GLOBAL OPTIMIATION OF HEAT ECHANGER NETWORK SYNTHESIS USING INTERVAL BASED TECHNIQUE

Karittha Kittijirakul

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science

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Global Optimization of Heat Exchanger Network Synthesis Using Interval Based Technique

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การเพิมประสิทธิภาพของการสังเคราะห์เครือข่ายแลกเปลียนความร้อนเพือนาความร้อนส่วนเกิน กลับมาใช้ใหม่

น.ส.กริษฐา กิตติจิระกุล

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
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วิทยาลัยปิโตรเลียมและปิโตรเคมี จุฬาลงกรณ์มหาวิทยาลัย
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By	Miss Karittha Kittijirakul
Field of Study	Petrochemical Technology / Polymer Science
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อ.ที่ปรึกษาหลัก : ผศ. ดร.กิติพัฒน์ สีมานนท์

การสังเคราะห์เครือข่ายการแลกเปลี่ยนความร้อน(HEN) เป็นหัวข้อการวิจัยที่ใช้แนวคิดของเศรษฐกิจหมุนเวียน และมุ่งเน้นไปที่การนำความร้อนเหลือทิ้งกลับมาใช้ใหม่ โดยมีเป้าหมายในการลดของเสียให้เหลือน้อยที่สุดและเพิ่มการใช้ทรัพยากรผ่านการรีไซเคิล การสังเคราะห์ HEN ใช้วัตถุประสงค์การออกแบบในการลดต้นทุนรวมต่อปี(TAC)ให้เหลือน้อยที่สุด โดยการวางตำแหน่งเครื่องแลกเปลี่ยนความร้อนในกระบวนการผลิตอย่างเหมาะสม เพื่อประหยัดการใช้สาธารณูปโภคและต้นทุนจากขนาดของเครื่องแลกเปลี่ยนความร้อน งานวิจัยนี้ประกอบด้วยสองส่วน; กลยุทธ์การเพิ่มประสิทธิภาพการหาคำตอบดีที่สุดและแบบจำลองการสังเคราะห์HENแบบจำลองโครงสร้างแบบ stage-wise เป็นพื้นฐานสำหรับการสังเคราะห์ HEN ซึ่งใช้เทคนิคการโปรแกรมจำนวนเต็มแบบไม่เชิงเส้นแบบผสม (MINLP) ในส่วนของของกลยุทธ์การหาคำตอบดีที่สุดโดยการแบ่งพลังงานร้อนออกเป็นหลายช่วง และนำมาใช้เพื่อให้มั่นใจว่า HEN ที่ สังเคราะห์มานั้นให้ค่าTAC ต่ำที่สุด เป้าหมายหลักคือการสังเคราะห์ HEN ที่มีค่า TAC ต่ำที่สุดโดยใช้กลยุทธ์การหาคำตอบดีที่สุด ผลลัพธ์แสดงให้เห็นว่าในตัวอย่างขนาดเล็ก การเพิ่มประสิทธิภาพการหาคำตอบที่ดีที่สุดสามารถลด TAC ได้อย่างมากเมื่อเทียบกับกรณีศึกษาจากงานวิจัยอื่น อย่างไรก็ตาม ในกรณีตัวอย่างที่ใหญ่ขึ้น การเพิ่มประสิทธิภาพโดยรวมด้วยการขยายจำนวนการแบ่งพาร์ติชันที่เพิ่มขึ้น สามารถลดค่าTAC โดยรวมได้อย่างมาก

สาขาวิชา เทคโนโลยีปิโตรเคมี	ลายมือชื่อนิสิต
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6478101363 : MAJOR PETROCHEMICAL TECHNOLOGY
KEYWOR D: Heat exchanger network synthesis/ Global optimization/ Mixed-integer nonlinear programming

Karittha Kittijirakul : Global Optimization of Heat Exchanger Network Synthesis Using Interval Based Technique. Advisor: Asst. Prof. Kitipat Siemanond, D.Eng.

Heat exchanger network (HEN) synthesis is a conventional research topic that utilizes the concept of Circular Economy and focuses on waste heat recovery with the goal of minimizing waste and enhancing resource utilization through recycling. HEN synthesis employs the design objectives of minimizing Total Annualized Cost (TAC) by optimally positioning heat exchangers in the process to save utility usage and capital cost from exchanger sizes. This work consists of two parts; Global optimization strategy and the HEN synthesis model. The stage-wise superstructure model is the basis for the HEN synthesis, which employs mixed integer nonlinear programming (MINLP) techniques in the general algebraic modeling system (GAMS). The ongoing challenge of global optimization strategy by partitioning the hot utility duty into several intervals is utilized to assure globally optimal HENS solutions. The primary goal is to synthesize HEN with minimum TAC using global optimization. The results show that in small cases, global optimization can significantly reach minimum TAC as ones from the case study from publications. However, in larger cases, global optimization with the extension of increasing partitioning numbers can significantly reduce TAC close to ones from publications.

Field of Study:	Petrochemical Technology	Student's Signature ....
Academic Year:	2023	Advisor's Signature ....

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Karittha Kittijirakul

TABLE OF CONTENTS

Page

LIST OF TABLES

Page

LIST OF FIGURES

Page

CHAPTER 1
INTRODUCTION

The development of Thailand towards Thailand 4.0 must overcome many problems and obstacles such as degradation of resources, overflowing garbage, and global warming. Ministry of Science and Technology aims to drive Bio-Circular-Green Eco-nomic Model (BCG), which is a new economic development model that accelerates economic growth by leaps and bounds on the basis of sustainable development. Over the past several decades, the Thai economy has grown slowly. The government therefore needs to accelerate the Thai economy by shifting the model of Thai economic and social development to a new model called the BCG Economy Model, which will be an important mechanism in driving the Thai economy to grow by leaps and bounds. The new economy covers three key areas, with a brief guideline as follows;

1. Bioeconomy focuses on applying high-level knowledge in biotechnology and biodiversity costs.
2. Circular Economy: Emphasis is placed on the utilization of raw materials throughout the life cycle and the use of old waste materials to create products, thereby reducing waste and overall environmental impact.
3. Green Economy that focuses on environmental benefits and sustainable development is the ultimate goal.

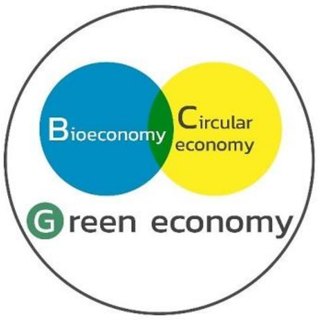

Figure 1.1 The relationship of the biological economy, circular economy and green economy. (NSTDA (Thailand), 2020).

Nowadays, the trend of energy conservation continues to be popular, due to sustainable development approach which is a development model that focuses on sustainability goals that do not cause negative effects on society and the environment or have the least effect on enhancing economy. So, we can follow sustainable development to conserve energy, save the environment by reducing the emission, and solve the global warming problem. Another trend to support the energy conservation is circular integration that applies the closed-loop material systems concept to reduce the resource and energy consumption for the sustainable production of the product in industrial operation and consists of process integration, industrial ecology, and circular economy (Walmsley, 2019).

Figure 1.2 The framework of circular integration incorporating the ideas of circular economy, industrial ecology, and process integration.(T. Gordon et. al.,2017).

Many industrial processes can reduce energy consumption by using a heat exchanger with the counter-current flow between a couple of hot and cold process streams to transfer the heat from hot to cold streams, reducing hot or cold utilities and satisfying the target temperatures of both streams. As a result, this process of heat integration is called HEN synthesis which helps save energy consumption in terms of mitigating operation costs and the environmental impact.

HEN synthesis employs the design objectives of minimizing TAC by optimally positioning heat exchangers in the process. The first HEN synthesis was developed by using Pinch Technology (PT) to sequentially optimize the network (Linnhoff B, 1983). The next HEN model called the stage-wise superstructure (SWS) model was introduced by simultaneous optimization HEN (Yee TF, 1990). The SWS model objectives are to minimize the TAC to synthesize a local-optimum HEN.

Global optimization and the HEN synthesis model compensate for our two-part strategy to synthesize a global-optimum HEN. First, the SWS model is the basis for the HEN synthesis, which employs MINLP techniques with outer approximation DICOPT. The sub second strategy of global optimization by partitioning the utility heat duty into several intervals is utilized to assure global-optimum HENS solutions. The primary goal is to synthesize HEN with minimum TAC using global optimization in comparison to published case studies. The process optimization approach can further be applied to the Bio-Circular-Green Economic Model (BCG) to develop more environmentally friendly processes.

CHAPTER 2
LITERATURE REVIEW

2.1 Heat Exchanger Network Synthesis (HENS)

Heat exchanger network synthesis is a conventional research topic in Process Systems Engineering, with the goal of reducing annual operating costs and capital costs by positioning heat exchangers optimally in the network. HENS synthesis can be characterized as highly combinatorial, nonlinear, and nonconvex optimization problem, all of which contribute to computing challenges manifested as extended calculation times or the identification of suboptimal global solutions. Consequently, over the last 40–50 years, numerous design technologies and approaches have been developed with substantial applicability to practical practice. HENS has been studied since the mid-twentieth century (Broeck HT, 1944), and numerous models have been proposed to address these problems since its introduction, as mentioned in (Furman KC, 2002) review articles on heat exchanger network synthesis, followed by (Klemeš JJ, 2013) and (Yuen, 2020) research publications. (Morar M, 2010) also offered a literature review until 2008. The Pinch Analysis is an extensively utilized HENS technology (Linnhoff B, 1983). Its concepts have been continuously improved over the years with the goal of addressing a wide range of challenges, such as HEN retrofit (Piacentino, 2011) and total site integration (Bandyopadhyay S, 2010). It is argued, however, that mathematical programming techniques capable of dealing with HENS problems offer the most effective way to efficiently incorporate all the aspects.

2.2 Pinch Technology (PT)

The Pinch Technology (PT) technique was created, with goals of maximizing heat recovery, minimizing utilities, reducing the number of stream matches, and reducing exchanger areas (Linnhoff B, 1983). The network is then designed to become as close to the goals as possible by locating thermodynamic bottlenecks, also known as pinch points, by constructing a composite curve between hot and cold streams that can inform about minimum hot utilities, minimum cold utilities, and maximum heat recovery at a predetermined minimum temperature difference. The next objective was to formulate mathematical programming to simultaneously optimize the trade-offs of operating cost and capital investment cost.

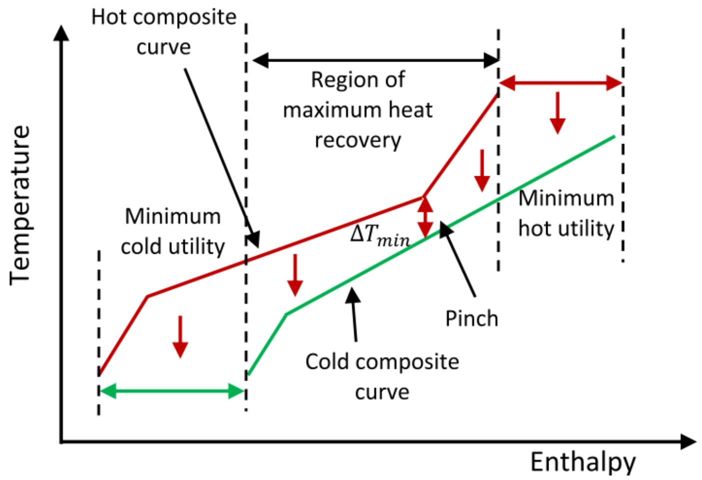

Figure 2.1 HENS hot and cold stream composite curves. (Linnhoff et. al., 1983).

2.3 Stochastic-based Approaches

Procedures for solving problems can be approached in a variety of ways. The majority of stochastic-based approaches (metaheuristics-based methods) are not included in this evaluation. A comparison of our global solutions to those discovered in the literature revealed that many stochastic-based algorithms do not guarantee global optimality, despite the fact that they frequently achieve it in practice. These types of algorithms are also known to require substantial human interaction in other words, they are not automated. Most of these approaches, such as genetic algorithms (Fieg G, 2009) and (Aguitoni MC, 2018), simulated algorithms (Peng F, 2015) and (Pavao LV, 2017), particle swarm optimization (Silva AP, 2010) and (Huo Z, 2013), and hybridization between different algorithms (Pavao LV, 2016) and (Pavao LV, 2018), are worth highlighting since they are capable of handling large-scale problems. We do not go into detail on the literature review of stochastic-based approaches, which cannot ensure global optimality and require specific parameter adjustment for high computational performance. In this study, we focus on the usage of the MINLP techniques.

2.4 Stagewise Superstructure Model (SWS)

The stage-wise superstructure (SWS) model was developed as a solution to synthesize heat exchanger networks than the previous method, which used the general algebraic modeling system or GAMS, which was well-known in the optimization research study field (Yee TF, 1990). The model was solved using mixed-integer non-linear programming (MINLP), which includes non-linear equations, binary variables, the basic heat transfer equation, and logical restrictions for approach temperature in the model and utilities at the network's extreme ends. The binary variables introduced first in this model for heat exchanger network synthesis's field can be used to determine network topology, heat exchanger location, and utilities between hot and cold streams, which are governed by the assumption of isothermal mixing after the streams exit the heat exchanger.

Furthermore, however unlike old model, this technique does not require a minimum temperature difference before optimization and can discover an area for an exchanger, but the old model cannot. To avoid numerical issues, they used approximate logarithm mean temperature difference (LMTD) in this model (Chen JJJ, 1987), then utilities cost, exchanger area, and stream matching are optimized concurrently with the objective function of minimizing the TAC, which includes annual operating cost, area cost, and investment cost. Furthermore, this work served as the foundation for subsequent literature on heat exchanger network synthesis.

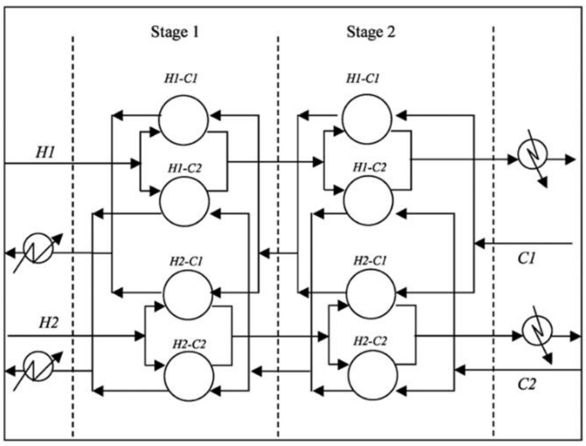

Figure 2.2 Two-stage network superstructure. (Yee TF, 1990).

.Objective function

$$min\left[\sum_{i\in H} CUCqc_i + \sum_{j\in C} HUCqh_j + CF\left(\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} z_{i,j,k} + \sum_{i\in H} zcu_i + \sum_{j\in C} zhu_j\right)\right.$$
$$+\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} AC\left(\frac{q_{i,j,k}}{(U)(LMTD_{i,j,k})}\right)^{AE} + \sum_{i\in H} AC\left(\frac{qc_i}{(U_i)(LMTD_i)}\right)^{AE}$$
$$\left.+\sum_{j\in C} AC\left(\frac{qh_j}{(U_j)(LMTD_j)}\right)^{AE}\right]$$

From the above equation, The first and second terms in the following equation are the utility costs for cold and hot utilities, respectively. The third term is fixed cost, which is calculated by summing binary variables and includes fixed costs for heat exchangers, cold utilities, and hot utilities. The final three terms are heat exchanger, cold utility, and hot utility area charges. The fundamental diagram from this study depicts all possible stream matching scenarios for hot and cool streams with a counter-current pattern.

2.5 Mixed Integer Non-linear Programming (MINLP)

HENS models can be divided into sequential synthesis and simultaneous synthesis (Furman KC, 2002). Models are solved sequentially by sequential synthesis; the solution of an intermediate model parameterizes the subsequent model. A sequential synthesis approach is illustrated by the linear programming (LP) transshipment model, the mixed-integer linear programming (MILP) transshipment model (Papoulias, 1983), and the nonlinear programming (NLP) superstructure model (Floudas CA, 1986); these models are solved sequentially and aim to minimize the utility cost, the number of matches, and the investment cost, respectively. A sequential method does not imply that the global solution will be optimal; for particular, the global solution may not have the lowest potential utility cost. Simultaneous synthesis models, such as the MINLP model, eliminate the limitations of the sequential approach by focusing exclusively on the operating cost (Yee TF, 1990). Due to the possibility that simultaneous optimization models have a more desirable global optimum than sequential synthesis models (Escobar M., 2013).

Among all prior studies on HENS, the technique that has gained the greatest attraction is one that offers a superstructure in collaboration with the development of a mixed integer nonlinear model (MINLM) that can be solved using mixed integer nonlinear programming (MINLP) methods. Many of the most remarkable attempts in the last five years that do not target global optimization include those of (Hong X, 2017), which established a novel transshipment model that incorporates stream splitting, by-passing, and recycling, as well as nonisothermal mixing and counting exchangers, in a way similar to that described by (Barbaro A, 2005). A novel HENS linearization technique based on stage-wise superstructure terminating in a MILP problem was developed by (Beck A, 2018) with the goal of reducing solution time. The solution of this MILP problem is then used to initialize the MINLP model. (Nemet A, 2019) proposed a two-step technique in which the first phase is to establish a structure by solving a MILP in order to identify various answers in an acceptable amount of time. In the following stage, they evaluate a reduced MINLP model , in which unsatisfactory possibilities from the previous step are prohibited. Finally, (Ziyatdinov NN, 2020) proposed an optimal heat exchanger network synthesis method based on sequential splitting of process streams.

Numerous techniques to solving the HENS mixed integer nonlinear model (MINLM) utilizing MINLP approaches; some employ Lagrangian decomposition, a large number use outer approximation (DICOPT), and still others use global optimization solvers that ensure globally optimum solutions that have been published recently. (Bogataj M, 2012) proposed an alternative approach for generating globally optimum solutions to the HENS issues utilizing an aggregated substructure to reduce the number of nonconvex terms that are constrained by large-scale structures. The approach incorporates convex approximation and under-estimators in order to narrow the gap between the lower and upper bounds. Another extension concerning staged superstructures,(Jongsuwat P, 2014)proposed incorporating substages and nonisothermal mixing, which was later solved globally by (Kim SY, 2017). Utilizing RYSIA, (Faria D., 2015) solved HENS problems to globally optimal by a bound contraction methodology based on the isothermal mixing stagewise superstructure with both small- and medium-scale instances were examined and global optimality could be ensured.

$$\min \boldsymbol{Z} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}) \quad \textit{Objective Function}$$

$$\textit{s.t.} \quad \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{y}) \le 0 \quad \textit{Inequality Constraints}$$

$$\boldsymbol{x} \in \boldsymbol{X}, \boldsymbol{y} \in \boldsymbol{Y}$$

$$\boldsymbol{X} = \{\boldsymbol{x} \mid \boldsymbol{x} \in \boldsymbol{R}^n, \boldsymbol{x}^L \le \boldsymbol{x} \le \boldsymbol{x}^U, \boldsymbol{Bx} \le \boldsymbol{b}\}$$

$$\boldsymbol{Y} = \{\boldsymbol{y} \mid \boldsymbol{y} \in \{0,1\}^m, \boldsymbol{Ay} \le \boldsymbol{a}\}$$

where, **x** is the vector of continuous variables;
y is the vector of integer (usually binary) variables;

Figure 2.3 A typical MINLP model. (CMU-IBM cyber).

Later, (Mistry M, 2016) showed that the reverse logarithmic mean temperature difference (RLMTD) is convex and proposed an outer approximation that works well for small problems. The original HEN model was approximated using a mixed-integer linear model (MILM), which was run iteratively and resolved to the global optimum of the original problem. (Beck A, 2018) developed a method for iteratively handling various MILP and NLP subproblems that enables the stagewise HEN model to be tightened by additional inequality constraints and tighter variable bounds. These approaches could allow solvers to locate the global optimum and significantly reduce duality gaps. While the approach is acceptable for small-scale problems, the methods are inefficient for large-scale applications. Finally, (Chenglin Chang, 2020) proposed a series of articles on the globally optimal synthesis of heat exchanger networks with non-isothermal mixing stagewise superstructure in minimal and non-minimal networks. All of the models outlined above, however, are based on the concept of isothermal mixing, which exaggerates heat exchanger area and limits the trade-off between capital and operating expenses.

2.6 Extention of Stagewise Superstructure Model on Global Optimization

The technique that dominates all prior efforts on HENS is the one that combines mathematical programming and the usage of superstructures. The two most common superstructures utilized in prior publications are the generalized superstructure developed by (Floudas CA, 1986), which allows for the employment of many exchangers between two streams. The former was a further generalized new superstructure for HENS that was solved globally by (Kim SY, 2016). Another popular superstructure formulation was published in the early 1990s, which permits simultaneous consideration of the number of heat exchangers, their corresponding heat exchanger area required, and utility costs. Stagewise superstructure is based on a set of assumptions; it assumes isothermal mixing and displays different stages in which multiple matches between streams occur (Yee TF, 1990).

The concept of staged superstructure has become a cornerstone of MINLP-based HENS research. With the restriction that no stream splits are allowed, (Zamora, 1998) proposed an outer approximation branch and bound algorithm that uses convex underrelaxations to solve the non-convex Mixed Integer Nonlinear Programming (MINLP) superstructure introduced by (Yee TF, 1990) to global optimality. (Björk KM, 2002) devised a global optimization strategy for the same superstructure model that allows for stream splits and non-isothermal mixing by convexifying signomial terms with an extended cutting plane method and constructing convex subproblems. Extensions of the stagewise superstructure that incorporate recycle inside each stage as well as partial bypasses of the stages are available in a variety of configurations (Huang KF, 2013). A superstructure with bypasses and recycles, as well as numerous exchangers in series on each branch, was developed by using transshipment-type equations to generate a rigorous linear model (Barbaro A, 2005). (Huang KF, 2012) discovered MINLP model solutions based on a hyperstructure of HEN stagewise stream superstructure. There are some diverse approaches to the HEN staged superstructure model: (Escobar M., 2013), (Onishi VC., 2014), (Na J., 2015).

