAC than other methods in literature.

A further change to the original SYNHEAT model is the exclusion of stream splits. This was done in order to account for the pressure drops in the way described above. If stream splits would have been included, a new variable would have been needed that would have added to the complexity of the model by optimizing the stream splits.

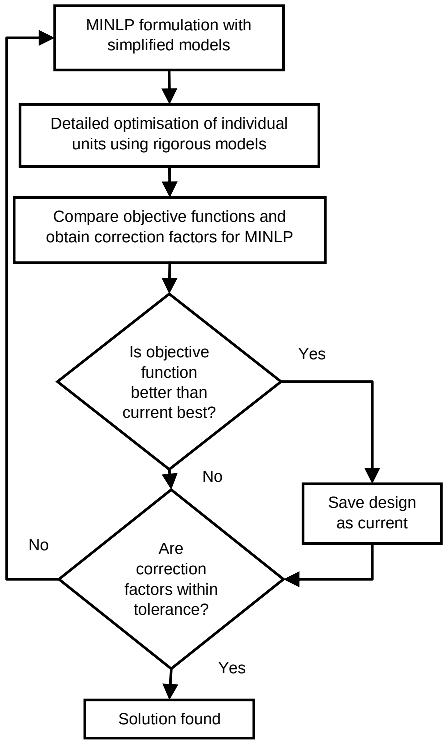
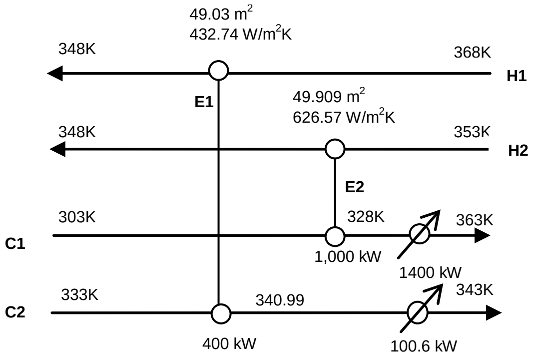


Figure 1: The proposed iterative procedure used in this study



Area cost ($/y) = 5,631.685, pumping cost ($/y) = 1,491.632, utility cost ($/y)

Figure 2: Optimal network for example 1

After the initial SWS model is solved in GAMS with the additions mentioned above, the network is modelled using heuristics in an Excel spreadsheet using the Bell-Delaware method as well as heuristics described by Serth (2007). Note that this means that exchangers are not rigorously optimised, but rather that practical considerations and empirical data is used to do the design in this paper. This can be changed to include detailed calculations, as this step is performed outside of the topology optimisation routine. Once the detailed designs are obtained, the correction factors are solved for. These factors, detailed above, are limited to a change of some number to avoid the solution space being too drastically altered and potential solutions excluded. In the examples detailed below, the change was restricted to

10 % for each of the factors. Note that this would mean that the shell pass correction factor will have non-integer values in the iterations, however they will converge upon integer values by the end of the algorithm. These correction factors are now inputted as parameters into the MINLP model and the model is re-solved. If the generated network is identical to the previous network and the new correction factors are the same as the previous correction factors, the procedure is stopped. If the network is new, this network is designed using the heuristic procedure again and new correction factors are derived. The iterative algorithm is shown graphically in Figure 1.

Table 1: Data for Example 1 and 2, taken from Mizutani et al. (2003b)

EXAMPLE 1				EXAMPLE 2			
	m (kg/s)	T_{in} (K)	T_{out} (K)		*m* (kg/s)	T_{in} (K)	T_{out} (K)
H1	8.15	368	348	H1	134	413	313
H2	81.5	353	348	H2	235	433	393
C1	16.3	303	363	H3	12.1	483	318
C2	20.4	333	343	H4	28.5	533	333
HU		500	500	H5	102	553	483
CU		300	320	H6	14.2	623	443
				H7	38.9	653	433
				C1	235	543	658
				C2	143	403	543
				C3	104	293	403
				CU		293	298
				HU		700	700

Where ΔT_{min} is 10 K. Area cost = 1,000 (number of shells) + $60.A^{0.6}$ \$/y, where A = m^2.
Pumping cost = $0.7(\Delta P_t m_t/\rho_t + \Delta P_s m_s/\rho_s)$, where ΔP = Pa, m = kg/s, and ρ = kg/m^3. Cooling Water

Table 2: Stream data for Example 1 and 2, taken from Mizutani et al (2003b)

$\mu(kg/m^3)$	$\rho(kg/m^3)$	$C_p(J/kg)$	$k(W/(m.K))$	$r_d(W/(m.K))$
2.4×10^{-4}	634	2,454	0.114	1.7×10^{-4}

3. Results

Two examples are used to illustrate the proposed methodology described above.