1. Global Optimization of the Stage-wise Superstructure (Faria D., 2015)

This article introduced bound contraction methodology for global optimization of bilinear MINLP models to solve the stage-wise superstructure model for heat exchanger networks. The additional contribution in this paper is the extension of the method used to underestimate bilinear terms only and bound contract discretized variables developed by Faria and Bagajewicz, to the underestimation of terms containing nonconvex monotone functions. Instead of introducing several new variables to convert the problem into a quadratic one, we use a different relaxation of monotone functions that does not require reformulation and addition of new variables beyond the integers needed for discretization.

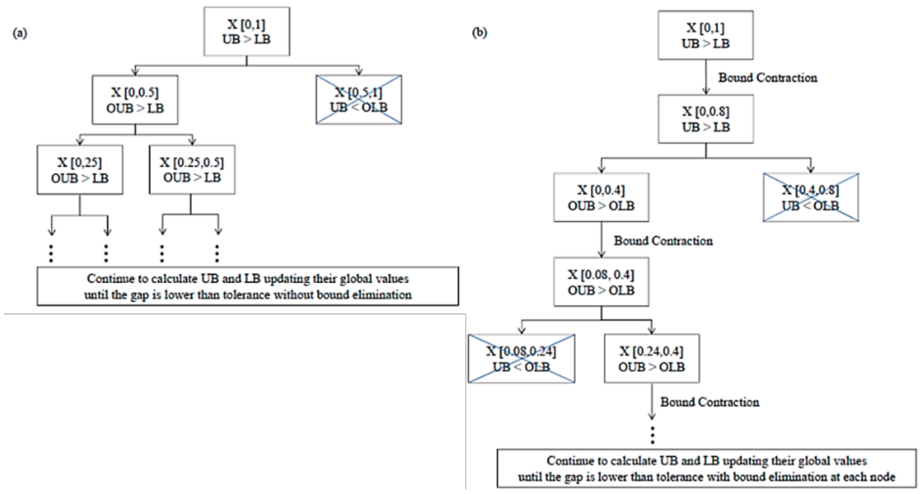

Figure 2.4 Illustration of the branch and bound procedures (a) without bound contraction and (b) with bound contraction at each node. (Faria et. al., 2015).

The bound contraction procedure used is the interval elimination strategy presented by Faria and Bagajewicz. The basic strategy is summarized next. Further details of different strategies can be found in the original paper.

1.1. Run the lower bounding model (presented in section 4) to obtain a lower bound of the problem and identify the intervals containing the solution of the lower bounding model. Update the overall lower bound (OLB).

1.2. Run the original MINLP initialized by the solution of the lower bounding model (previous step) to find an upper bound solution. If a solution is found, update the overall upper bound value (OUB).

1.3. Calculate the gap between update OUB and OLB. If the gap is lower than the tolerance, the solution was found. Otherwise go to the step 4.

1.4. Run the lower bounding model forbidding the intervals selected in step 1. All previously forbidden intervals are set free. If the LB is infeasible, or its value is larger than the current OUB, then all the intervals that have not been forbidden for this variable are eliminated. The surviving feasible region between the new bounds is repartitioned.

1.5. Repeat step 4 for all the other variables, one at a time.

1.6. Go back to step 1 (a new iteration using contracted bounds starts).

In the branch and bound with the bound contraction, our bound contraction procedure is applied to only one iteration at each node before variables are branched. This method may sometimes take a longer or shorter time depending on the success of the bound contraction step. The result show that the model is significantly faster for the big problem that They tested as compared to the branch and bound options. In fact, they can say that for the problem tested, the branch and bound with or without bound contraction, using their lower bound model is not efficient.

2. Global Optimization of the Stagewise Superstructure (Chenglin Chang, 2020)

This article introduces the concept of minimal structure (MSTR) and presents an enumeration algorithm for the synthesis of heat exchanger networks based on MSTR. Minimal Structures refer to a class of heat exchanger networks featuring acyclic heat transfer networks without energy loops. The enumerations used are either exhaustive or smart with a stopping criterion. Without loss of generality, they use the isothermal mixing Synheat model, that is, the method applies identically to other superstructures, with likely variations in the optimization models associated to each step. A conjecture is used to state that the algorithm renders solutions that are globally optimal. Literature examples are used to demonstrate the capabilities of the enumeration algorithm. Most of our solutions compare favorably with the best reported ones in literature, with exceptions where the reported solution is not minimal.

Example 1 Table 1 shows data consists of two hot and two cold streams from Faria et al. The data is given in Table 1. The fixed annual cost of units is $5,500 and the annual area cost coefficient is 150 $/m2. One feasible structure with five exchangers for this problem is shown in Figure 2.5.

Stream	T_{IN} (K)	T_{OUT} (K)	h (kW/m^{2}K)	Fcp (kW/K)
H1	650.0	370.0	1.0	10.0
H2	590.0	370.0	1.0	20.0
C1	410.0	650.0	1.0	15.0
C2	350.0	500.0	1.0	13.0
CU	300.0	320.0	1.0	_
HU	680.0	680.0	5.0	_
$EMAT_{Min}$	10.0 K			
Utility cost coefficients		$Chu_j = 80$ \$/kWy; $Ccu_i = 15$ \$/kWy;		
Fixed cost coefficients		$\hat{C}f_{i,j} = \hat{C}cuf_i = \hat{C}huf_j =$ \$5,500; $\hat{n}y=1$		
Area cost coefficients		$\hat{a}_{i,j} = \hat{a}cu_i = \hat{a}hu_j = 150$ \$/m^2 $\hat{b}_{i,j} = \hat{b}cu_i = \hat{b}hu_j = 1$		

Figure 2.5 Data of example 1 (Chenglin Chang, 2020).

They verify that the MSTR of Figure 2.6 is only feasible for values of energy between EMin = 575 kW and EMax = 2,750 kW. They correspond to HRATmin = 18.3 K and HRATmax = 129.3 K. These values can be verified using the pinch method. Figure 2.7 shows that the minimum TAC takes place at E = 1,117.3 kW.

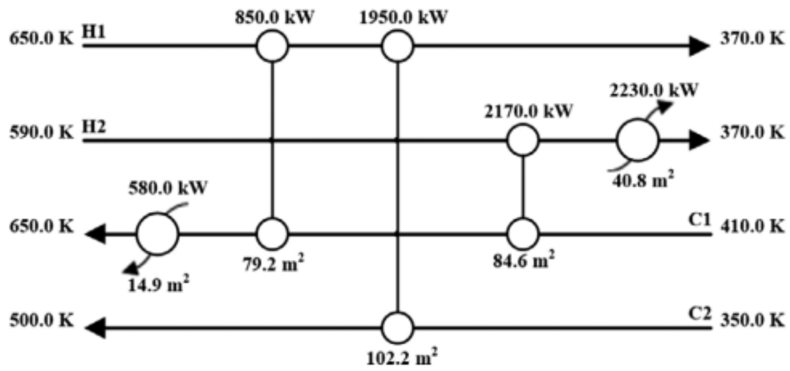

Figure 2.6 One heat transfer structure for example 1 (Chenglin Chang, 2020)

A new concept of Minimal HEN structures is presented and an algorithm to obtain globally optimal solutions for these types of networks is crafted. The algorithm is based on enumerating all possible structures, with or without a stopping criterion. The models are all linear. The strategy is based on the fact that for each structure, the total cost is a unimodal continuous function of E with one and only one global minimum. A Golden Search is employed to find the best solution with the lowest TAC for each minimal structure. There are in total four alternative options for the proposed algorithm, each with advantages and disadvantages. Sixteen examples are tested for illustration purpose and most of our solutions compare favorably with literature results. The algorithm guarantees global optimality over the proposed search space.

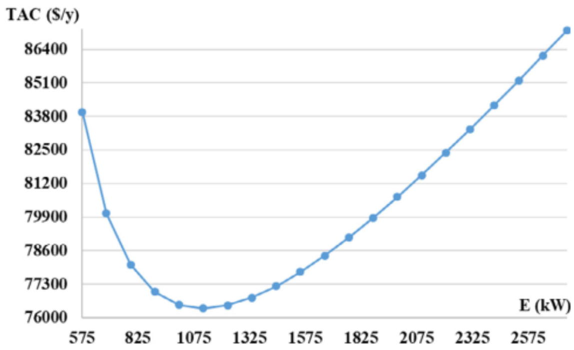

Figure 2.7 TAC vs. E for a fixed structure of example 1 and reduced energy cost. (Chenglin Chang, 2020).

3. Global optimization of heat exchanger networks using a new generalized superstructure (Kim SY, 2016)

They present an extension of a previously presented superstructure (Floudas CA, 1986) for heat exchanger network grassroots design. This extension is such that it includes several matches between two streams, activates splitting control and allows for mixing temperature control. They solve this model globally using RYSIA, a recently developed method bound contraction procedure (Faria D., 2015). They also add a new RYSIA feature called Lifting Partitioning. Results show structures that cannot be obtained using the stages model (Yee TF, 1990) or other similar restrictive models.

The HEN design model of the heat exchanger network uses the superstructure model developed by Floudas CA (1986). In order to describe how the HEN design model can be developed, we address a simple network, which has one hot stream and two cold streams in figure 9. Without loss of generality, we assume there are two heat exchangers per hot/cold stream match and they are not necessarily contiguous or in series. figure 9 illustrates the nature of the superstructure for just one hot stream and two cold streams and two exchangers per pair of streams, although the model can have many exchangers. In the original formulation by Floudas CA (1986), the feasible space is defined by nonlinear constraints, many of which are bilinear, and other purely nonconvex functions. Bilinear functions are included in the heat balances equations of heat exchangers and mixers. Nonconvex functions are the part of heat exchanger area calculations. The non-convex and bilinear MINLP model presented in this paper differs slightly from the original formulation.

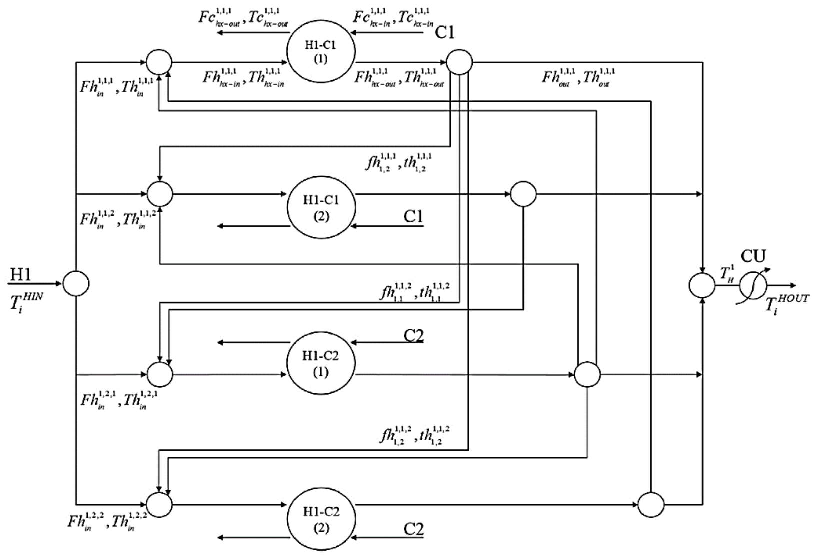

Figure 2.8 Heat exchanger network superstructure; two exchangers per match. (Kim et. al., 2016).

In conclusion, recognizing that local solvers like DICOPT cannot obtain solutions, often rendering infeasible if no goo initial point is provided, they solve it globally using RYSIA, our bound contraction method for bilinear problems extended to monotone functions by Faria et al. (2015). When applying these versions of RYSIA, they found that the lower bound model is too relaxed and therefore the bound contraction takes a long number of iterations. To fix this problem, they introduce so-called "lifting partitioning", which helps the lower bound render higher values. They compare with the bilinear reformulation and branch and bound and They present results that highlight features in the HEN that other models cannot model.

CHAPTER 3
METHODOLOGY

Materials and Equipment

Equipment:

1. Laptop Intel(R) Core (TM) i5-7300HQ CPU @ 2.50GHz, Ram 16.0 GB
2. Laptop Intel(R) Core (TM) i7-7700HQ CPU @ 2.80GHz, Ram 12.0 GB

Software:

1. General Algebraic Modelling System (GAMS)
2. Aspen Energy Analyzer (AspenTech)
3. Microsoft Excel

Experimental Procedures

Our two-part strategy is composed by global optimization and the HEN synthesis model.

3.1 HEN Synthesis Model

The stage-wise superstructure (SWS) model was developed as a solution to synthesize heat exchanger networks and was well-known in the optimization research study field (Yee TF, 1990). The model was solved using mixed-integer non-linear programming (MINLP), which includes non-linear equations, binary variables, the basic heat transfer equation, and logical restrictions for approach temperature in the model and utilities at the network's extreme ends. The binary variables introduced first in this model for heat exchanger network synthesis's field can be used to determine network topology, heat exchanger location, and utilities between hot and cold streams, which are governed by the assumption of isothermal mixing after the streams exit the heat exchanger.

In this study, the SWS model is for the HEN synthesis, which employs MINLP techniques in GAMS. The indexes as I for hot streams, J for cold streams, and K for the stages are set. The first step is the declaration of parameters and variables derived from information on hot streams and cold streams, such as stream characteristics, cost factors, and stream temperatures. Then, the equations in SWS model are declared with their names, including the objective function of TAC, the energy balance, and logical constraints.

3.1.1 Nomenclature

	Sets
I	Hot streams
J	Cold streams
K	The stages
HP	Hot process streams
CP	Sold process streams
ST	stages

	Parameters
CUcost	Cold utility cost ($/kW)
HUcost	Hot utility cost ($/kW)
Fcost	Fixed cost ($)
AC	Area cost coefficient ($/m^2)
AE	Area cost exponent
Tin_I	Supply temperature of hot stream I (K)
Tin_J	Supply temperature of cold stream J (K)
$Tout_I$	Target temperature of hot stream I (K)
$Tout_J$	Target temperature of cold stream J (K)
Thuin	Inlet temperature of hot utility (K)
Thuout	Outlet temperature of hot utility (K)
Tcuin	Inlet temperature of cold utility (K)
Tcuout	Outlet temperature of cold utility (K)
U	Overall heat transfer coefficient (W/m^{2}K)
h	Individual heat transfer coefficient of stream (W/m^{2}K)
Cp	Specific heat capacity (kJ/kgK)
p	Density of fluid (kg/m^3)
M_I	Mass flow rate for hot streams (kg/s)

M_J	Mass flow rate for cold streams (kg/s)
NOK	Number of stages
EMAT	Exchanger minimum approach temperature (K)
Ω_I	Upper bound for heat exchanged of hot stream (kW)
Ω_J	Upper bound for heat exchanged of cold stream (kW)
$\Gamma_{I,J}$	Upper bound for temperature difference (K)

Variables

TAC	Total annual cost ($)
$q_{I,J,K}$	Heat exchange between hot and cold streams (kW)
qcu_I	Heat exchange between cold utilities and hot streams (kW)
qhu_J	Heat exchange between hot utilities and cold streams (kW)
$t_{I,K}$	Intermediate temperature of hot stream I at stage K (K)
$t_{J,K}$	Intermediate temperature of cold stream J at stage K (K)
$dt_{I,J,K}$	Approach temperature for stream matching (K)
$dtcu_I$	Approach temperature between cold utility and hot stream (K)
$dthu_J$	Approach temperature between hot utility and cold stream (K)
$LMTD_{I,J,K}$	Logarithm mean temperature difference (K)
$A_{I,J,K}$	Area of heat exchangers (m^2)
Acu_I	Area of cold utilities (m^2)
Ahu_J	Area of hot utilities (m^2)

Binary variables

$z_{I,J,K}$	Binary variables represent exchanger matching
zcu_I	Binary variables represent cold utility matching
zhu_J	Binary variables represent hot utility matching

3.1.2 Objective Function

The objective of this step is to minimize an objective function of TAC which comprises six terms shown in Equation 1.

$$TAC = CUcost \sum_I qcu_I + HUcost \sum_J qhu_J + Fcost[\sum_I \sum_J \sum_K Z_{I,J,K} + \sum_J zcu_I + \sum_J zhu_J] + \sum_I \sum_J \sum_K AC \cdot (A_{I,J,K})^{AE} + \sum_I AC \cdot (Acu_I)^{AE} + \sum_J AC \cdot (Ahu_J)^{AE} \quad \text{(Equation 1)}$$

The first term is cold utility costs, the second term is hot utility costs, the third term is fixed costs for process heat exchangers and the utilities, the fourth term is area costs for process heat exchangers, the fifth term is area cost for cold utilities, and the last term is area cost for hot utilities, where $Fcost$ represent the cost parameters of the units, $CUcost$ and $HUcost$ is the utility cost factor, and qcu_I and qhu_J represent the heat load of a hot utility for a cold stream j and a cold utility for a hot stream i, respectively. The heat transfer model of HENs is similar to the stage-wise superstructure of Yee and Grossman (1990), as shown in Figure 2.2. The annual interest rate in this study is set to 0%, and the project life time is one year.

3.1.3 <u>Constraints</u>

Overall heat balance for each stream:

$$M_I \cdot Cp \cdot (Tin_I - Tout_I) = \Sigma_J \Sigma_K q_{I,J,K} + qcu_I \qquad I \in HP \qquad \text{(Equation 2)}$$

$$M_J \cdot Cp \cdot (Tout_J - Tin_I) = \Sigma_I \Sigma_K q_{I,J,K} + qhu_J \qquad J \in CP \qquad \text{(Equation 3)}$$

Stage heat balance:

$$M_I \cdot Cp \cdot (t_{I,K} - t_{I,J,K+1}) = \Sigma_J q_{I,J,K} \qquad K \in ST, I \in HP \qquad \text{(Equation 4)}$$

$$M_J \cdot Cp \cdot (t_{J,K} - t_{I,J,K+1}) = \Sigma_I q_{I,J,K} \qquad K \in ST, J \in CP \qquad \text{(Equation 5)}$$

Superstructure inlet temperatures:

$$Tin_I = t_{I,1} \qquad I \in HP \qquad \text{(Equation 6)}$$

$$Tin_J = t_{J,NOK+1} \qquad J \in CP \qquad \text{(Equation 7)}$$

Feasibility of temperatures (monotonic decrease in temperatures):

$$t_{I,K} \geq t_{I,K+1} \qquad K \in ST, I \in HP \qquad \text{(Equation 8)}$$

$$t_{J,K} \geq t_{J,K+1} \qquad K \in ST, J \in CP \qquad \text{(Equation 9)}$$

$$Tout_I \leq t_{I,NOK+1} \qquad I \in HP \qquad \text{(Equation 10)}$$

$$Tout_J \geq t_{J,1} \qquad J \in CP \qquad \text{(Equation 11)}$$

Hot and cold utility load:

$$M_I \cdot Cp \cdot (t_{I,NOK+1} - Tout_I) = qcu_I \qquad I \in HP \qquad \text{(Equation 12)}$$

$$M_J \cdot Cp \cdot (Tout_J - t_{J,1}) = qhu_J \qquad J \in CP \qquad \text{(Equation 13)}$$

Approach temperatures:

$$dt_{I,J,K} \leq (t_{I,K} - t_{J,K}) + \Gamma_{I,J} \cdot (1 - z_{I,J,K}) \qquad K \in ST, I \in HP, J \in CP \qquad \text{(Equation 14)}$$

$$dt_{I,J,K+1} \leq (t_{I,K+1} - t_{J,K+1}) + \Gamma_{I,J} \cdot (1 - z_{I,J,K}) \qquad K \in ST, I \in HP, J \in CP \qquad \text{(Equation 15)}$$

$$dtcu_I \leq (t_{I,NOK+1} - Tcuout) \qquad I \in HP \qquad \text{(Equation 16)}$$

$$dthu_J \leq (Thuout - t_{J,1}) \qquad J \in CP \qquad \text{(Equation 17)}$$

$$\Gamma_{I,J} = max\,[Tin_I - Tin_J,\ Tout_I - Tin_J,\ Tin_I - Tout_J,\ Tout_J - Tout_I] \qquad \text{(Equation 18)}$$

Minimum approach temperature (lower bounds):

$$dt_{I,J,K} \geq EMAT \qquad K \in ST, I \in HP, J \in CP \qquad \text{(Equation 19)}$$

Logical constraints:

$$q_{I,J,K} - min\,[\Omega_I, \Omega_J] \cdot z_{I,J,K} \leq 0 \qquad K \in ST, I \in HP, J \in CP \qquad \text{(Equation 20)}$$

$$qcu_I - \Omega_I \cdot zcu_I \leq 0 \qquad I \in HP \qquad \text{(Equation 21)}$$

$$qhu_J - \Omega_J \cdot zcu_J \leq 0 \qquad J \in CP \qquad \text{(Equation 22)}$$

$$\Omega_I = M_I \cdot Cp \cdot (Tin_I - Tout_I) \qquad \text{(Equation 23)}$$

$$\Omega_J = M_J \cdot Cp \cdot (Tout_J - Tin_J) \qquad \text{(Equation 24)}$$

Area calculations using Chen's (1987) approximation for the logarithmic mean temperature difference:

$$A_{I,J,K} = \frac{q_{I,J,K}}{U_{ij} \cdot \left[\frac{2}{3}\left(dt_{I,J,K} \cdot dt_{I,J,K+1}\right)^{0.5} + \frac{1}{3}\left(\frac{dt_{I,J,K} + dt_{I,J,K+1}}{2}\right)\right]} \qquad \text{(Equation 25)}$$

$$Acu_I = \frac{qcu_I}{U_{CU} \cdot \left[\frac{2}{3}(dtcu_I(Tout_I - Tcuin))^{0.5} + \frac{1}{3}\left(\frac{(dtcu_I(Tout_I - Tcuin))}{2}\right)\right]} \qquad \text{(Equation 26)}$$

$$Ahu_J = \frac{qhu_J}{U_{HU} \cdot \left[\frac{2}{3}\left(dthu_J \cdot (Thuin - Tout_J)\right)^{0.5} + \frac{1}{3}\left(\frac{dthu_J \cdot (Thuin - Tout_J)}{2}\right)\right]} \qquad \text{(Equation 27)}$$

Where, $U_{ij} = \left[\frac{1}{h_i} + \frac{1}{h_j}\right]^{-1}$; $U_{CU} = \left[\frac{1}{h_i} + \frac{1}{h_{CU}}\right]^{-1}$; $U_{HU} = \left[\frac{1}{h_{HU}} + \frac{1}{h_j}\right]^{-1}$ (Equation 28)

3.2 Global Optimization Strategy

3.2.1 Pinch Analysis

The feasible hot utility range between minimum and maximum hot utility for each network is identified using pinch analysis. The network is designed by locating thermodynamic bottlenecks or pinch point, by constructing a composite curve between hot and cold streams that can inform about minimum hot utilities, minimum cold utilities, and maximum heat recovery at a predetermined minimum temperature difference. The minimum hot utility is identified by set the cold utility to zero or set the maximum heat recovery. For the maximum hot utility is defined by set the heat recovery to zero.

3.2.2 Initialization

The maximum number of iterations for solving the local optimum is taken into consideration as the terminating criteria after the minimum and maximum hot utility ranges have been founded. The hot utility range will be divided into n intervals by the defined heat duty interval. The maximum number of iterations is calculated from the hot utility range and defined heat duty interval as shown in equation 29.

$$\text{Maximum number of iterations} = \frac{\text{Maximum hot utility} - \text{Minimum hot utility}}{\text{Defined heat duty interval}} \qquad \text{(Equation 29)}$$

The upper and lower limits of the hot utility at each heat duty interval i are shown in Fig 3.1. The local-optimum HEN is generated at each sub interval between the upper and lower limits of hot utilities until reaching the maximum iteration number. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations or all intervals. In some cases, we could include the Global Optimization with Extension with less defined heat duty interval to reach lower-TAC HEN, considered as global optimum.

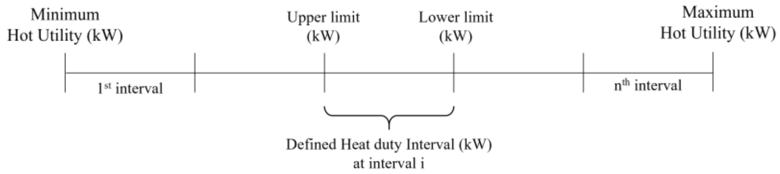

Figure 3.1 A comprehensive clarification of the heat duty partition.

3.2.3 Global Optimization Algorithm

The global optimization algorithm is divided into two parts: the regular global optimization and the global optimization with extension.

3.2.3.1 Regular Global Optimization

Regular global optimization is the starting global optimization using the initial set of defined hot utility intervals and number of iterations. The initial value and bound to variables in the denominator of constraints are set to avoid division-by-zero error. After that, the SWS model is solved by DICOPT to get the local optimal HEN design using a new initialization and boundary to shorten the computational time. If the local optimal HEN solution is found with the TAC less than previous local optimal HEN, the lower-TAC HEN results and topology will be saved as global-optimal HEN candidate before carrying out the subsequent step.

The parameters for the stream properties and all of the SWS model's equations are first set according to the flowchart of the global optimization algorithm in Figure 3.2. Then, heat duty intervals are defined to partition the feasible hot utility range into n intervals. For the first solving iteration with the hot-utility interval i = 1, we set objective of TAC as target at i = 1 equal to very large value. Then, we run the SWS model by varying the hot utility heat duty at interval i to calculate the optimal TAC solutions for each iteration step. For iteration i, if the optimal HEN solution has TAC_i lower than the previous solution, the TAC will be set as target TAC_i at updated target HEN_i. We will continue run the model by varying the hot utility upper and lower limit until reaching the maximum number of iterations, the optimal HEN solution with updated target TAC will be a global optimal solution (Target TAC, P) for this regular global optimization step.

3.2.3.2 Global Optimization with Extension

Global optimization with extension is the subsequent step using the different set of defined hot utility intervals and number of iterations. After get a global optimal solution (Target TAC, P) from the previous step, if the previous hot utility duty solution (Target Q_h) is not equal to zero, the program will try to run the global optimization with extension 1 by setting a smaller heat duty interval and change hot utility range around the previous hot utility result (Target Q_h). The program will run through the regular global optimization step again to synthesize a global optimal solution of extension 1 (Target TAC, 1). If Target TAC, P is less than Target TAC, P-1, we could run the global optimization again with extension as shown in Fig 3.2. To guarantee a global optimal solution (Target TAC, P-1), the program will terminate when the global optimal solution with upper extension step provides a solution larger or equal to the previous extension step.

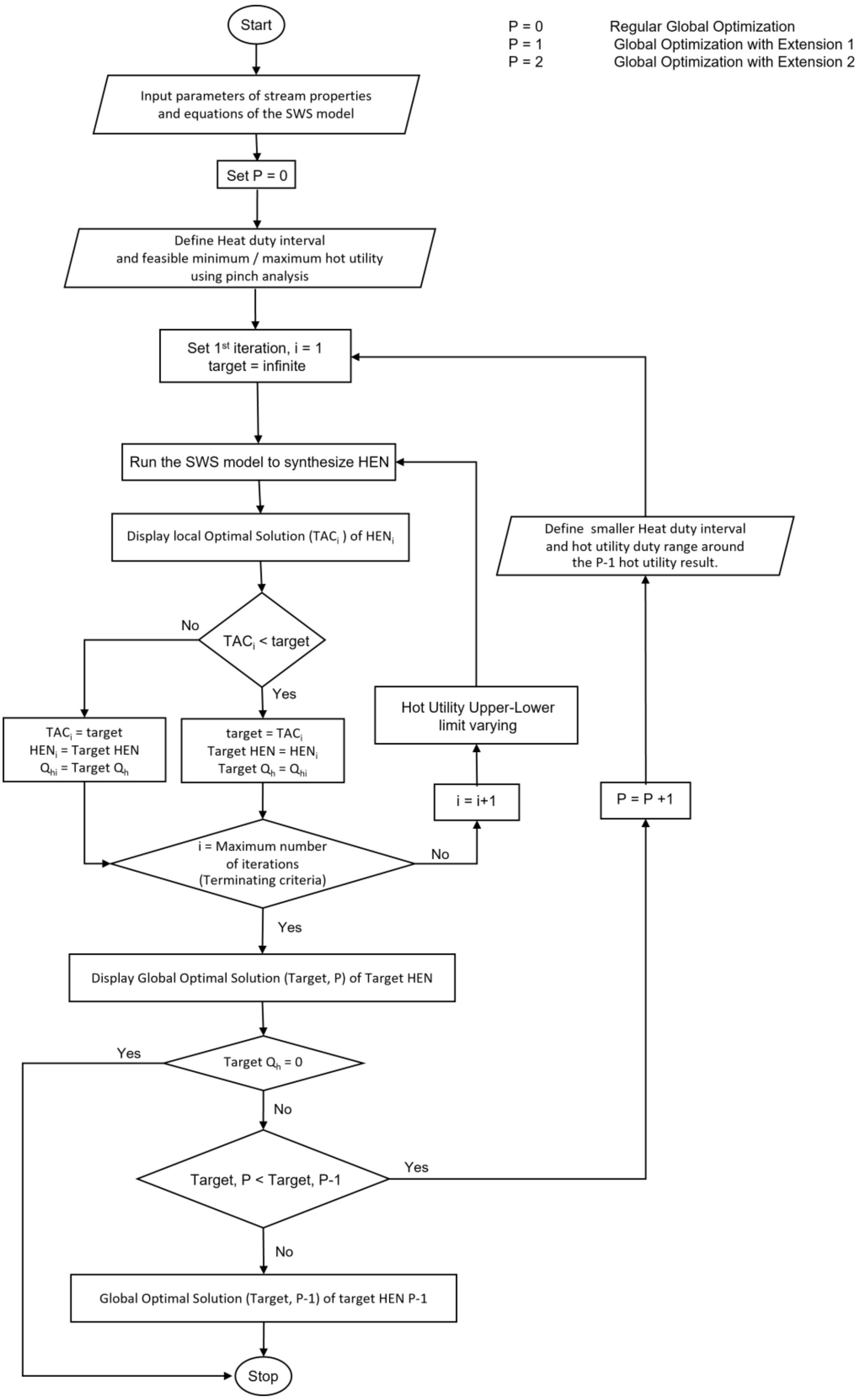

Figure 3.2 The flowchart of global optimization algorithm.

CHAPTER 4
RESULTS AND DISCUSSION

This section presents seven HEN examples of various sizes from the literature for comparison with our HEN synthesis. Our HEN synthesis model coding was implemented in GAMS (version 24.2.1) (Brooke, 2007.) and solved using CPLEX (version 12.3) as the MIP solver and DICOPT (Viswanathan, 1990) as the MINLP solver on a PC machine (i7 2.8 GHz, 12 GB RAM).

The overall summary results for each example from publications are shown in Table 4.1. For Examples 1, 2, and 3 of small-sized HEN with two hot and two cold streams. Our method with global optimization strategy gave the same or slightly better solutions than those from the literature, indicating that the methods used in this literature identify solutions close to the global ones with less computational time. For examples 4, 5, 6, and 7 of various sized HEN, the literature global optimum is better than our solution, although our computational time are much lower.

Table 4.1 Results of all examples

Example	Item	Base case (Maximum iteration = 1)	Global with 1kw interval (without Extend technique)	Our optimal solution for HENs			Optimal topology from literature	Percentage difference	Literature source
				Global	Global with Extend 1	Global with Extend 2			
1 (2H,2C)	Theoretical TAC ($/y)	95,373	95,373	95,373			95,350	0.02%	Mizutani et al. (2003)
	Heat Duty Interval (kW)	1,400	1	100			-		Not guarantee global optimum
	Time (s)	0.8	447	5.2			N/A		
2 (2H,2C)	Theoretical TAC ($/y)	154,865	154,865	154,865			154,902	0.02%	Faria et al. (2015)
	Heat Duty Interval (kW)	5,180	1	200			-		Guarantee global optimum
	Time (s)	0.3	1923	22.5			250		
3 (2H,2C)	Theoretical TAC ($/y)	270,370	261,140	261,140			261,787	0.25%	Esocobar et al. (2013)
	Heat Duty Interval (kW)	5,100	1	100			-		Guarantee global optimum
	Time (s)	0.3	1791	19.1			80.1		
4 (4H,5C)	Theoretical TAC ($/y)	551,421,924	551,433,624	551,427,124			99,605,219	138.8%	Faria et al. (2015)
	Heat Duty Interval (kW)	1,845	1	100			-		Guarantee global optimum
	Time (s)	225	246	73			108		
5 (5H,5C)	Theoretical TAC ($/y)	121,672	85,534	112,447	85,809	73,434	-	-	Mistry et al. (2016)
	Heat Duty Interval (kW)	6,042	1	100	10	1	-		Not guarantee global optimum
	Time (s)	0.2	2265	16.8	9.2	10.4	9,600		
6 (5H,5C)	Theoretical TAC ($/y)	111,520	110,869	111,491	110,869		110,848	0.02%	Daichendt et al. (2016)
	Heat Duty Interval (kW)	1,630	1	100	10		-		Guarantee global optimum
	Time (s)	1.2	769	12.7	6.6		2,252.0		
7 (6H,4C)	Theoretical TAC ($/y)	6,365,859	5,945,951	6,222,161	5,960,899		5,788,187	2.94%	Pavao et al. (2016)
	Heat Duty Interval (kW)	32,803	1	1,000	200		-		Guarantee global optimum
	Time (s)	29.4	21558	224.0	69.0		N/A		

Theoretical TAC is the total annualized cost calculated using equation 25 to 27, the theoretical area and the logarithmic mean temperature difference approach (LMTD).

4.1 Example 1 (M.A.S.S. Ravagnani, 2007)

The first example consists of two cold and two hot process streams. The stream data and parameters are given in Table 4.2. This example is used to illustrate the proposed approach in detail. A relatively large number of partitioning intervals was chosen to ensure that only one interval elimination loop is needed to satisfy the convergence criterion.

Table 4.2 Data and parameters of example 1 (M.A.S.S. Ravagnani, 2007)

Stream	T_{in} (K)	T_{out} (K)	FC_p (kW/K)
H1	368	348	20.0
H2	353	348	200.0
C1	303	363	40.0
C2	333	343	50.1
HU	500	500	
CU	300	320	
Parameters	**Unit**		
Cold utility cost (CUcost)	\$/kW	6	
Hot utility cost (HUcost)	\$/kW	60	
Fixed cost (Fcost)	\$	1000	
Area cost coefficient (AC)	\$/m^2	60	
Area cost exponent (AE)	-	0.6	
Overall heat transfer coefficients (U)	W/m^2 K	444	
Exchanger minimum approach temperature (EMAT)	K	10	
Annual interest rate	%	0	
Life time	year	1	

The example was solved using a 3-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 K. Using the Pinch analysis, we verify that the network is only feasible for energy values between Minimum hot utility = 1500 kW and Maximum hot utility = 2900 kW. We then define a heat duty interval of 100 kW and a maximum number of iterations of 14 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The optimal HEN solution is presented in Fig 4.1.

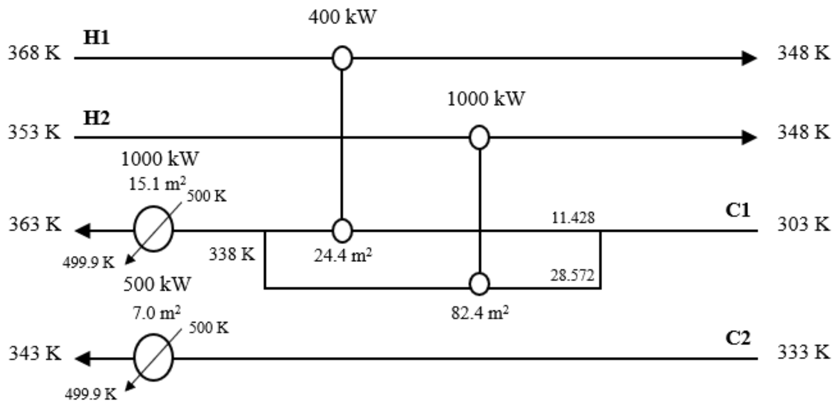

Figure 4.1 Our optimal HEN solution of example 1 with theoretical area.

Figure 4.2 shows that the TAC is monotone increasing and therefore a minimum TAC exhibit within the range of feasible energy value. In this case, the minimum TAC takes place at Hot utility = 1500.6 kW with the globally optimal solution features an annualized cost of $95,373/year. The total CPU time needed to obtain the solution was 5.2 sec.

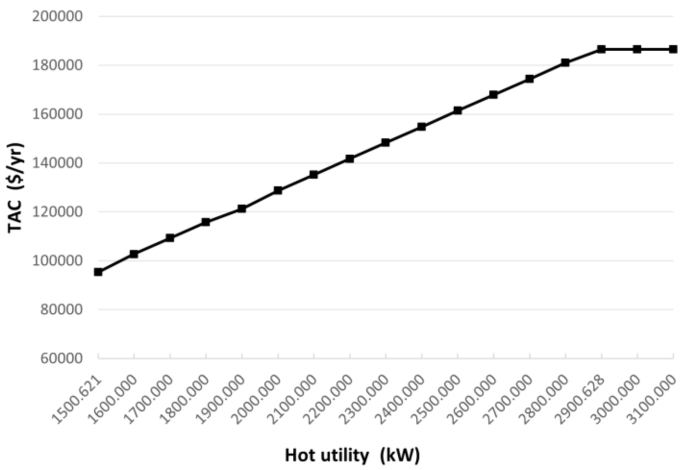

Figure 4.2 TAC vs. hot utility for a structure of example 1.

Table 4.3 summarize the results for different number of partitioning intervals. Our regular global solution is $95,373 per year which is slightly higher than the one from literature. The program then tries to run the global optimization with extension 1. The TAC solution is not lower than the previous solution, so the program stops and report the regular global solution.

By generating a network with the same hot utility range (1500 to 2900 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case provides the exact same TAC solution as our regular global optimization result, but with much less CPU time.

Table 4.3 Results for different partitioning interval numbers

Items	Base case (Maximum iteration = 1)	Global with 1kw interval (without Extend technique)	Our optimal solution		Optimal Results from literature
			Global	Global with Extend 1	
Maximum number of iterations	1	1,400	14		
Minimum Hot Utility (kW)	1500	1,500	1500		
Maximum Hot Utility (kW)	2900	2,900	2900	-	
Defined Heat Duty Interval	1,400	1	100		
CPU time	0.8 s	7 m 27 s	5.2 s		N/A
TAC ($/yr)	**95,373**	**95,373**	**95,373**		**95,350**
Hot Utility (kW)	**1,500.7**	**1,500.7**	**1,500.7**		**1,500**

The HEN topology solution from paper of (M.A.S.S. Ravagnani, 2007), the original research specifically studied on the equipment details design and did not ensure global optimization. The values for area are utilized to determine the best HEN global annual cost, which is $95,350/year. The optimal HEN topology solution with theoretical area is shown in Figure 4.3. The comparation of HEN topology solution of the paper and our solution shown in Figure 4.1 are exactly the same with two heat exchanger and two hot utility devices.

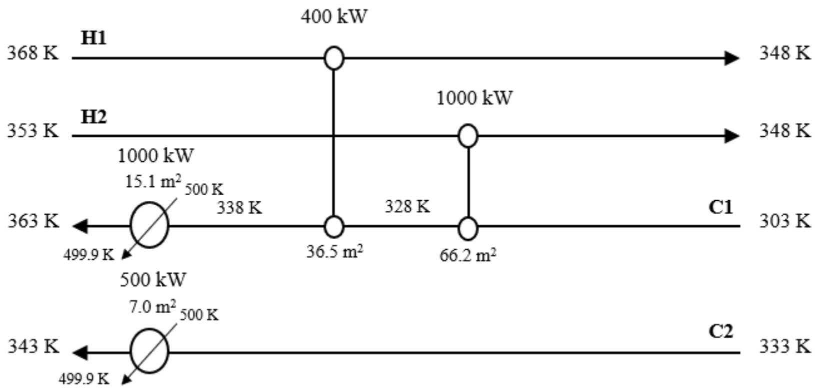

Figure 4.3 The optimal HEN topology solution (M.A.S.S. Ravagnani, 2007) with theoretical area.

We calculate Mizutani's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Mizutani's Theoretical Area value, the theoretical TAC of $95,350/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Mizutani and our result are presented in Table 4.4. Despite the fact that the configuration is exactly the same, our optimal solution is slightly higher than the original literature due to a difference in area cost calculation. However, the variation is not significant, indicating that it is near to the global optimum.

Table 4.4 Theoretical area for optimal HEN topology from our optimal HEN (a), base case HEN (b), and Mizutani et al. (2003) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m^2)	$A_{H1\text{-}C1}$	24.352
	$A_{H1\text{-}C2}$	82.439
	$A_{C1\text{-}HU}$	15.1
	$A_{C2\text{-}HU}$	6.962
Fixed cost ($)		4,000
Area cost ($)		1,373
Hot utility cost ($/yr)		90,000
Cold utility cost ($/yr)		0
TAC Calculation ($/yr)		**95,373**

(b)

Item	Base case
Fixed cost ($)	4,000
Area cost ($)	1,373
Hot utility cost ($/yr)	90,000
Cold utility cost ($/yr)	0
TAC Calculation ($/yr)	**95,373**

(c)

Item	Exchanger	Topology from literature Mizutani et al. (2003)
Theoretical Area (m^2)	$A_{H1\text{-}C1}$	36.528
	$A_{H1\text{-}C2}$	66.192
	$A_{C1\text{-}HU}$	15.1
	$A_{C2\text{-}HU}$	6.967
Fixed cost ($)		4,000
Area cost ($)		1,350
Hot utility cost ($/yr)		90,000
Cold utility cost ($/yr)		0
TAC Calculation ($/yr)		**95,350**

4.2 Example 2 (Faria D., 2015)

The example consists of two cold and two hot process streams. This example is taken from (Faria D., 2015) and the stream data and parameters are given in Table 4.5.

Table 4.5 Data and parameters of example 2 (Faria D., 2015)

Stream	T_{in} (K)	T_{out} (K)	h (kW/m²K)	FC_p (kW/K)
H1	650	370	1.0	10.0
H2	590	370	1.0	20.0
C1	410	650	1.0	15.0
C2	350	500	1.0	13.0
HU	680	680	5.0	
CU	300	320	1.0	
Parameters			**Unit**	
Cold utility cost (CUcost)			\$/kW	15
Hot utility cost (HUcost)			\$/kW	80
Fixed cost (Fcost)			\$	5500
Area cost coefficient (AC)			\$/m²	150
Area cost exponent (AE)			-	1.0
Exchanger minimum approach temperature (EMAT)			K	10
Annual interest rate			%	0
Life time			year	1

The example was solved using a 3-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 K. Therefore, we verify that the structure obtained from the optimization is only feasible for values of energy between Minimum hot utility = 320 kW and Maximum hot utility = 5,500 kW. These values can be confirmed using the pinch analysis. We then define a heat duty interval of 200 kW and a maximum number of iterations of 26 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The optimal HEN solution is presented in Fig 4.4.