3.1 Example 1

The first example is from Mizutani et al. (2003b) and involves the optimisation of a heat exchanger network involving two hot streams and two cold streams with one hot and one cold utility available. The data for the problem is presented in Table 1, with stream data presented in Table 2.

As discussed in the methodology, the implicit factors that are added into the model are initialised at values that underestimate the objective function, so the $NSP_{i,j,k}$ is initialised at 1 pass, $CorF_{i,j,k}$ begins at 1, $U_{i,j,k}$ at 750 W/m^2K, and the pressure drops, $delPc_{j,k}$ and $delPh_{i,k}$, are initialized at 10,000 Pa.

The proposed algorithm generates the final network shown in Figure 2 with a global annual cost of \$97,159.32 after 11 iterations. The optimal HEN topology was identified in the first iteration and stayed constant throughout the procedure. Due to the 10 % maximum allowable change per iteration for each factor that is inputted from outside the optimization loop, it took some time for the pressure drops and heat transfer coefficients to converge upon the design obtained.

While the topology is the same, the objective function values differ to other authors. The comparisons are presented in Table 4. The differences are due to the method of individual exchanger design described in Section 2. The designs are overdesigned by 1 % and 4.4 % for exchanger 1 and 2 compared to the actual minimum area required for the heat transfer. This could be the reason for pumping costs being higher than other solutions. Added to this is the fact that the other authors used a rigorous optimisation for the individual exchangers that involved an objective function that focused on minimising area and pumping costs, whereas the method presented here uses heuristics to get a practical design that looks to maximise heat transfer and uses practical considerations. Particularly important is that the designs in Mizutani et al. (2003b) do not consider multiple tube passes and therefore underestimate the pressure drops by a potentially large amount.

Interestingly, the correction factors, $\mathrm{CorF}_{i,j,k}$, converge upon 1.08298 and 1.06382 for exchanger E1 and E2, showing that the SYNHEAT model alone cannot predict the actual areas of the exchangers obtained through detailed modelling. It is vital that the topology optimisation has access to these non-ideal factors so that a realistic optimum can be obtained. The next example further illustrates the usefulness of this approach.

3.2 Example 2

The second example is also taken from Mizutani et al. (2003b) and involves the optimisation of a heat exchanger network involving seven hot streams and three cold streams with one hot and one cold utility available. The data for the problem is presented in Table 1, with stream data in Table 2, and the initialisations for this example are identical to example 1, except for the number of shell passes initialised to 2 to speed convergence as the exchangers are large in this example and often require 2 shell passes. The initial SYNHEAT model has 136 discrete variables. During the solution procedure 7 separate topologies were found and the procedure converged after 31 iterations. The optimal solution, however was found at iteration 21, and that network is shown in Figure 3. The solution is also compared to Mizutani et al. (2003b) in Table 3.

Table 3: Comparison of solutions with other authors for Example 1 and 2

Cost ($/y)	Example 1			Example 2		
	Mizutani et al. (2003b)	Ravagnani and Caballero (2007b)	This paper	Mizutani et al. (2003b)	This paper (optimal)	This paper (converged)
Total annual cost	95,852.0	96,137.71	97,159.3	5,159,098	4,203,057	4,403,365
Area cost	5,608.0	5,675.52	5,631.68	24,123	64,982	67,676
Pumping cost	244.0	462.19	1,491.63	4,807	46,099	47,593
Utility cost	90,000.0	90,000.0	90,036.0	5,154,291	4,091,975	4,288,095

The solution obtained has significantly higher pumping and area costs in comparison to Mizutani et al (2003b). This is expected due to the considerations of this study, namely the fact that the fixed cost of the exchangers are multiplied by the number of shells that need to be installed and that the pressure drops consider multiple tube and shell passes, a consideration that will have significant consequences compared to the assumption of 1 shell pass and 1 tube pass made by Mizutani et al. (2003b).