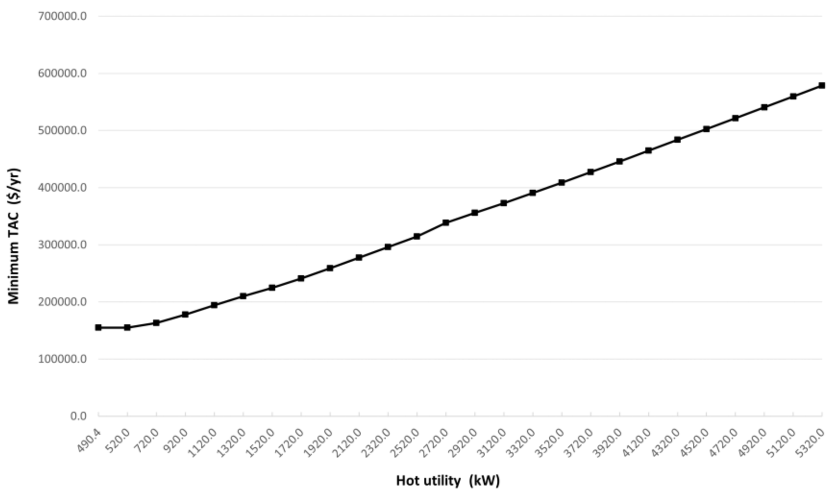

Figure 4.4 TAC vs. hot utility for a structure of example 2.

The globally optimal solution, depicted in Figure 4.5, has an annualized cost of $154,865 after 22.5 s of CPU time. In this case, the minimum TAC takes place at hot utility = 490.4 kW.

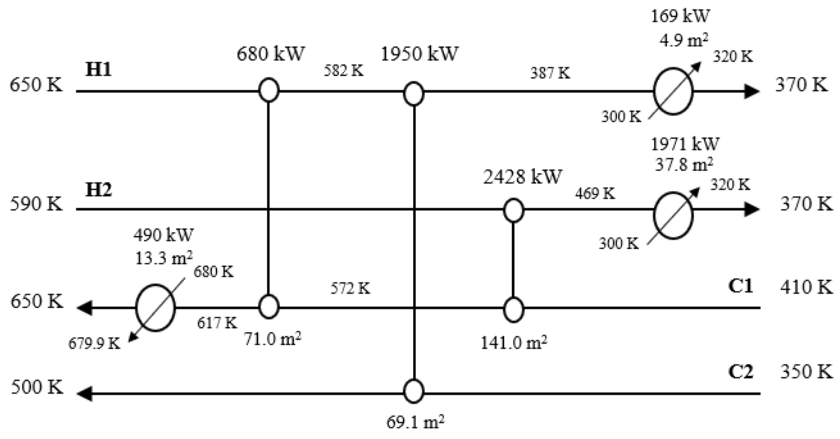

Figure 4.5 Our optimal HEN solution of example 2 with theoretical area.

Table 4.6 summarize the results for different number of partitioning intervals. Our regular global solution is $154,865 per year which is slightly lower than the one from literature, due to the hot utility duty consume 0.7 kW less. The program then tries to run the global optimization with extension 1. The TAC solution is not lower than the previous solution, so the program stops and report the regular global solution.

By generating a network with the same hot utility range (320 to 5,500 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case provides the exact same TAC solution as our regular global optimization result, but with much less CPU time.

Table 4.6 Results for different partitioning interval numbers

Items	Base case (Maximum iteration = 1)	Global with 1kw interval (without Extend technique)	Our optimal solution		Optimal Results from literature
			Global	Global with Extend 1	
Maximum number of iterations	1	5,180	26		
Minimum Hot Utility (kW)	320	320	320		
Maximum Hot Utility (kW)	5,500	5,500	5,500	-	
Defined Heat Duty Interval	5,180	1	200		
CPU time	0.3 s	32 m 3 s	22.5 s		250 s
TAC ($/yr)	**154,865**	**154,865**	**154,865**		**154,902**
Hot Utility (kW)	**490.4**	**490.4**	**490.4**		**491.1**

The HEN topology solution from paper of Faria et al. (2015), the original research performed optimization by difference approach, modified their bound contraction methodology for global optimization of bilinear MINLP models to solve the stage-wise superstructure model for heat exchanger networks. The optimal TAC obtained in the paper is $154,902/year and it was obtained in 4 min 10 s of CPU time. The optimal HEN topology solution with theoretical area is shown in Figure 4.6. The comparation of HEN topology solution of the paper and our solution shown in Figure 4.5 are quite similar with three heat exchanger and three utility devices.

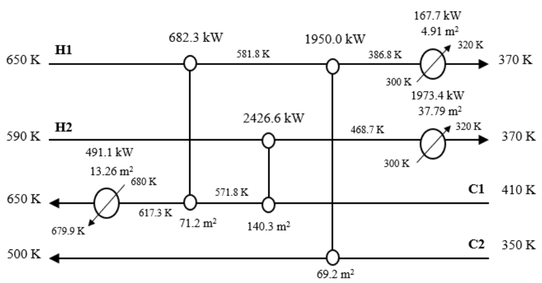

Figure 4.6 The optimal HEN topology solution from Faria et al. (2015) with theoretical area.

We calculate Faria's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Faria's Theoretical Area value, the theoretical TAC of $154,902/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Faria and our result are presented in Table 4.7, our global optimal theoretical TAC is $154,865/year at number of iterations of 26. The optimal solution HEN configuration is similar with the one obtained by Faria et al. (2015). Our best global annual cost, on the other hand, is slightly lower, showing that our optimal solution network is close to the global optimum while requiring significantly less computational time.

Table 4.7 Theoretical area for optimal HEN topology from our optimal HEN (a), base case HEN (b), and Faria et al. (2015) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m^2)	A_{H1-C1}	71.0
	A_{H1-C2}	69.1
	A_{H2-C1}	141.0
	A_{C1-HU}	13.3
	A_{H1-CU}	4.9
	A_{H2-CU}	37.8
Fixed cost ($)		33,000
Area cost ($)		50,565
Hot utility cost ($/yr)		39,200
Cold utility cost ($/yr)		32,100
TAC Calculation ($/yr)		**154,865**

(b)

Item	Base case
Fixed cost ($)	33,000
Area cost ($)	50,565
Hot utility cost ($/yr)	39,200
Cold utility cost ($/yr)	32,100
TAC Calculation ($/yr)	**154,865**

(c)

Item	Exchanger	Topology from literature (Faria et al., 2015)
Theoretical Area (m^2)	A_{H1-C1}	71.2
	A_{H2-C1}	140.3
	A_{H1-C2}	69.2
	A_{C1-HU}	13.26
	A_{H1-CU}	4.90
	A_{H2-CU}	37.79
Fixed cost ($)		33,000
Area cost ($)		50,498
Hot utility cost ($/yr)		39,288
Cold utility cost ($/yr)		32,116
TAC Calculation ($/yr)		**154,902**

4.3 Example 3 (Escobar M., 2013)

The third example consists of two cold and two hot process streams. This example is taken from Escobar et al. (2013). The stream data and parameters are given in Table 4.8.

Table 4.8 Data and parameters of example 3 (Escobar M., 2013)

Stream	T_{in} (°C)	T_{out} (°C)	h (kW/m²°C)	FC_p (kW/°C)
H1	270	160	1	18
H2	220	60	1	22
C1	50	210	1	20
C2	160	210	1	50
HU	250	250	1	
CU	15	20	1	
Parameters			**Unit**	
Cold utility cost (CUcost)			\$/kW	20
Hot utility cost (HUcost)			\$/kW	200
Fixed cost (Fcost)			\$	4000
Area cost coefficient (AC)			\$/m²	500
Area cost exponent (AE)			-	0.83
Exchanger minimum approach temperature (EMAT)			°C	10
Annual interest rate			%	0
Life time			year	1

The example was solved using a 3-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 °C. Using the pinch analysis, we verify that the network is only feasible for energy values between Minimum hot utility = 600 kW and Maximum hot utility = 5700 kW. We then define a heat duty interval of 100 kW and a maximum number of iterations of 51 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The optimal HEN solution is presented in Fig 4.7.

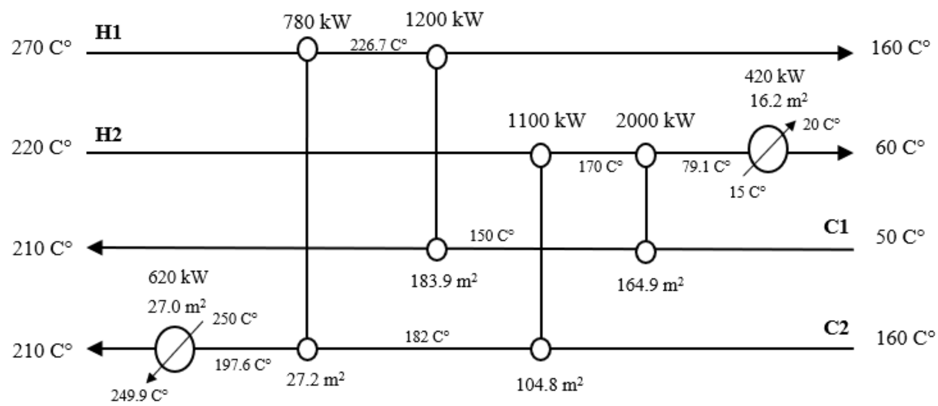

Figure 4.7 Our optimal HEN solution of example 3 with theoretical area.

Figure 4.8 shows that the TAC is monotone increasing and therefore a minimum TAC exhibit within the range of feasible energy value. In this case, the minimum TAC takes place at Hot utility = 620 kW with the globally optimal solution features an annualized cost of $261,140/year. The total CPU time needed to obtain the solution was 19.1 sec.

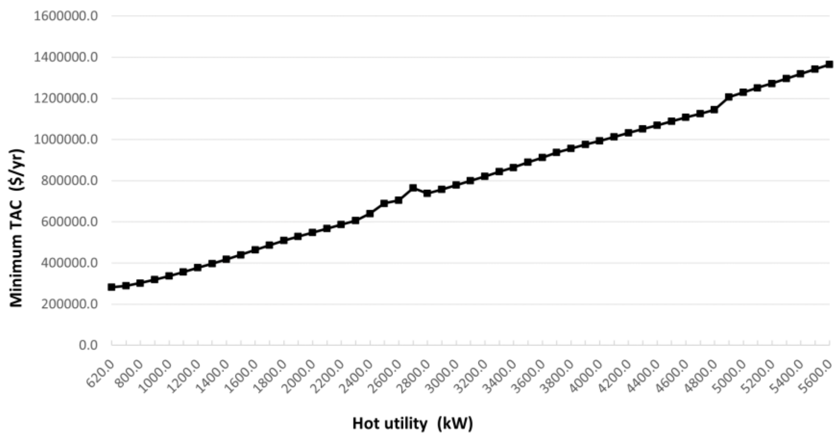

Figure 4.8 TAC vs. hot utility for a structure of example 3.

Table 4.9 summarize the results for different number of partitioning intervals. Our regular global solution is $261,140 per year, which is slightly lower than the one from literature which is $261,787 per year, although the hot utility duty consume only 20 kW more. The program then tries to run the global optimization with extension 1. The TAC solution is not lower than the previous solution, so the program stops and report the regular global solution.

By generating a network with the same hot utility range (600 to 5,700 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case provides the slightly higher TAC solution than our regular global optimization result, but with much less CPU time.

Table 4.9 Results for different partitioning interval numbers

Items	Base case (Maximum iteration = 1)	Global with 1kw interval (without Extend technique)	Our optimal solution		Optimal Results from literature
			Global	Global with Extend 1	
Maximum number of iterations	1	5,100	51		
Minimum Hot Utility (kW)	600	600	600		
Maximum Hot Utility (kW)	5,700	5,700	5,700	-	
Defined Heat Duty Interval	5,100	1	100		
CPU time	0.3 s	29 m 51 s	19.1 s		80.1 s
TAC ($/yr)	**270,370**	**261,140**	**261,140**		**261,787**
Hot Utility (kW)	**700.0**	**620.0**	**620.0**		**600**

The HEN topology solution from paper of Escobar et al. (2013), the original research performed optimization by difference approach, SBB (M.R. Bussiek, 2001) combines a standard Branch and Bound method with some NLP solvers in GAMS. The values for area are utilized to determine the best HEN global annual cost, which is $261,787/year with 80.1 sec CPU time. The optimal HEN topology solution with theoretical area is shown in Figure 4.9. Although, the comparation of HEN topology solution of the paper and our solution shown in Figure 4.7 are quite similar with four heat exchanger and two utility devices, but there is a large difference in the TAC result.

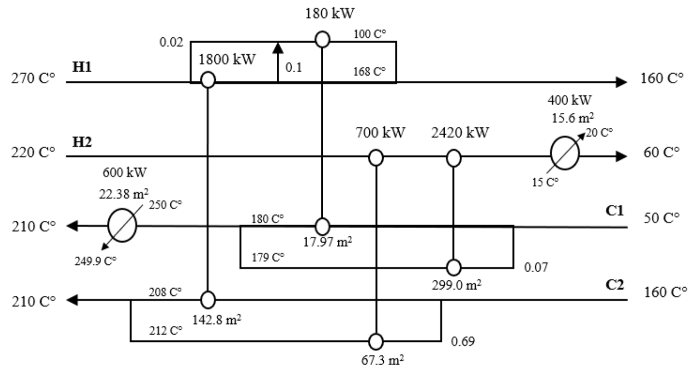

Figure 4.9 HEN topology using hyperstructure (Escobar M., 2013) with theoretical area.

We calculate Escobar's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Escobar's theoretical area value, the theoretical TAC of $261,787/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Escobar and our result are presented in Table 4.10, our global optimal theoretical TAC is $261,140/year at maximum number of iterations of 51. Our theoretical TAC solution is slightly lower than the original literature, the necessary compute time is significantly less, demonstrating that there are several alternative solutions close to the global optimum.

Table 4.10 Theoretical area for optimal HEN topology from our optimal HEN (a), base case HEN (b), and Escobar et al., 2013 (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m²)	$A_{H1\text{-}C2}$	27.2
	$A_{H1\text{-}C1}$	183.9
	$A_{H2\text{-}C2}$	104.8
	$A_{H2\text{-}C1}$	164.9
	$A_{H2\text{-}CU}$	16.2
	$A_{C2\text{-}HU}$	27.0
Fixed cost ($)		24,000
Area cost ($)		104,740
Hot utility cost ($/yr)		124,000
Cold utility cost ($/yr)		8,400
TAC Calculation ($/yr)		**261,140**

(b)

Item	Base case
Fixed cost ($)	20,000
Area cost ($)	110,370
Hot utility cost ($/yr)	140,000
Cold utility cost ($/yr)	10,000
TAC Calculation ($/yr)	**270,370**

(c)

Item	Exchanger	Topology from literature (Escobar M., 2013)
Theoretical Area (m²)	$A_{H1\text{-}C1}$	17.97
	$A_{H1\text{-}C2}$	142.8
	$A_{H2\text{-}C1}$	299.0
	$A_{H2\text{-}C2}$	67.3
	$A_{H2\text{-}CU}$	15.6
	$A_{C1\text{-}HU}$	22.38
Fixed cost ($)		24,000
Area cost ($)		109,787
Hot utility cost ($/yr)		120,000
Cold utility cost ($/yr)		8,000
TAC Calculation ($/yr)		**261,787**

4.4 Example 4 (Faria D., 2015)

The example consists of four cold and five hot process streams. This example is taken from Faria et al. (2015) and the stream data and parameters are given in Table 4.11.

Table 4.11 Data and parameters of example 4 (Faria D., 2015)

Stream	T_{in} (K)	T_{out} (K)	h (kW/m²K)	FC_p (kW/K)
H1	433.15	366.15	0.06	2.634
H2	522.15	411.15	0.06	3.162
H3	500.15	339.15	0.06	4.431
H4	472.15	339.15	0.06	5.319
C1	333.15	433.15	0.06	2.286
C2	389.15	495.15	0.06	1.824
C3	311.15	494.15	0.06	2.532
C4	355.15	450.15	0.06	5.184
C5	366.15	478.15	0.06	4.170
HU	544.15	422.15	0.06	
CU	311.15	355.15	0.06	
Parameters			**Unit**	
Cold utility cost (CUcost)			\$/kW	53349
Hot utility cost (HUcost)			\$/kW	566167
Fixed cost (Fcost)			\$	5291.9
Area cost coefficient (AC)			\$/m²	77.79
Area cost exponent (AE)			-	1.0
Exchanger minimum approach temperature (EMAT)			K	10
Annual interest rate			%	0
Life time			year	1

The example was solved using a 5-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 K. Therefore, we verify that the structure obtained from the optimization is only feasible for values of energy between minimum hot utility = 0 kW and maximum hot utility = 1,845 kW. These values can be confirmed using the pinch analysis. We then define a heat duty interval of 100 kW and a maximum number of iterations of 19 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals

until reaching the maximum number of iterations. The optimal HEN solution is presented in Fig 4.10.

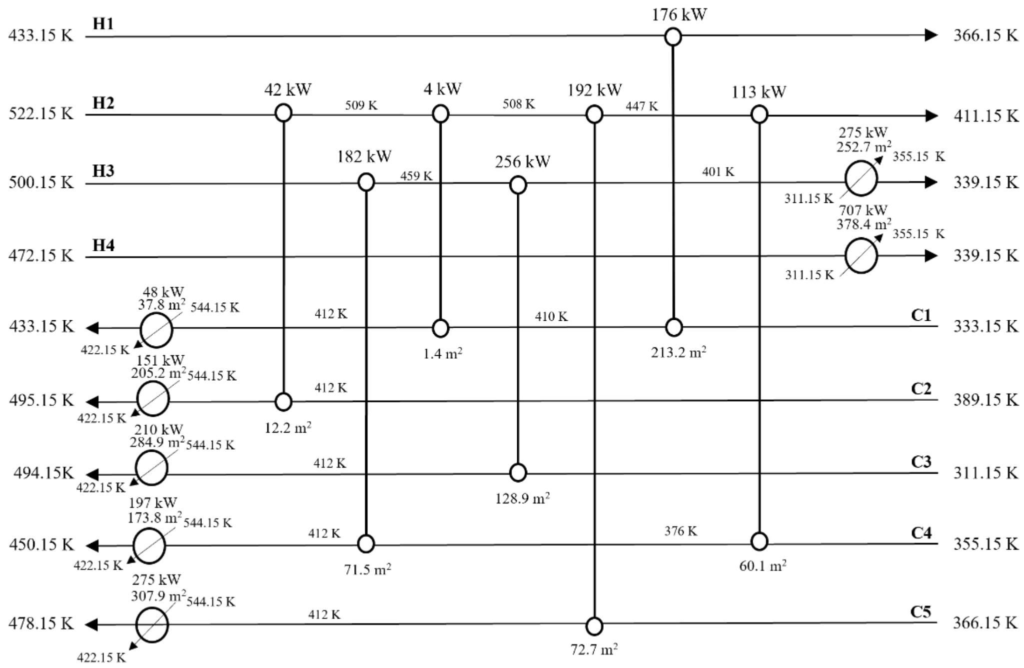

Figure 4.10 Our optimal HEN solution of example 4 with theoretical area.

Figure 4.11 shows that the TAC is monotone increasing and therefore a minimum TAC exhibit within the range of feasible energy value. In this case, the minimum TAC takes place at hot utility = 811.8 kW with the globally optimal solution features an annualized cost of $551,427,124/year.

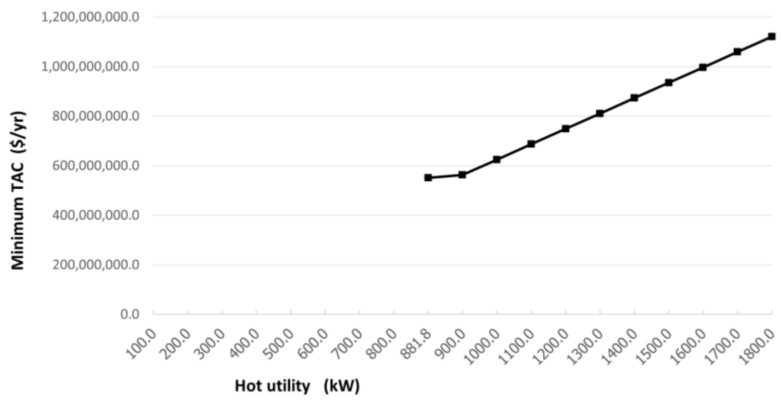

Figure 4.11 TAC vs. hot utility for a structure of example 4.

The optimal TAC obtained in the paper of Faria et al. (2015) is \$99,605,219/year and it was obtained in 108 sec of CPU time. While our global optimal TAC solution is \$551,427,124/year after 73 sec of CPU time. Despite the fact that the required computational time is less, our best TAC is considerable higher than the original literature, showing that our optimal solution network is different from the global optimum.

Table 4.12 summarize the results for different number of partitioning intervals. Our regular global solution is \$551,427,124 per year, which is extremely higher than the one from literature, due to our hot utility duty consume 660.4 kW more than the paper. So that makes a large effect on hot utility cost calculation and the TAC value. This different could be due to the difference in SWS model and the linearization technique used in the literature. The program then tries to run the global optimization with extension 1. The TAC solution is not lower than the previous solution, so the program stops and report the regular global solution. By generating a network with the same hot utility range (0 to 1,845 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case provides slightly lower TAC solution than our regular global optimization result, but with much less CPU time.

Table 4.12 Results for different partitioning interval numbers

Items	**Base case** (Maximum iteration = 1)	**Global with 1kw interval** (without Extend technique)	**Our optimal solution**		**Optimal Results from literature**
			Global	**Global with Extend 1**	
Maximum number of iterations	1	1,845	19		
Minimum Hot Utility (kW)	0	0	0		
Maximum Hot Utility (kW)	1,845	1,845	1,845	-	
Defined Heat Duty Interval	1,845	1	100		
CPU time	3 m 45 s	14 m 6 s	1 m 13 s		1 m 48 s
TAC (\$/yr)	**551,421,924**	**551,433,624**	**551,427,124**		**99,605,219**
Hot Utility (kW)	**811.8**	**811.8**	**811.8**		**151.4**

The HEN topology solution from paper of Faria et al. (2015), the original research performed optimization by difference approach, modified their bound contraction methodology for global optimization of bilinear MINLP models to solve the stage-wise superstructure model for heat exchanger networks. The values for area are utilized to determine the best HEN global annual cost, which is \$99,605,219/year with 108 sec CPU time. The optimal HEN topology solution with theoretical area is shown in Figure 4.12. The comparation of HEN topology solution of the paper and our solution shown in Figure 4.10 are difference, our topology has 4 more hot utility units and one more heat exchanger unit. This had a significant impact on the TAC value and the calculation of hot utility costs.

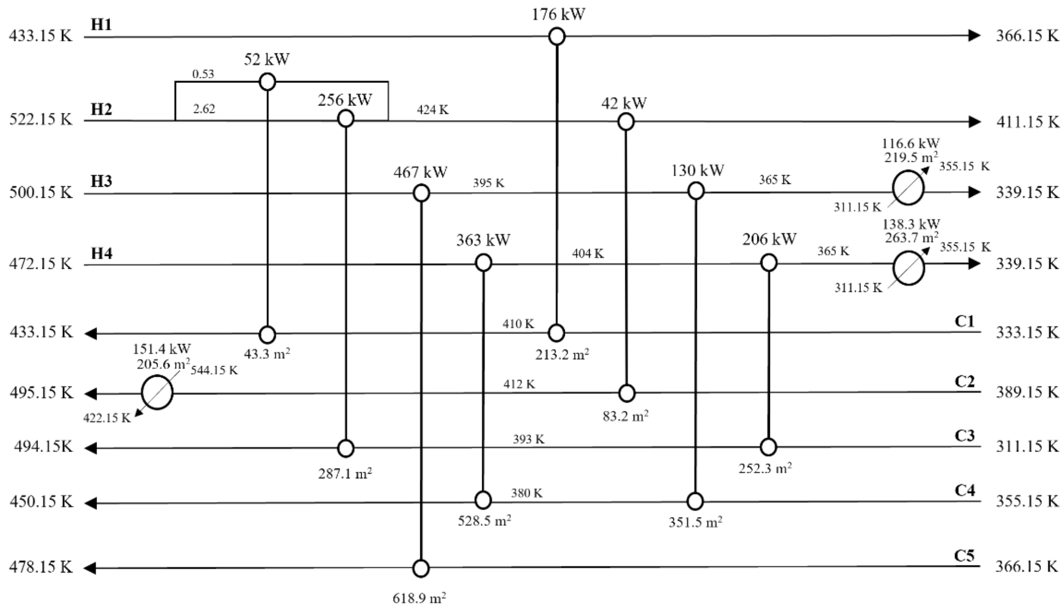

Figure 4.12 Improved topology solution with reduced MINLP from Faria et al. (2015) with theoretical area.

We calculate Faria's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Faria's theoretical area value, the theoretical TAC of \$99,605,219/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Faria and our result are presented in Table 4.13, our global optimal theoretical TAC is \$551,427,124/year at number of iterations of 19. Our optimal solution is extremely higher than the original literature, the necessary compute time is less, demonstrating that our optimal solution did not close to the global optimum. From Table 4.13, the calculated utility costs for both hot and cold can be seen to be significantly higher than those found in original research. As a result of this, the TAC value differs significantly.

Table 4.13 Theoretical area for optimal HEN topology from our optimal HEN (a), base case HEN (b), and Faria et al. (2015) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m²)	$A_{H2\text{-}C2}$	12.2
	$A_{H3\text{-}C4}$	71.5
	$A_{H2\text{-}C1}$	1.4
	$A_{H3\text{-}C3}$	128.9
	$A_{H2\text{-}C5}$	72.7
	$A_{H1\text{-}C1}$	213.2
	$A_{H2\text{-}C4}$	60.1
	$A_{H3\text{-}CU}$	252.7
	$A_{H4\text{-}CU}$	378.4
	$A_{HU\text{-}C1}$	37.8
	$A_{HU\text{-}C2}$	205.2
	$A_{HU\text{-}C3}$	284.9
	$A_{HU\text{-}C4}$	173.8
	$A_{HU\text{-}C5}$	307.9
Fixed cost ($)		74,086
Area cost ($)		171,193
Hot utility cost ($/yr)		52,388,718
Cold utility cost ($/yr)		498,793,127
TAC Calculation ($/yr)		**551,427,124**

(b)

Item	Base case
Fixed cost ($)	74,086
Area cost ($)	165,993
Hot utility cost ($/yr)	52,388,718
Cold utility cost ($/yr)	498,793,127
TAC Calculation ($/yr)	**551,421,924**

(c)

Item	Exchanger	Topology from literature Faria et al. (2015)
Theoretical Area (m²)	$A_{H2\text{-}C2}$	43.3
	$A_{H2\text{-}C3}$	287.1
	$A_{H3\text{-}C5}$	618.9
	$A_{H4\text{-}C4}$	528.5
	$A_{H1\text{-}C1}$	213.2
	$A_{H2\text{-}C2}$	83.9
	$A_{H3\text{-}C4}$	351.5
	$A_{H4\text{-}C3}$	254.0
	$A_{H3\text{-}CU}$	219.8
	$A_{H4\text{-}CU}$	264.1
	$A_{HU\text{-}C2}$	207.2
Fixed cost ($)		58,211
Area cost ($)		237,862
Hot utility cost ($/yr)		13,595,992
Cold utility cost ($/yr)		85,713,154
TAC Calculation ($/yr)		**99,605,219**

4.5 Example 5 (Mistry M, 2016)

The example consists of five cold and five hot process streams. This example is taken from Mistry et al. (2016) and the stream data and parameters are given in Table 4.14.

Table 4.14 Data and parameters of example 5 (Mistry M, 2016)

Stream	T_{in} (K)	T_{out} (K)	h (kW/m²K)	FC_p (kW/K)
H1	160.0	93.3	1.7	8.8
H2	248.9	137.8	1.7	10.6
H3	226.7	65.6	1.7	14.8
H4	271.1	148.9	1.7	12.6
H5	198.9	65.6	1.7	17.7
C1	60.0	160.0	1.7	7.6
C2	115.6	221.7	1.7	6.1
C3	37.8	211.1	1.7	8.4
C4	82.2	176.7	1.7	17.3
C5	93.3	204.4	1.7	13.9
HU	240.0	240.0	3.4	
CU	25.0	40.0	1.7	

Parameters	Unit	
Cold utility cost (CUcost)	\$/kW	10
Hot utility cost (HUcost)	\$/kW	200
Fixed cost (Fcost)	\$	4000
Area cost coefficient (AC)	\$/m²	146
Area cost exponent (AE)	-	0.6
Exchanger minimum approach temperature (EMAT)	K	10
Annual interest rate	%	0
Life time	year	1

The example was solved using a 5-stages superstructure model and assumed an exchanger minimum temperature approach EMAT of 10 K. Therefore, we verify that the structure obtained from the optimization is only feasible for values of energy between Minimum hot utility = 0 kW and Maximum hot utility = 6,042 kW. These values can be confirmed using the pinch analysis. We then define a heat duty interval of 100 kW and a maximum number of iterations of 61 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals

until reaching the maximum number of iterations. The optimal HEN solution is presented in Fig 4.13.

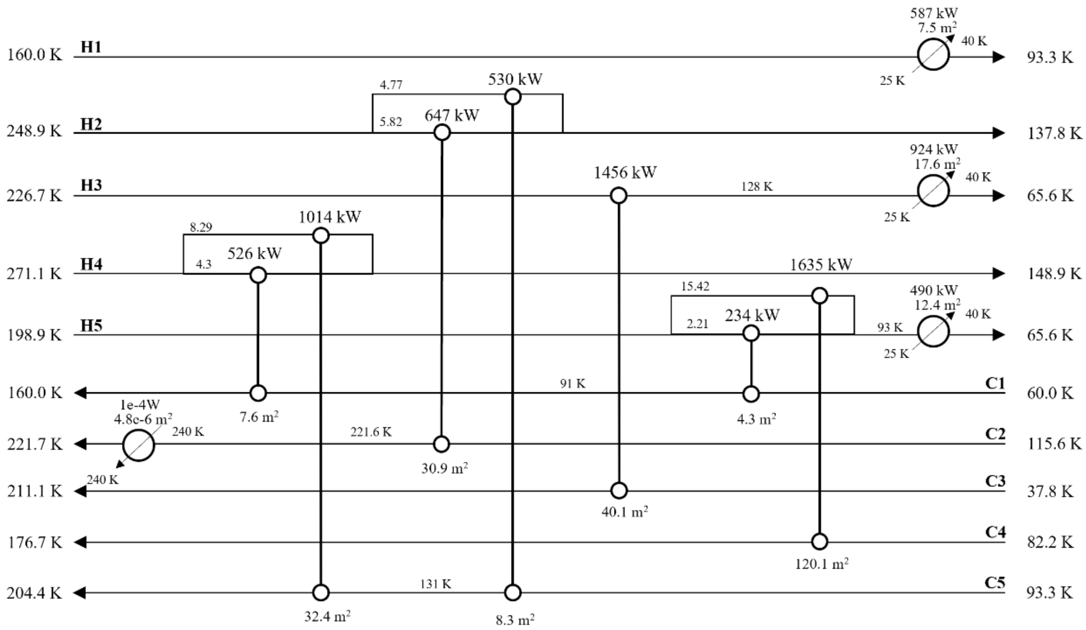

Figure 4.13 Our optimal HEN solution of example 5 with theoretical area.

Figure 4.14 shows that the TAC is monotone increasing and therefore a minimum TAC exhibit within the range of feasible energy value. In this case, the minimum TAC takes place at Hot utility = 100 kW with the globally optimal solution features an annualized cost of $112,447/year.

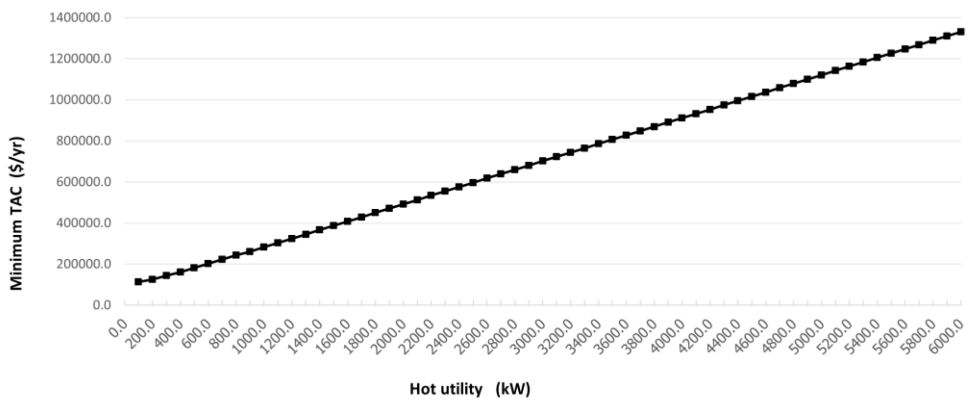

Figure 4.14 TAC vs. hot utility for a structure of example 5.

The optimal TAC obtained in the paper of Mistry et al. (2016) is \$64,138/year and it was obtained in 9,600s of CPU time. While our global optimal TAC solution is \$112,447/year after 16.8 s of CPU time. Despite the fact that the required computational time is significantly less, our best TAC is two times bigger than the original literature, showing that our optimal solution network is significantly different from the global optimum.

Therefore, we further expand our global optimization approach by solving for less TAC between minimum hot utility = 0 kW and maximum hot utility = 200 kW with a smaller heat duty interval of 10 kW. A maximum number of iterations of 21 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The example was resolved using a 5-stages superstructure and assumed a minimum temperature approach EMAT of 10 K. The extension 1 HEN solution is presented in Fig 4.15.

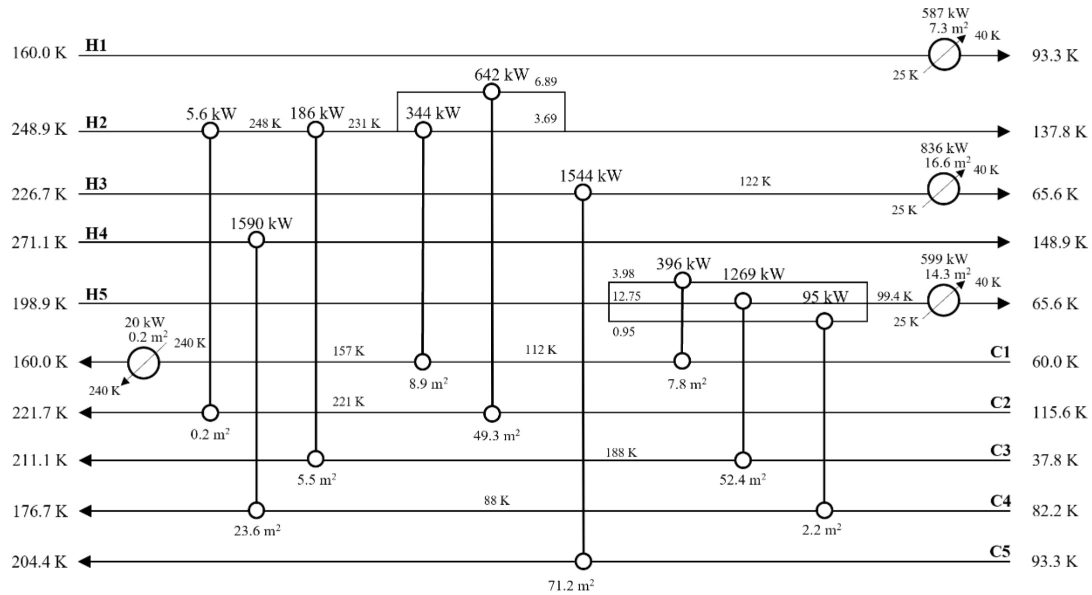

Figure 4.15 The optimal HEN solution of example 5 - extend 1.

After 9.2 sec CPU time, we get the minimum TAC takes place at hot utility = 20 kW with the globally optimal solution features an annualized cost of $85,809/year as shown in Figure 4.16.

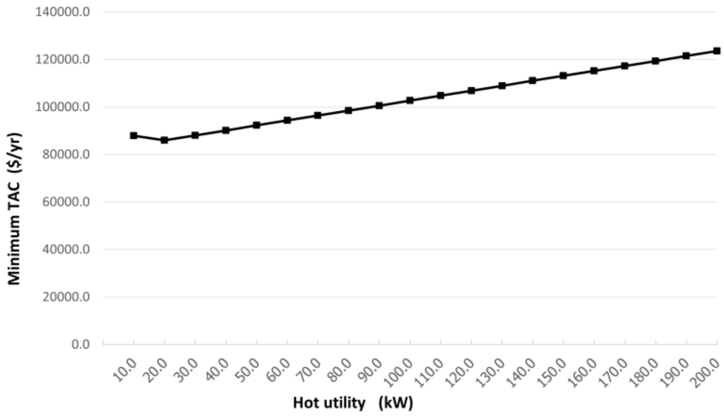

Figure 4.16 TAC vs. hot utility for a structure of example 5- extend 1.

For the second extension, we expand our global optimization approach by solving for less TAC between minimum hot utility = 0 kW and maximum hot utility = 40 kW with a smaller heat duty interval of 1 kW. A maximum number of iterations of 40 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The example was resolved using a 5-stages superstructure and assumed a minimum temperature approach EMAT of 10 K. The optimal HEN solution is presented in Fig 4.17.

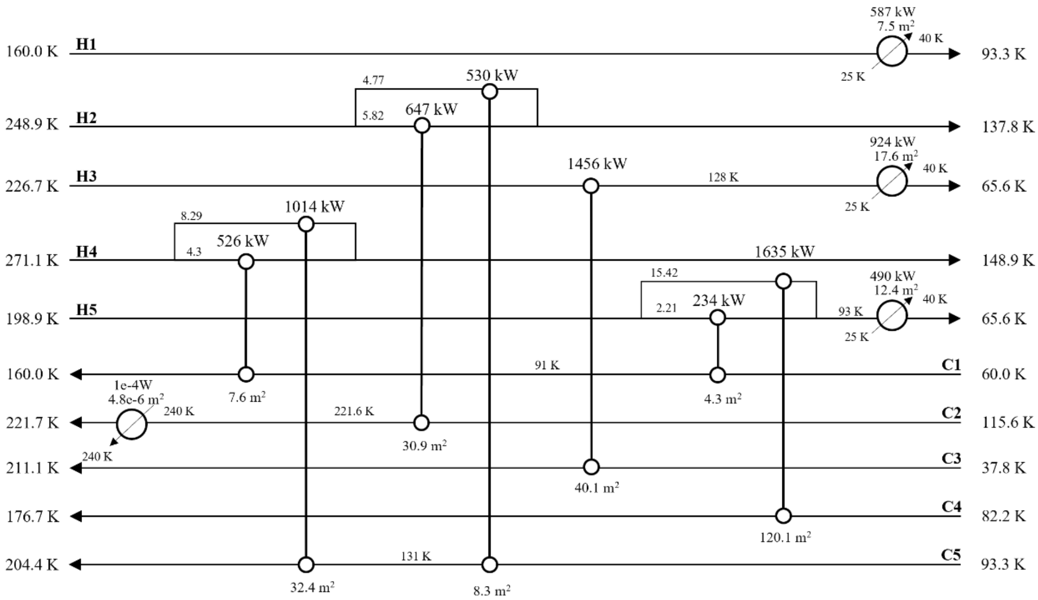

Figure 4.17 The optimal HEN solution of example 5 - extend 2.

After 10.4 sec CPU time, we get the minimum TAC takes place at hot utility near 0 kW with the globally optimal solution features an annualized cost of \$73,434/year as shown in Figure 4.18.

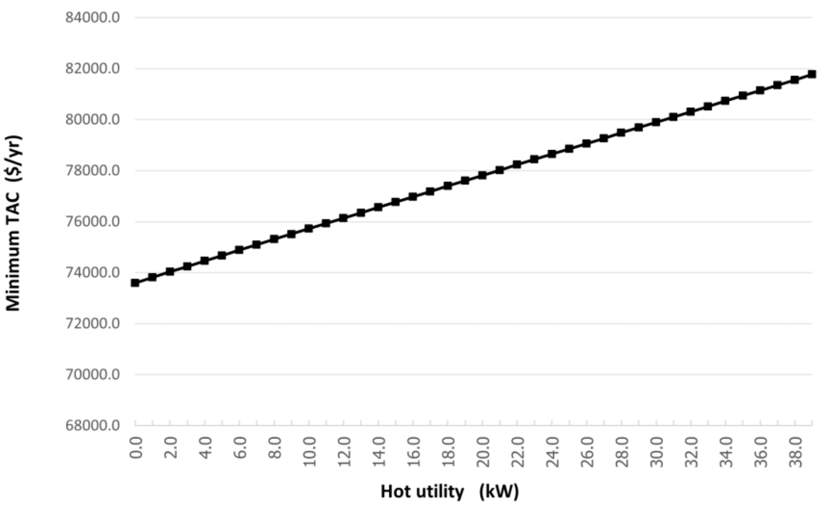

Figure 4.18 TAC vs. hot utility for a structure of example 5- extend 2.

Table 4.15 summarize the results for different number of partitioning intervals. Our regular global solution is $112,447 per year at hot utility 100 kW, which is two times higher than the one from literature. However, by decreasing the heat duty interval from 100 to 1 kw through the first step until the last extension step, our global optimization with extension significantly lowers the objective TAC value from $112,447 to $73,434 per year. The program tries to run the global optimization with extension 1. The TAC solution is much lower than previous solution with $85,809 per year at hot utility 20 kW, still higher than the one from literature. The program then continues running the global optimization with extension 2. The extension 2 solution is lower than previous solution with $73,434 per year at hot utility near 0 kW, but still higher than the one from literature. The program continues running the global optimization with extension 3, but TAC solution is not lower than the previous solution, so the program stops and report the extension 2 global solution. Our computational time summation is 36.4 second, substantially lower than the paper.

Table 4.15 Results for different partitioning interval numbers

Items	Base case (Maximum iteration = 1)	Global with 1kw interval (without Extend technique)	Our optimal solution			Optimal Results from literature
			Global	Global with Extend 1	Global with Extend 2	
Maximum number of iterations	1	6,042	61	20	40	
Minimum Hot Utility (kW)	0	0	0	0	0	
Maximum Hot Utility (kW)	6,042	6,042	6,042	200	40	
Defined Heat Duty Interval	6,042	1	100	10	1	
CPU time	0.2 s	37 m 45 s	16.8 s	9.2 s	10.4 s	9,600 s
TAC ($/yr)	**121,672**	**85,534**	**112,447**	**85,809**	**73,434**	**N/A**
Hot Utility (kW)	**200**	**2**	**100**	**20**	**1e-4**	**N/A**

By generating a network with the same hot utility range (0 to 6,042 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case shown in fig 4.19, presents a higher TAC solution than our regular global optimization result, demonstrating the efficiency of our method in achieving the optimal solution. To examine the effectiveness of the global optimization with extension, the global optimization with 1 kW interval is run without applying our extension technique. The TAC solution is $85,534 per year, higher than our extension 2 result with much higher computational time, demonstrating how our global optimization with extension is more effective in terms of both the computational time and the objective value.