When Mizutani et al. (2003b) solved this problem, the detailed design of the network contained 8,452 discrete variables, 16,939 equations, and 20,408 continuous variables. The size of this problem is very likely to have caused the non-optimal solution as the highly non-linear and combinatorial nature of the problem could have caused convergence upon local optima as opposed to the global optimum.

In this study, the reason that the optimal solution was found at iteration 21 and the final converged solution is different to the optimal solution is most likely due to the correction factors affecting the solution space and the final converged solution being a local optimum. It is therefore impossible to guarantee that this method can give a global optimum solution, however the generation of many potential networks and detailed evaluation of these networks is worthwhile. The inclusion of the external detailed design ensures that the networks are evaluated and allow for the MINLP network optimisation access to more detailed information implicitly.

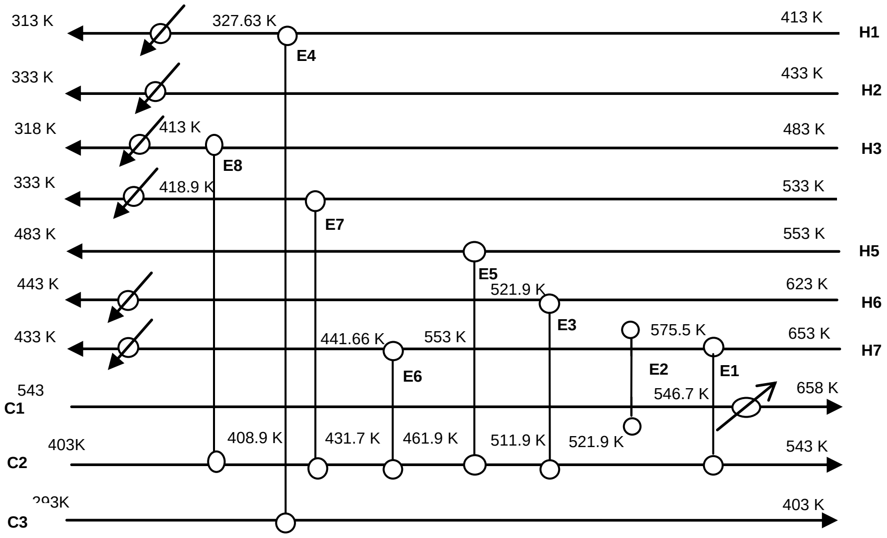
4. Conclusions

This paper presents a new algorithm for the synthesis of heat exchanger networks including detailed heuristic design of individual heat exchangers. The method combines 2 separate stages, namely network topology optimization and a design stage that models the individual exchangers. These 2 elements are combined with a novel algorithm that allows for the MINLP topology to converge upon the same network that is rigorously designed, allowing many potential networks to be evaluated and enhancing the chances of not only converging upon an optimal solution, but also a physically achievable solution.

The algorithm uses correction factors in the objective function to force the objective function towards the solution obtained for the same network that is rigorously designed externally. It uses initializations that underestimate the objective function for all correction factors and limits the change that can occur between iterations to avoid omitting potential networks.

The method was successful in finding potential networks and screening for competitive solutions for the examples tested.

It is also possible to automate this procedure using models similar to those of Mizutani et al. (2003b) and Ravagnani et al. (2007b) and incorporating the iterative procedure of this study. The solution is likely to be closer to the mathematical optimum, but without the use of heuristics the network may not be physically viable. The method presented can also be applied using any rigorous modelling software such as ASPEN HTRI or similar thermodynamic modelling to ensure that the network converges on a physically achievable solution.



Area cost ($/y) = 64,981.97, Pumping cost ($/y) = 46,099.06, Utility cost ($/y) = 4,091,975.98, Global annual cost ($/y) = 4,203,057.01

Figure 3: Optimal network for Example 2

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