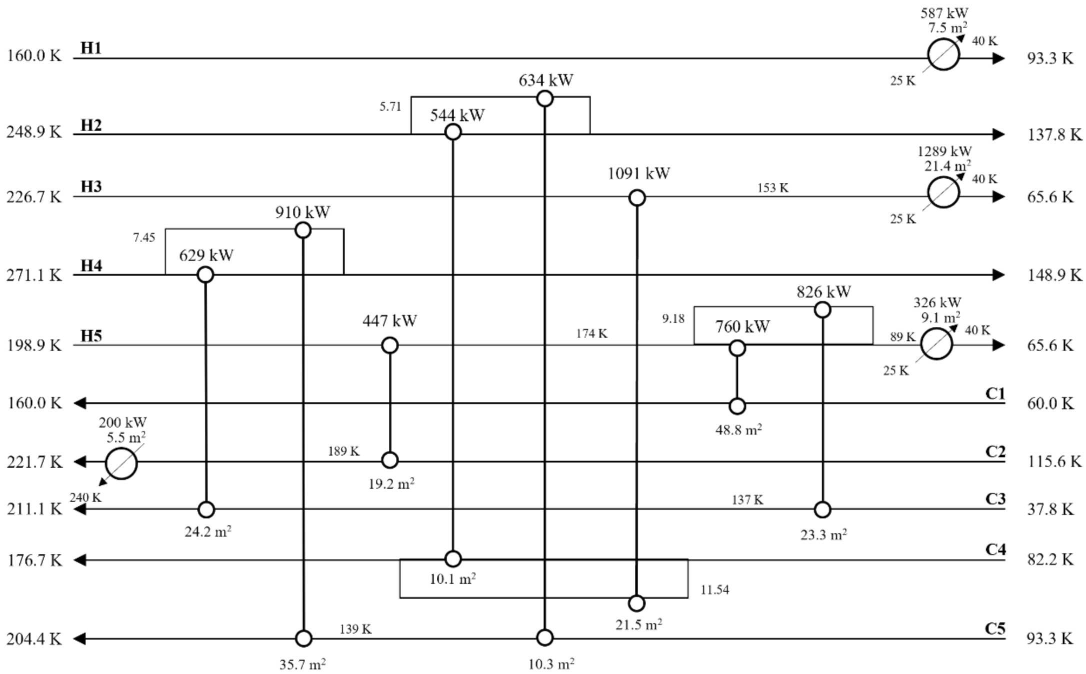

Figure 4.19 HEN solution of base case.

The HEN topology solution from paper of Mistry et al. (2016), the original research performed optimization by difference approach. This study did not present the optimal HEN configuration; therefore, we were unable to determine the theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Theoretical area data for Mistry and our global optimal theoretical TAC is $73,434/year at maximum number of iterations of 40. Although the extend 2 model results show a significant decrease in the global TAC value compared to the previous computation, our best TAC is still substantially larger than the original literature even though the necessary compute time is significantly less. As shown in Table 4.16, our optimal solution using the extension technique is significantly lower than the base case, owing primarily to lower hot utility costs.

Table 4.16 Result for optimal HEN topology from our optimal HEN (a), base case HEN (b), Mistry et al. (2016) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m²)	$A_{H4\text{-}C1}$	7.6
	$A_{H4\text{-}C5}$	32.4
	$A_{H2\text{-}C2}$	30.9
	$A_{H2\text{-}C5}$	8.3
	$A_{H3\text{-}C3}$	40.1
	$A_{H5\text{-}C1}$	4.3
	$A_{H5\text{-}C4}$	120.1
	$A_{C2\text{-}HU}$	4.8e-6
	$A_{H1\text{-}CU}$	7.5
	$A_{H3\text{-}CU}$	17.6
	$A_{H5\text{-}CU}$	12.4
Fixed cost ($)		44,000
Area cost ($)		9,424
Hot utility cost ($/yr)		0
Cold utility cost ($/yr)		20,010
TAC Calculation ($/yr)		**73,434**

(b)

Item	Exchanger	Base case
Theoretical Area (m²)	$A_{H4\text{-}C3}$	24.2
	$A_{H4\text{-}C5}$	35.7
	$A_{H5\text{-}C2}$	19.2
	$A_{H2\text{-}C4}$	10.1
	$A_{H2\text{-}C5}$	10.3
	$A_{H3\text{-}C4}$	21.5
	$A_{H5\text{-}C1}$	48.8
	$A_{H5\text{-}C3}$	23.3
	$A_{C2\text{-}HU}$	5.5
	$A_{H1\text{-}CU}$	7.5
	$A_{H3\text{-}CU}$	21.4
	$A_{H5\text{-}CU}$	9.1
Fixed cost ($)		48,000
Area cost ($)		11,662
Hot utility cost ($/yr)		40,000
Cold utility cost ($/yr)		22,010
TAC Calculation ($/yr)		**121,672**

(c)

Item	Exchanger	Topology from literature Mistry et al. (2016)
Theoretical Area (m²)	N/A	N/A
Fixed cost ($)		N/A
Area cost ($)		N/A
Hot utility cost ($/yr)		N/A
Cold utility cost ($/yr)		N/A
TAC Calculation ($/yr)		N/A

4.6 Example 6 (M. M. Daichendt, 1993)

The example consists of five cold and five hot process streams. This example is taken from Daichendt et al. (1993) and the stream data and parameters are given in Table 4.17.

Table 4.17 Data and parameters of esxample 6 (M. M. Daichendt, 1993)

Stream	T_{in} (K)	T_{out} (K)	h (kW/m^{2}K)	FC_p (kW/K)
H1	500	340	1.6	15
H2	460	400	1.6	3
H3	440	400	1.6	8
H4	350	310	1.6	9
H5	350	320	1.6	5
C1	300	340	1.6	8
C2	340	360	1.6	15
C3	340	400	1.6	8
C4	380	460	1.6	4
C5	460	560	1.6	6
HU	580	580	1.6	
CU	300	320	1.6	
Parameters			**Unit**	
Cold utility cost (CUcost)			$/kW	10
Hot utility cost (HUcost)			$/kW	125
Fixed cost (Fcost)			$	900
Area cost coefficient (AC)			$/m^2	300
Area cost exponent (AE)			-	1.0
Exchanger minimum approach temperature (EMAT)			K	10
Annual interest rate			%	0
Life time			year	1

The example was solved using a 5-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 K. Therefore, we verify that the structure obtained from the optimization is only feasible for values of energy between minimum hot utility = 390 kW and maximum hot utility = 2,020 kW. These values can be confirmed using the pinch analysis. We then define a heat duty interval of 100 kW and a maximum number of iterations of 17 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals

until reaching the maximum number of iterations. The optimal HEN solution is presented in Fig 4.20.

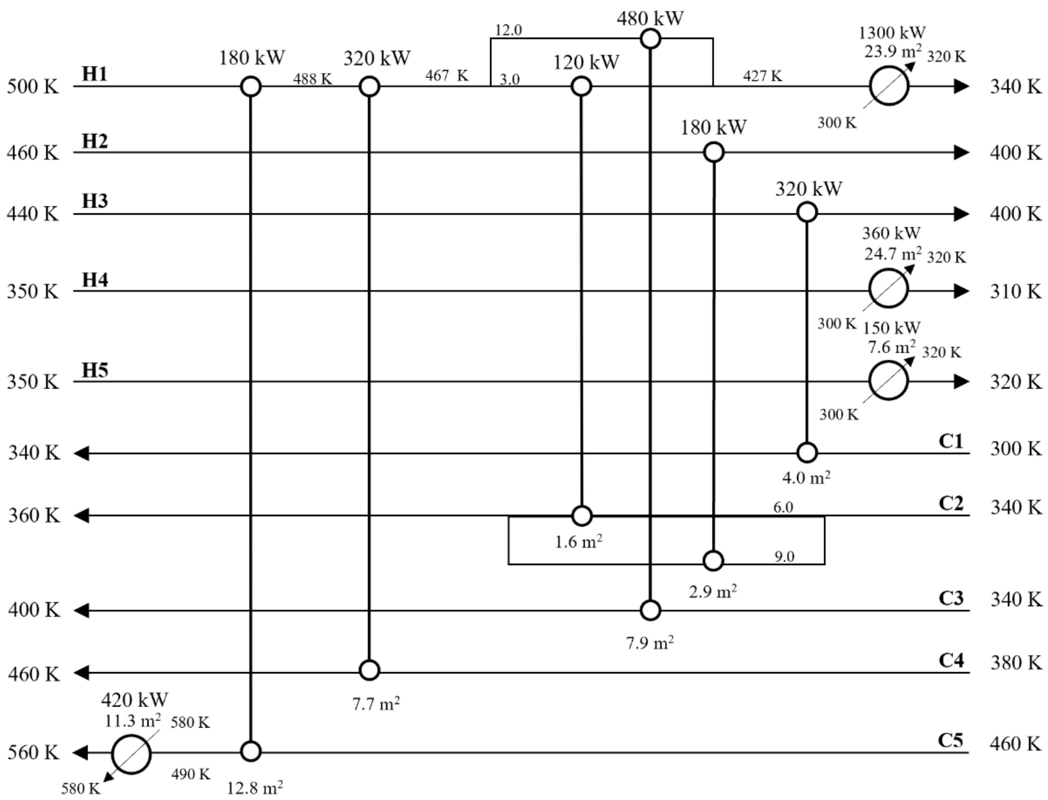

Figure 4.20 Our optimal HEN solution of example 6 with theoretical area.

Figure 4.21 shows that the TAC is monotone increasing and therefore a minimum TAC exhibit within the range of feasible energy value. In this case, the minimum TAC takes place at hot utility = 420 kW with the globally optimal solution features an annualized cost of $111,491/year.

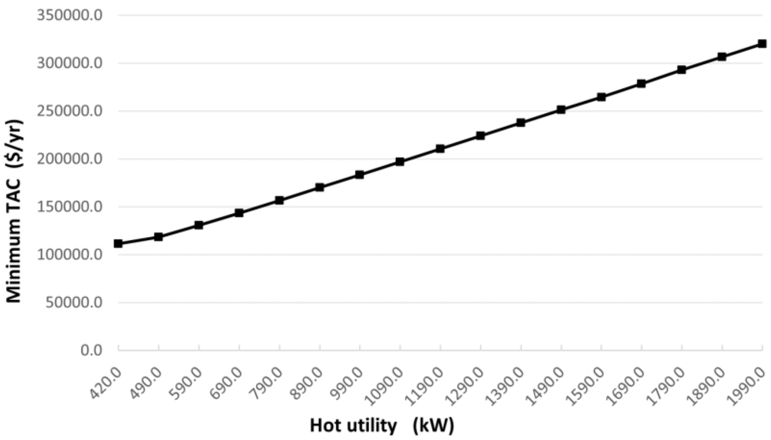

Figure 4.21 TAC vs. hot utility for a structure of example 6.

The optimal TAC obtained in the paper of Daichendt et al. (1993) is $110,848/year and it was obtained in 2,252 sec of CPU time. While our global optimal TAC solution is $111,491/year after 12.7 sec of CPU time. Despite the fact that the required computational time is significantly less, our best TAC is slightly higher than the original literature, showing that our optimal solution network is fairly different from the global optimum.

Therefore, we further expand our global optimization approach by solving for less TAC between minimum hot utility = 390 kW and maximum hot utility = 500 kW with heat duty interval of 10 kW. A maximum number of iterations of 11 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The optimal HEN solution is presented in Fig 4.22.

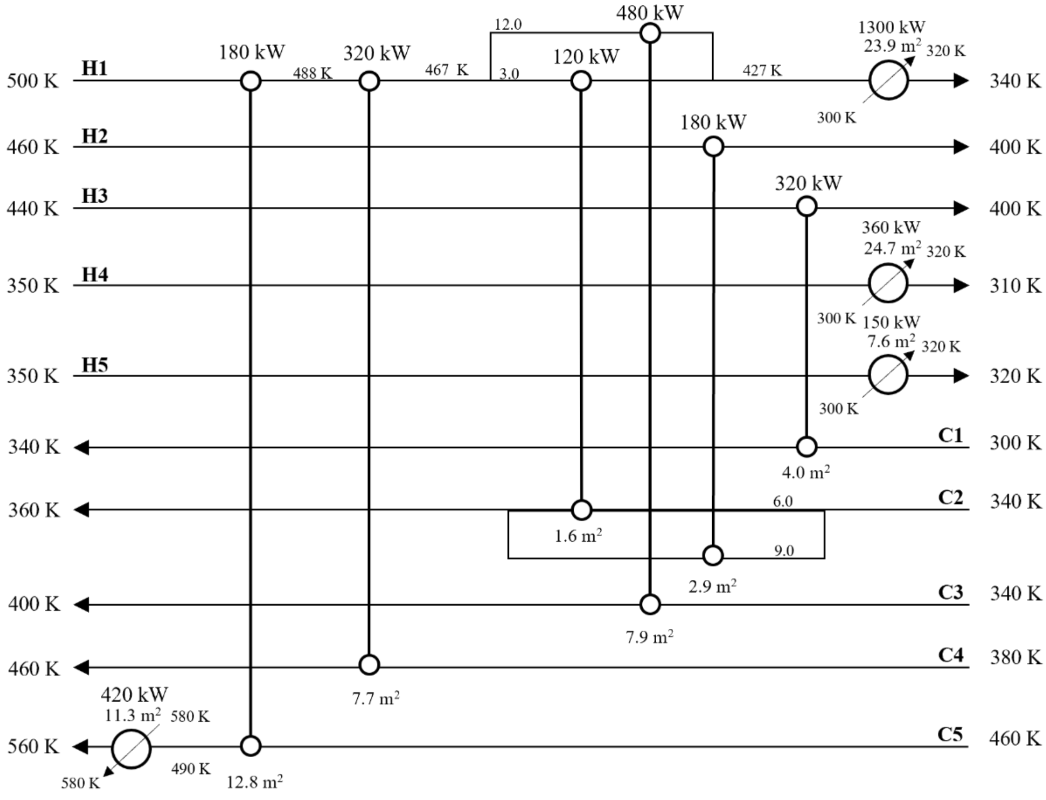

Figure 4.22 The optimal HEN solution of example 6 - extend 1.

As we use less intervals, the maximum number of iterations tends to diminish and the time decrease. After 6.6 sec CPU time, we get the minimum TAC takes place at hot utility = 420 kW with the globally optimal solution features an annualized cost of $110,869/year as shown in Figure 4.23.

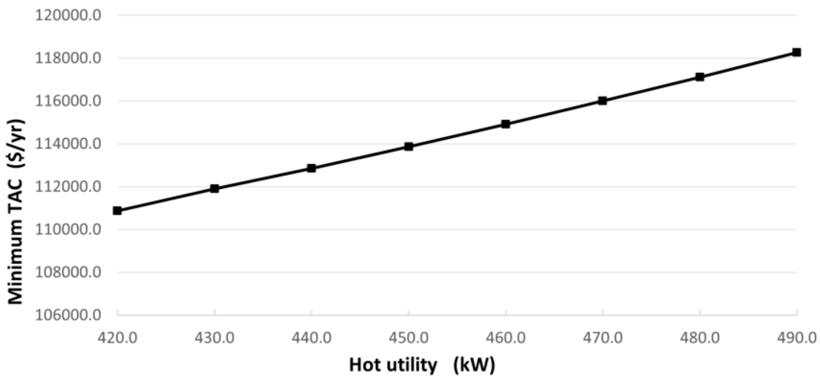

Figure 4.23 TAC vs. hot utility for a structure of example 6- extend 1.

Table 4.18 summarize the results for different number of partitioning intervals. Our regular global solution is $111,491 per year, which is higher than the one from literature. However, by decreasing the heat duty interval from 100 to 10 kw through the first step until the last extension step, our global optimization with extension significantly lowers the objective TAC value from $111,491 to $110,869 per year. The program tries to run the global optimization with extension 1. The TAC solution is much lower than previous solution with $110,869 per year, still slightly higher than the one from literature with $110,848 per year. The hot utility duty is equality at 420kW. The program then continues running the global optimization with extension 2, but TAC solution is not lower than the previous solution, so the program stops and report the extension 1 global solution. Our computational time summation is 19.1 second, substantially lower than the paper.

Table 4.18 Results for different partitioning interval numbers

Items	**Base case** (Maximum iteration = 1)	**Global with 1kw interval** (without Extend technique)	**Our optimal solution**		**Optimal Results from literature**
			Global	**Global with Extend 1**	
Maximum number of iterations	1	1,630	17	11	
Minimum Hot Utility (kW)	390	390	390	390	
Maximum Hot Utility (kW)	2,020	2,020	2,020	500	
Defined Heat Duty Interval	1,630	1	100	10	
CPU time	1.2 s	12 m 49 s	12.7 s	6.6 s	2,252 s
TAC ($/yr)	**111,520**	**110,869**	**111,491**	**110,869**	**110,848**
Hot Utility (kW)	**420.0**	**420.0**	**420.0**	**420.0**	**420.0**

By generating a network with the same hot utility range (390 to 2,020 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case shown in Fig 4.24, presents a higher TAC solution than our global optimization with extension 1 result, demonstrating the efficiency of our method in achieving the optimal solution. To examine the effectiveness of the global optimization with extension, the global optimization with 1 kW interval is run without applying our extension technique. The TAC solution is $110,869 per year, exact same as our extension 1 result with much higher computational time, demonstrating how our global optimization with extension is more effective in terms of both the computational time and the objective value.

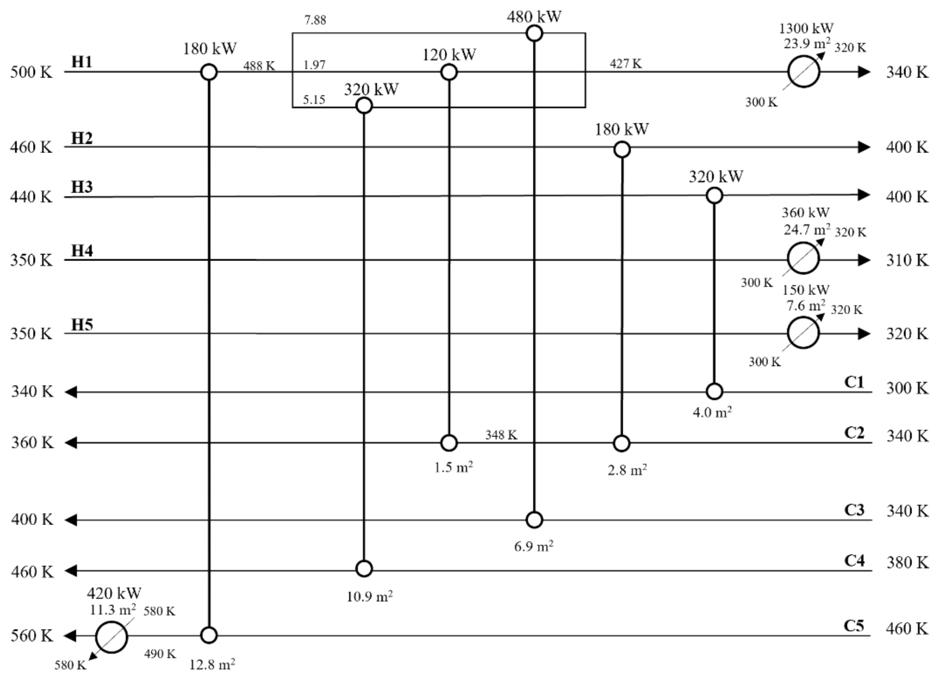

Figure 4.24 HEN solution of base case.

The HEN topology solution from paper of Daichendt et al. (1993), the original research performed optimization by difference approach, modified reduced superstructures and improved robustness by elimination of poor solutions for HENS. The values for area are utilized to determine the best HEN global annual cost, which is $110,848/year with 2,252.0 sec CPU time. The optimal HEN topology solution with theoretical area is shown in Figure 4.25. The comparation of HEN topology solution of the paper and our extension 1 solution shown in Figure 4.22 are similar with six heat exchanger units and three utility units at exact same stream. As a result, our TAC results and paper are exceptionally comparable.

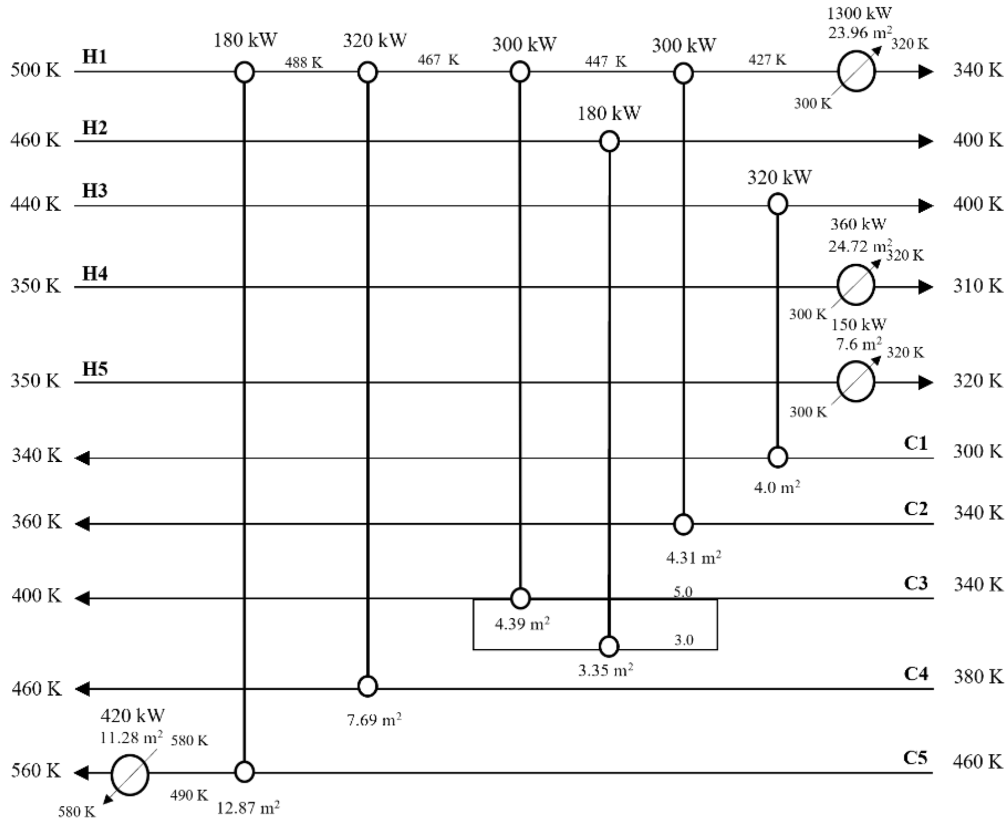

Figure 4.25 Improved topology solution with reduced MINLP from Daichendt et al. (1993) with theoretical area.

We calculate Daichendt's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Daichendt's theoretical area value, the theoretical TAC of $110,848/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Daichendt and our result are presented in Table 4.19. Our global optimal theoretical TAC is $110,869/year at number of iterations of 11, which is slightly higher than the original literature due to the difference in area cost, the necessary compute time is significantly less, showing that our optimal solution network is close to the global optimum while requiring significantly less computational time.

Table 4.19 Result for optimal HEN topology from our optimal HEN (a), base case HEN (b), Daichendt et al. (1993) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m²)	$A_{H1\text{-}C5}$	12.8
	$A_{H1\text{-}C4}$	7.7
	$A_{H1\text{-}C2}$	1.6
	$A_{H1\text{-}C3}$	7.9
	$A_{H2\text{-}C2}$	2.9
	$A_{H3\text{-}C1}$	4.0
	$A_{H5\text{-}HU}$	11.3
	$A_{H1\text{-}CU}$	23.9
	$A_{H4\text{-}CU}$	24.7
	$A_{H5\text{-}CU}$	7.6
Fixed cost ($)		9,000
Area cost ($)		31,269
Hot utility cost ($/yr)		52,500
Cold utility cost ($/yr)		18,100
TAC Calculation ($/yr)		**110,869**

(b)

Item	Exchanger	Base case
Theoretical Area (m²)	$A_{H1\text{-}C5}$	12.8
	$A_{H1\text{-}C4}$	10.9
	$A_{H1\text{-}C2}$	1.5
	$A_{H1\text{-}C3}$	6.9
	$A_{H2\text{-}C2}$	2.8
	$A_{H3\text{-}C1}$	4.0
	$A_{H5\text{-}HU}$	11.3
	$A_{H1\text{-}CU}$	23.9
	$A_{H4\text{-}CU}$	24.7
	$A_{H5\text{-}CU}$	7.6
Fixed cost ($)		9,000
Area cost ($)		31,920
Hot utility cost ($/yr)		52,500
Cold utility cost ($/yr)		18,100
TAC Calculation ($/yr)		**111,520**

(c)

Item	Exchanger	Topology from literature Daichendt et al. (1993)
Theoretical Area (m²)	$A_{H1\text{-}C5}$	12.870
	$A_{H1\text{-}C4}$	7.686
	$A_{H1\text{-}C3}$	4.389
	$A_{H2\text{-}C3}$	3.347
	$A_{H1\text{-}C2}$	4.310
	$A_{H3\text{-}C1}$	4.000
	$A_{H5\text{-}HU}$	11.281
	$A_{H1\text{-}CU}$	23.956
	$A_{H4\text{-}CU}$	24.718
	$A_{H5\text{-}CU}$	7.602
Fixed cost ($)		9,000
Area cost ($)		31,248
Hot utility cost ($/yr)		52,500
Cold utility cost ($/yr)		18,100
TAC Calculation ($/yr)		**110,848**

4.7 Example 7 (Pavao LV C. C., 2016)

The last example consists of six cold and fore hot process streams. This example is taken from Pavao et al. (2016). The stream data and parameters are given in Table 4.20.

Table 4.20 Data and parameters of example 7

Stream	T_{in} (K)	T_{out} (K)	h (kW/m²K)	FC_p (kW/K)
H1	85	45	0.05	156.3
H2	120	40	0.05	50
H3	125	35	0.05	23.9
H4	56	46	0.05	1250
H5	90	85	0.05	1200
H6	225	75	0.05	50
C1	40	55	0.05	466.7
C2	55	65	0.05	600
C3	65	165	0.05	180
C4	10	170	0.05	81.3
HU	200	199	0.05	
CU	15	25	0.05	
Parameters			**Unit**	
Cold utility cost (CUcost)			$/kW	15
Hot utility cost (HUcost)			$/kW	100
Fixed cost (Fcost)			$	8000
Area cost coefficient (AC)			$/m²	60
Area cost exponent (AE)			-	1.0
Exchanger minimum approach temperature (EMAT)			K	1
Annual interest rate			%	0
Life time			year	1

The example was solved using a 4-stages superstructure model and assumed a exchanger minimum temperature approach EMAT of 10 K. Therefore, we verify that the structure obtained from the optimization is only feasible for values of energy between minimum hot utility = 11,205 kW and maximum hot utility = 44,008 kW. These values can be confirmed using the pinch analysis. We then define a heat duty interval of 1,000 kW and a maximum number of iterations of 33 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The optimal HEN solution is presented in Fig 4.26.

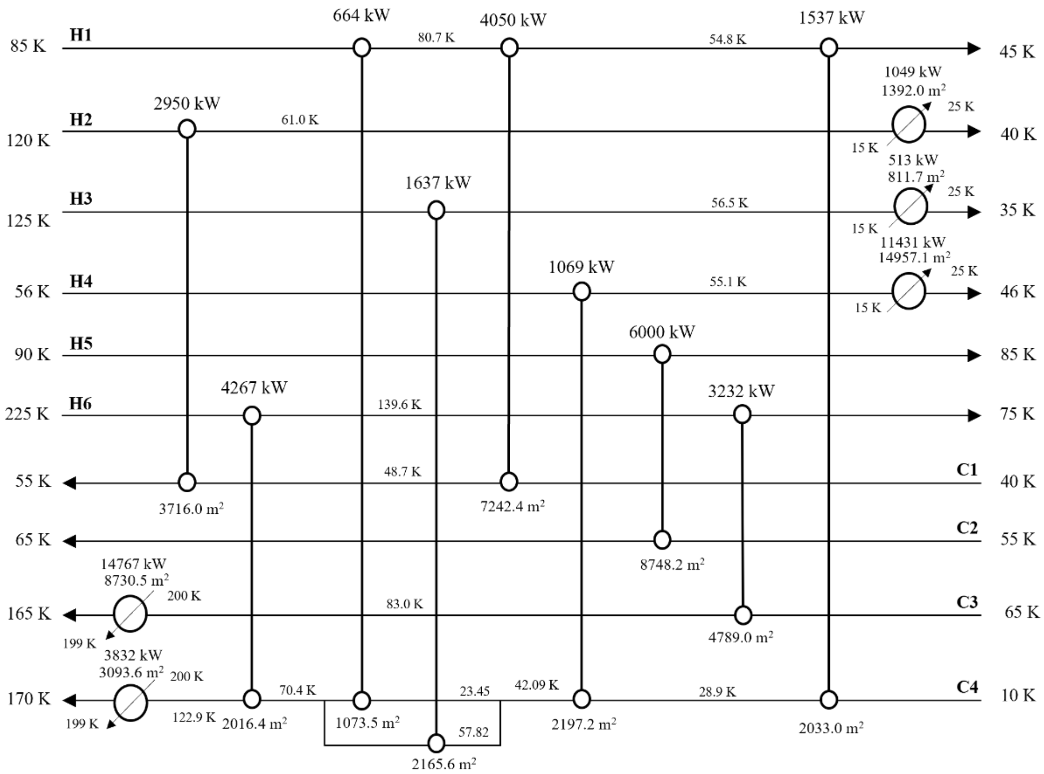

Figure 4.26 Our optimal solution network of example 7 with theoretical area.

Figure 4.27 shows that the TAC is fluctuating and tend to increase with the energy value. The minimum TAC exhibit within the range of this feasible energy value, takes place at hot utility = 19,224 kW with the globally optimal solution features TAC of $6,222,161/year.

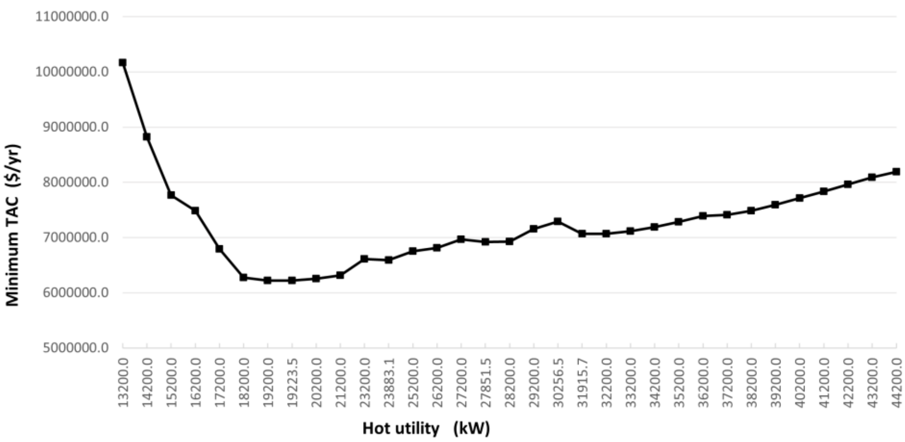

Figure 4.27 TAC vs. hot utility for a structure of example 7.

The optimal TAC obtained in the paper of Pavao et al. (2016) is $ 5,788,187/year. While our global optimal TAC solution is $6,222,161/year with 3 min 44 sec of CPU time. Our best TAC is significantly higher than the original literature, showing that our optimal solution network is fairly different from the global optimum.

Therefore, we further expand our global optimization approach by solving for less TAC between minimum hot utility = 17,000 kW and maximum hot utility = 23,200 kW with heat duty interval of 200 kW. A maximum number of iterations of 31 that will be considered as terminating criteria. The local-optimum HENs are synthesized at several intervals until reaching the maximum number of iterations. The global optimum HEN is the local optimal HEN with the lowest TAC of all iterations. The example was resolved using a 4-stages superstructure and assumed a minimum temperature approach EMAT of 10 K. The optimal HEN solution is presented in Fig 4.28.

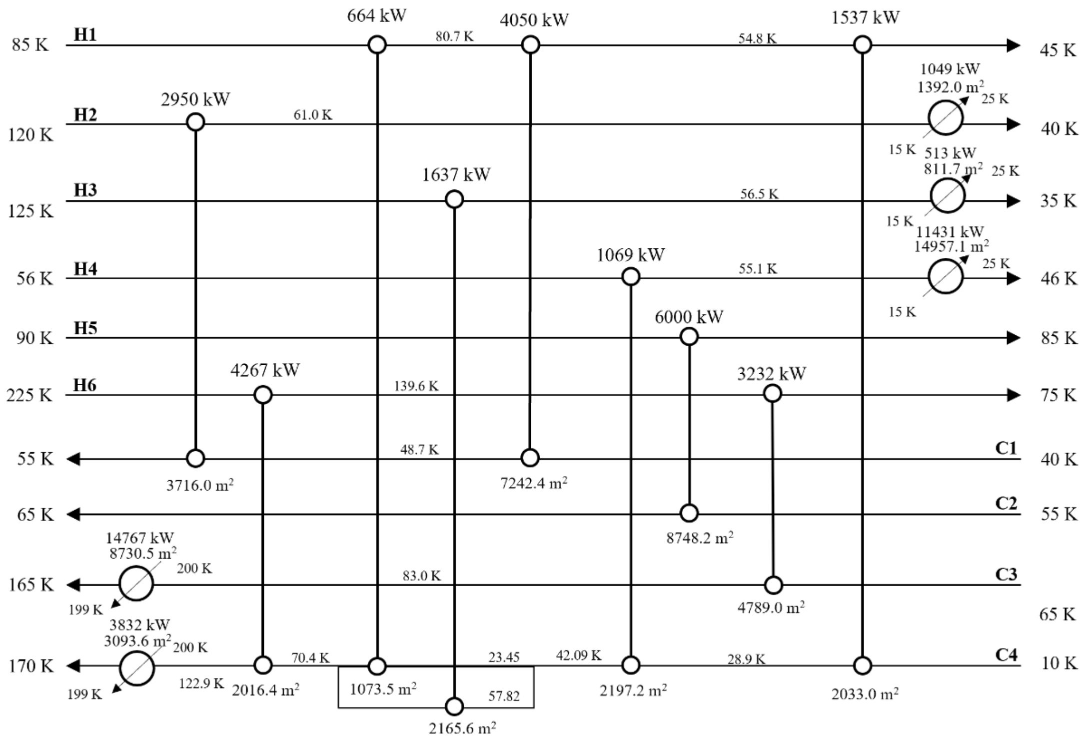

Figure 4.28 The optimal HEN solution of example 7 - extend 1.

As we use less intervals, the maximum number of iterations tends to diminish and the time decrease. After 1 min 3 sec of CPU time, we get the minimum TAC takes place at hot utility = 18,600 kW with the globally optimal solution features TAC of 5,960,899/year as shown in Figure 4.29. While the optimal TAC obtained in the paper of Pavao et al. (2016) is $ 5,788,187/year. The extend 1 model results show a significant decrease in the global TAC value compared to the previous computation. Although our best TAC is still slightly larger than the original literature, demonstrating that there are several alternative solutions close to the global optimum.

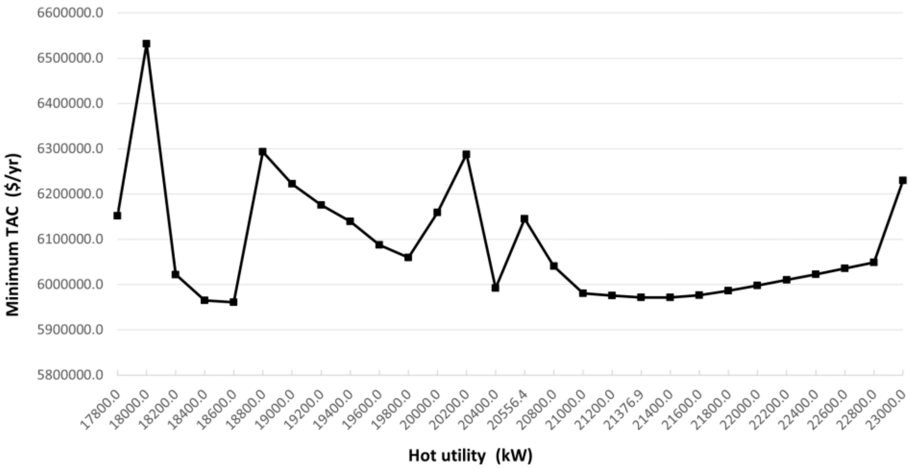

Figure 4.29 TAC vs. hot utility for a structure of example 7- extend 1.

Table 4.21 summarize the results for different number of partitioning intervals. Our regular global solution is $6,222,161 per year, which is higher than the one from literature. However, by decreasing the heat duty interval from 1,000 to 200 kw through the first step until the last extension step, our global optimization with extension significantly lowers the objective TAC value from $6,222,161 to 5,960,899$ per year. The program tries to run the global optimization with extension 1. The TAC solution is much lower than previous solution with $5,960,899 per year, still slightly higher than the one from literature with $5,788,187 per year. The program then continues running the global optimization with extension 2, but TAC solution is not lower than the previous solution, so the program stops and report the extension 1 global solution.

Table 4.21 Results for different partitioning interval numbers

Items	**Base case** (Maximum iteration = 1)	**Global with 1kw interval** (without Extend technique)	**Our optimal solution**		**Optimal Results from literature**
			Global	**Global with Extend 1**	
Maximum number of iterations	1	32,803	33	31	
Minimum Hot Utility (kW)	11,205	11,205	11,205	17,000	
Maximum Hot Utility (kW)	44,008	44,008	44,008	23,200	
Defined Heat Duty Interval	32,803	1	1,000	200	
CPU time	29.4 s	5 h 59 m 18 s	3 m 44 s	1 m 3 s	N/A
TAC ($/yr)	**6,365,859**	**5,945,951**	**6,222,161**	**5,960,899**	**5,788,187**
Hot Utility (kW)	**18,842**	**19,295**	**19,224**	**18,600**	**20,320**

By generating a network with the same hot utility range (11,205 to 44,008 kW), the base case is used to evaluate the effectiveness of the regular global optimization method. The base case shown in Fig 4.30, presents a higher TAC solution than our global optimization result, demonstrating the efficiency of our method in achieving the optimal solution. To examine the effectiveness of the global optimization with extension, the global optimization with 1 kW interval is run without applying our extension technique. The TAC solution costs $5,945,951 per year, which is slightly less than our extension 1 result, but comes with a much longer computational time. This demonstrating how our global optimization with extension is more effective in terms of both the computational time and the objective value.

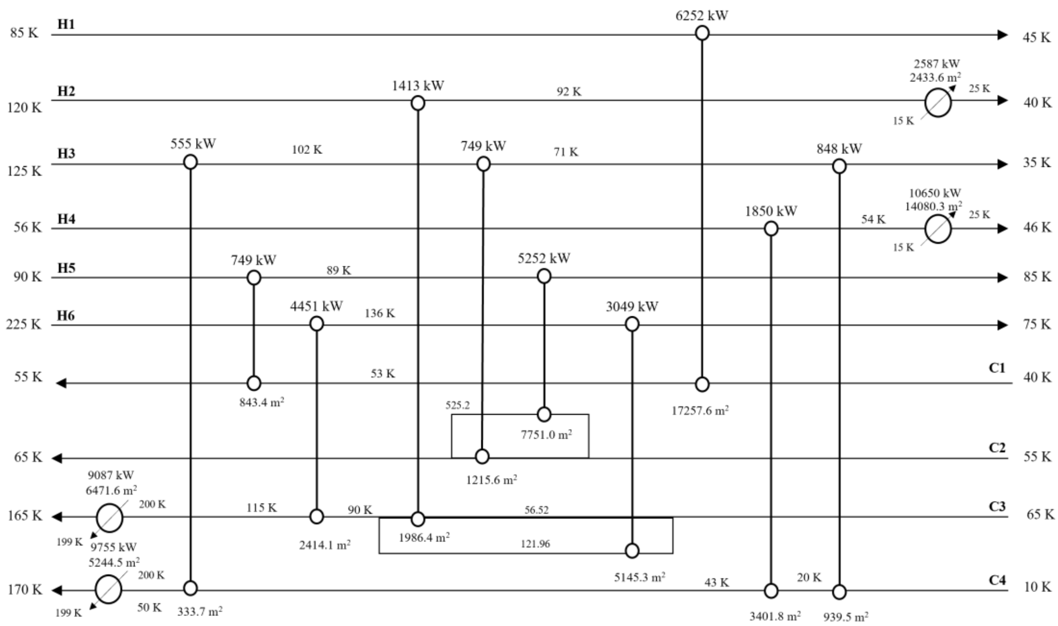

Figure 4.30 HEN solution of base case.

The HEN topology solution from paper of Pavao et al. (2016), the original research performed optimization by difference approach, hybrid meta-heuristic method and simple Simulated Annealing approach is used for the combinatorial level, while a strategy named rocket fireworks optimization is developed and applied to the continuous domain. The algorithm was written in C++. The values for area are utilized to determine the best HEN global annual cost, which is $ 5,788,187/year. The optimal HEN topology solution with theoretical area is shown in Figure 4.31. The comparation of HEN topology solution of the paper and our extension 1 solution shown in Figure 4.28 are quite different, although our hot utility duty consumes 1720 kW less than the paper but our TAC solution is significantly larger.

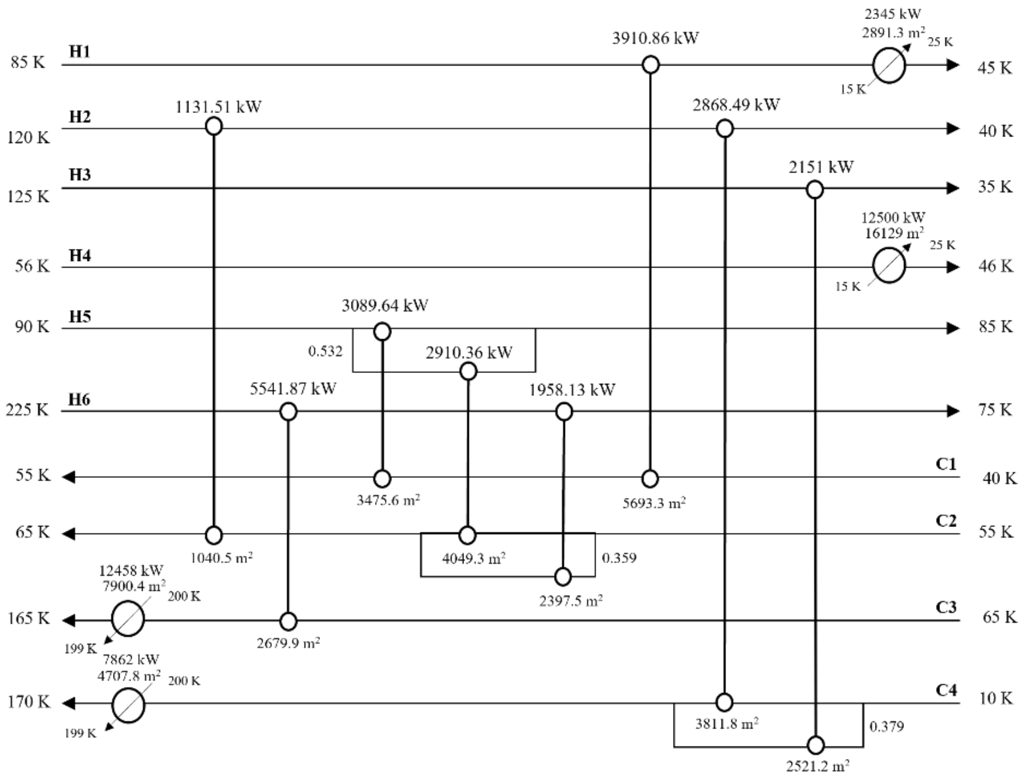

Figure 4.31 Improved topology solution with reduced MINLP from Pavao et al. (2016) with theoretical area.

We calculate Pavao's theoretical area for each heat exchanger by using our LMTD and area formular, presented in equation 25 to 27. Using Pavao's theoretical area value, the theoretical TAC of $5,788,187/year is defined in order to compare with our theoretical TAC value. Theoretical area data for Pavao and our result are presented in Table 4.22. Our global optimal theoretical TAC is $5,960,899/year at number of iterations of 31. The extend 1 result show a significant decrease in the global TAC value compared to the previous computation. Although our best TAC is still slightly larger than the original literature, demonstrating that there are several alternative solutions close to the global optimum. However, our optimal solution with extension technique is much lower than the base case, mainly lower in area cost.

Table 4.22 Result for optimal HEN topology from our optimal HEN (a), base case HEN (b), Pavao et al. (2016) (c)

(a)

Item	Exchanger	Our Result
Theoretical Area (m^2)	A_{H2-C1}	3716.0
	A_{H6-C4}	2016.4
	A_{H1-C4}	1073.5
	A_{H3-C4}	2165.6
	A_{H1-C1}	7242.4
	A_{H4-C4}	2197.2
	A_{H5-C2}	8748.2
	A_{H6-C3}	4789.0
	A_{H1-C4}	2033.0
	A_{C3-HU}	8730.5
	A_{C4-HU}	3093.6
	A_{H2-CU}	1392.0
	A_{H3-CU}	811.7
	A_{H4-CU}	14957.1
Fixed cost ($)		122,000
Area cost ($)		3,784,104
Hot utility cost ($/yr)		1,859,900
Cold utility cost ($/yr)		194,895
TAC Calculation ($/yr)		**5,960,899**

(b)

Item	Exchanger	Base case
Theoretical Area (m^2)	A_{H3-C4}	333.7
	A_{H5-C1}	843.4
	A_{H6-C3}	2414.1
	A_{H2-C3}	1986.4
	A_{H3-C2}	1215.6
	A_{H5-C2}	7751.0
	A_{H6-C3}	5145.3
	A_{H1-C1}	17257.6
	A_{H4-C4}	3401.8
	A_{H3-C4}	939.5
	A_{C3-HU}	6471.6
	A_{C4-HU}	5244.5
	A_{H2-CU}	2433.6
	A_{H4-CU}	14080.3
Fixed cost ($)		112,000
Area cost ($)		4,171,104
Hot utility cost ($/yr)		1,884,200
Cold utility cost ($/yr)		198,555
TAC Calculation ($/yr)		**6,365,859**

(c)

Item	Exchanger	Topology from literature Pavao et al. (2016)
Theoretical Area (m^2)	A_{H2-C2}	1040.5
	A_{H6-C3}	2679.9
	A_{H5-C1}	3475.6
	A_{H5-C2}	4049.3
	A_{H6-C2}	2397.5
	A_{H1-C1}	5693.3
	A_{H2-C4}	3811.8
	A_{H3-C4}	2521.2
	A_{H1-CU}	2891.3
	A_{H4-CU}	16129.0
	A_{C3-HU}	7900.4
	A_{C4-HU}	4707.8
Fixed cost ($)		96,000
Area cost ($)		3,437,520
Hot utility cost ($/yr)		2,032,000
Cold utility cost ($/yr)		222,667
TAC Calculation ($/yr)		**5,788,187**

CHAPTER 5
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

This study proposes a global optimization strategy for the synthesis of HEN, which must be applied to numerous industrial processes requiring heat integration to save energy. For small problems of example 1,2, and 3, the methods used in our work generate optimal HEN solutions using less computational time with TACs close to the global ones from literatures. The large problems of example 5 to 7 are solved by our global optimization with extension technique and it generates global-optimum HENs with larger TAC than ones from literatures. However, the optimal results from example 4 are significantly larger in TAC than the literature. It could be due to differences in the stage-wise superstructure model and the linearization technique used in the literature. Our Global optimization performance could be improved by lowering the problem's computational complexity. Implementing further thermodynamic theory-based constraints to tighten the convex relaxation is another technique that may be beneficial to improve the algorithm's performance. All these initiatives are part of ongoing work.

5.2 Recommendations

Consider Example 4 to be our challenging case. Previously, we obtained infeasible results and reduced gradient less than tolerance. Since the initial value was far from the converging point, the relaxed NLP was infeasible. We must test our model to ensure that it solves correctly as an RMINLP model. Despite our computational time being substantially smaller, the literature's results are marginally better than ours.

APPENDICES / APPENDIX

GRAPHICAL ABSTRACT

Appendix A

EXAMPLE 7 GAMS CODE

Stage-wise superstructure model

```
Sets
        I hot streams /H1, H2, H3, H4, H5, H6/
        J cold streams /C1, C2, C3, C4/
        K stage NO. /K1, K2, K3, K4, K5/ ;

Parameter
        TinI(I)         K /H1 =85 , H2 =120 , H3 =125 , H4 =56 , H5 =90 , H6 =225 /
        TinJ(J)         K /C1 =40 , C2 =55 , C3 =65 , C4 =10 /
        ToutI(I)        K /H1 =45 , H2 =40 , H3 =35 , H4 =46 , H5 =85, H6 =75 /
        ToutJ(J)        K /C1 =55 , C2 =65 , C3 =165 , C4 =170  /

        FcpI(I)         kW per K /H1 =156.3 , H2 =50 , H3 =23.9 , H4 =1250 , H5 =1200 , H6 =50 /
        FcpJ(J)         kW per K /C1 =466.7 , C2 =600 , C3 =180 , C4 =81.3 /
        hI(I)           kW per m2*K /H1 =0.05 , H2 =0.05 , H3 =0.05 , H4 =0.05 , H5 =0.05 , H6 =0.05 /
        hJ(J)           kW per m2*K /C1 =0.05 , C2 =0.05 , C3 =0.05 , C4 =0.05 /

        EMAT            HE minimum approch temperature (K) /1/
        OMEGAI(I)       upper bound for HE
        OMEGAJ(J)       upper bound for HE
        GAMMA(I,J)      upper bound for temp different

        Thuin           Temp inlet for Hot Utility (K) /200/
        Thuout          Temp outlet for Hot Utility (K) /199/
        Tcuin           Temp inlet for Cold Utility (K) /15/
        Tcuout          Temp outlet for Cold Utility (K) /25/

        U               overall heat transfer coeff for HE (kW per m2*K) /0.025/
        Uc              overall heat transfer coeff for coldU (kW per m2*K) /0.025/
        Uh              overall heat transfer coeff for HotU (kW per m2*K) /0.025/

        Fcost           Unit fixed cost (Dollar) /8000/
        HUcost          Hot utility cost coeff (Dollar per kW) /100/
        CUcost          Cold utility cost coeff (Dollar per kW) /15/
        AC              Area cost coefficient ($ per m2) /60/
        AE              Area cost exponential   /1/
;
```

```
Variables
         dt(I,J,K)          approach temperature
         dtcu(I)            approach temperature between cold utility and hot stream
         dthu(J)            approach temperature between hot utility and cold stream
         q(I,J,K)           heat exchanged between hot I and cold J
         qcu(I)             heat exchanged between cold utility and hot I
         qhu(J)             heat exchanged between hot utility and cold J
         ti(I,K)            temperature of hot stream I at hot end of stage K
         tj(J,K)            temperature of cold stream J at hot end of stage K
         z(I,J,K)           exchanger matching between hot I and cold J at stage K
         zcu(I)             cold utility matching with hot I
         zhu(J)             hot utility matching with cold J
         ZZ                 TAC when fixed E

         qcs                Vary sum cold utility
         qhs                Range sum Hot utility

         A(I,J,K)           area of heat exchangers
         TA                 sum of area of heat exchangers only
         Acost              area cost for heat exchanger only

         Acu(I)             cold utility area
         Ahu(J)             hot utility area
         AUcost             area cost for utilities only ;


Positive variables          dt(I,J,K), dtcu(I), dthu(J), q(I,J,K), qcu(I), qhu(J), ti(I,K), tj(J,K), A(I,J,K)  ;

Binary variables            z(I,J,K), zcu(I), zhu(J) ;
```

```
Equations
        MINU            objective function minimize utilities and matching

        HOTI(I)         heat balance in hot streams I
        COLDJ(J)        heat balance in cold streams J

        HOTK1(I)        heat balance of hot at stage K1
        HOTK2(I)        heat balance of hot at stage K2
        HOTK3(I)        heat balance of hot at stage K3
        HOTK4(I)        heat balance of hot at stage K4

        COLDK1(J)       heat balance of cold at stage K1
        COLDK2(J)       heat balance of cold at stage K2
        COLDK3(J)       heat balance of cold at stage K3
        COLDK4(J)       heat balance of cold at stage K4

        TINHOT(I)       hot temperature in
        TINCOLD(J)      cold temperature in

        FEHOTK1(I)      feasibility of hot temperature at stage K1
        FEHOTK2(I)      feasibility of hot temperature at stage K2
        FEHOTK3(I)      feasibility of hot temperature at stage K3
        FEHOTK4(I)      feasibility of hot temperature at stage K4

        FECOLDK1(J)     feasibility of cold temperature at stage K1
        FECOLDK2(J)     feasibility of cold temperature at stage K2
        FECOLDK3(J)     feasibility of cold temperature at stage K3
        FECOLDK4(J)     feasibility of cold temperature at stage K4

        FEHOTOUT(I)     feasibility of hot temperature out
        FECOLDOUT(J)    feasibility of cold temperature out

        HOTU(I)         hot utility load
        COLDU(J)        cold utility load

        LogicK1(I,J)    logical constraint at stage K1
        LogicK2(I,J)    logical constraint at stage K2
        LogicK3(I,J)    logical constraint at stage K3
        LogicK4(I,J)    logical constraint at stage K4

        LogicHOT(J)     logical constraint hot utility
        LogicCOLD(I)    logical constraint cold utility
```

```
Equations
        ApproK1(I,J)     approach temperature at stage K1
        AApproK1(I,J)    the other approach temperature at stage K1
        ApproK2(I,J)     approach temperature at stage K2
        AApproK2(I,J)    the other approach temperature at stage K2
        ApproK3(I,J)     approach temperature at stage K3
        AApproK3(I,J)    the other approach temperature at stage K3
        ApproK4(I,J)     approach temperature at stage K4
        AApproK4(I,J)    the other approach temperature at stage K4

        Approdthu(J,K)
        Approdtcu(I,K)

        EMATdt(I,J,K)    exchanger minimum approach temperature constraint

        qcsum,qhsum     sum utility

**For Area Cost**
        AreaK1(I,J)      area of heat exchangers at stage K1
        AreaK2(I,J)      area of heat exchangers at stage K2
        AreaK3(I,J)      area of heat exchangers at stage K3
        AreaK4(I,J)      area of heat exchangers at stage K4

        TotalArea        summation of area of heat exchangers
        Areacost
        AreaCU(I)
        AreaHU(J)
        AreaUcost
;
```

```
MINU            .. ZZ =e= CUcost*sum(I,qcu(I)) + HUcost*sum(J,qhu(J))
                       + Fcost*sum((I,J,K),z(I,J,K)) + Fcost*sum(I,zcu(I)) + Fcost*sum(J,zhu(J))
                       + sum((I,J,K),(AC*((A(I,J,K))**AE)))
                       + sum((I),(AC*((Acu(I))**AE))) + sum((J),(AC*((Ahu(J))**AE))) ;


HOTI(I)         .. (TinI(I)-ToutI(I))*FcpI(I) =e= sum((J,K),q(I,J,K))+qcu(I) ;
COLDJ(J)        .. (ToutJ(J)-TinJ(J))*FcpJ(J) =e= sum((I,K),q(I,J,K))+qhu(J) ;

HOTK1(I)        .. (ti(I,'K1')-ti(I,'K2'))*FcpI(I) =e= sum(J,q(I,J,'K1')) ;
HOTK2(I)        .. (ti(I,'K2')-ti(I,'K3'))*FcpI(I) =e= sum(J,q(I,J,'K2')) ;
HOTK3(I)        .. (ti(I,'K3')-ti(I,'K4'))*FcpI(I) =e= sum(J,q(I,J,'K3')) ;
HOTK4(I)        .. (ti(I,'K4')-ti(I,'K5'))*FcpI(I) =e= sum(J,q(I,J,'K4')) ;

COLDK1(J)       .. (tj(J,'K1')-tj(J,'K2'))*FcpJ(J) =e= sum(I,q(I,J,'K1')) ;
COLDK2(J)       .. (tj(J,'K2')-tj(J,'K3'))*FcpJ(J) =e= sum(I,q(I,J,'K2')) ;
COLDK3(J)       .. (tj(J,'K3')-tj(J,'K4'))*FcpJ(J) =e= sum(I,q(I,J,'K3')) ;
COLDK4(J)       .. (tj(J,'K4')-tj(J,'K5'))*FcpJ(J) =e= sum(I,q(I,J,'K4')) ;


TINHOT(I)       .. TinI(I) =e= ti(I,'K1') ;
TINCOLD(J)      .. TinJ(J) =e= tj(J,'K5') ;

FEHOTK1(I)      .. ti(I,'K1') =g= ti(I,'K2') ;
FEHOTK2(I)      .. ti(I,'K2') =g= ti(I,'K3') ;
FEHOTK3(I)      .. ti(I,'K3') =g= ti(I,'K4') ;
FEHOTK4(I)      .. ti(I,'K4') =g= ti(I,'K5') ;

FECOLDK1(J)     .. tj(J,'K1') =g= tj(J,'K2') ;
FECOLDK2(J)     .. tj(J,'K2') =g= tj(J,'K3') ;
FECOLDK3(J)     .. tj(J,'K3') =g= tj(J,'K4') ;
FECOLDK4(J)     .. tj(J,'K4') =g= tj(J,'K5') ;

FEHOTOUT(I)     .. ToutI(I) =l= ti(I,'K5') ;
FECOLDOUT(J)    .. ToutJ(J) =g= tj(J,'K1') ;

HOTU(I)         .. (ti(I,'K5')-ToutI(I))*FcpI(I) =e= qcu(I) ;
COLDU(J)        .. (ToutJ(J)-tj(J,'K1'))*FcpJ(J) =e= qhu(J) ;
```

```
LogicK1(I,J)    .. q(I,J,'K1')-min(OMEGAI(I),OMEGAJ(J))*z(I,J,'K1') =l= 0 ;
LogicK2(I,J)    .. q(I,J,'K2')-min(OMEGAI(I),OMEGAJ(J))*z(I,J,'K2') =l= 0 ;
LogicK3(I,J)    .. q(I,J,'K3')-min(OMEGAI(I),OMEGAJ(J))*z(I,J,'K3') =l= 0 ;
LogicK4(I,J)    .. q(I,J,'K4')-min(OMEGAI(I),OMEGAJ(J))*z(I,J,'K4') =l= 0 ;

LogicHOT(J)     .. qhu(J)-OMEGAJ(J)*zhu(J) =l= 0 ;
LogicCOLD(I)    .. qcu(I)-OMEGAI(I)*zcu(I) =l= 0 ;

ApproK1(I,J)    .. dt(I,J,'K1') =l= (ti(I,'K1')-tj(J,'K1'))+GAMMA(I,J)*(1-z(I,J,'K1')) ;
AApproK1(I,J)   .. dt(I,J,'K2') =l= (ti(I,'K2')-tj(J,'K2'))+GAMMA(I,J)*(1-z(I,J,'K1')) ;
ApproK2(I,J)    .. dt(I,J,'K2') =l= (ti(I,'K2')-tj(J,'K2'))+GAMMA(I,J)*(1-z(I,J,'K2')) ;
AApproK2(I,J)   .. dt(I,J,'K3') =l= (ti(I,'K3')-tj(J,'K3'))+GAMMA(I,J)*(1-z(I,J,'K2')) ;
ApproK3(I,J)    .. dt(I,J,'K3') =l= (ti(I,'K3')-tj(J,'K3'))+GAMMA(I,J)*(1-z(I,J,'K3')) ;
AApproK3(I,J)   .. dt(I,J,'K4') =l= (ti(I,'K4')-tj(J,'K4'))+GAMMA(I,J)*(1-z(I,J,'K3')) ;
ApproK4(I,J)    .. dt(I,J,'K4') =l= (ti(I,'K4')-tj(J,'K4'))+GAMMA(I,J)*(1-z(I,J,'K4')) ;
AApproK4(I,J)   .. dt(I,J,'K5') =l= (ti(I,'K5')-tj(J,'K5'))+GAMMA(I,J)*(1-z(I,J,'K4')) ;

Approdthu(J,K)  .. dthu(J) =l= Thuout - tj(J,'K1') ;
Approdtcu(I,K)  .. dtcu(I) =l= ti(I,'K5') - Tcuout ;

EMATdt(I,J,K)   .. dt(I,J,K) =g= EMAT ;

qcsum .. qcs =e= sum(i,qcu(i));
qhsum .. qhs =e= sum(j,qhu(j));


* ---------------Add Value to parameter -------------------
OMEGAI(I) = (TinI(I)-ToutI(I))*FcpI(I) ;
OMEGAJ(J) = (ToutJ(J)-TinJ(J))*FcpJ(J) ;
GAMMA(I,J) = max(TinI(I) - TinJ(J), ToutI(I) - TinJ(J),
                 TinI(I) - ToutJ(J), ToutJ(J) - ToutI(I)) ;
```

```
**----------------------------For Area Cost--------------------------
AreaK1(I,J)     .. A(I,J,'K1') =e= q(I,J,'K1')/U/(0.01+ (2/3*((dt(I,J,'K1')*dt(I,J,'K2'))**0.5)+1/3*((dt(I,J,'K1')+dt(I,J,'K2'))/2)) );
AreaK2(I,J)     .. A(I,J,'K2') =e= q(I,J,'K2')/U/(0.01+ (2/3*((dt(I,J,'K2')*dt(I,J,'K3'))**0.5)+1/3*((dt(I,J,'K2')+dt(I,J,'K3'))/2)) );
AreaK3(I,J)     .. A(I,J,'K3') =e= q(I,J,'K3')/U/(0.01+ (2/3*((dt(I,J,'K3')*dt(I,J,'K4'))**0.5)+1/3*((dt(I,J,'K3')+dt(I,J,'K4'))/2)) );
AreaK4(I,J)     .. A(I,J,'K4') =e= q(I,J,'K4')/U/(0.01+ (2/3*((dt(I,J,'K4')*dt(I,J,'K5'))**0.5)+1/3*((dt(I,J,'K4')+dt(I,J,'K5'))/2)) );

TotalArea       .. TA =e= sum((I,J,K),A(I,J,K)) ;
Areacost        .. Acost =e= sum((I,J,K),(AC*((A(I,J,K))**AE)))  ;

AreaCU(I)       .. Acu(I) =e= qcu(I)/Uc/(2/3*((dtcu(I)*(ToutI(I)-Tcuin))**0.5)+1/3*((dtcu(I)+(ToutI(I)-Tcuin))/2)) ;
AreaHU(J)       .. Ahu(J) =e= qhu(J)/Uh/(2/3*((dthu(J)*(Thuin-ToutJ(J)))**0.5)+1/3*((dthu(J)+(Thuin-ToutJ(J)))/2)) ;
AreaUcost       .. AUcost =e= sum((I),(AC*((Acu(I))**AE))) + sum((J),(AC*((Ahu(J))**AE))) ;

*Force(I,J)       .. z('H1','C1','K2') =e= 1 ;

**--------------------- Initialization------------------------------
  dt.l(I,J,K) = TinI(I) - TinJ(J) ;
*dt.lo(I,J,K) = EMAT ;
dt.up(I,J,K) =  Max( EMAT, abs(TinI(I) - TinJ(J)) ) ;

  ti.l(I,'K1') = TinI(I) ;                tj.l(J,'K5') = TinJ(J) ;
  dthu.l(J) = Thuout - TinJ(J) ;          dthu.lo(J) = EMAT ;
  dtcu.l(I) = TinI(I) - Tcuout ;          dtcu.lo(I) = EMAT ;
  q.up(I,J,K) = min((TinI(I)-ToutI(I))*FcpI(I),(ToutJ(J)-TinJ(J))*FcpJ(J)) ;
```

Base case

```
*------------global optimization------------------
scalar n ;
scalar globminZZ  Global minimum cost, f  to Range qhs lower bound (E=11200 to 44000 kw) ;
globminZZ = inf ;
f = 9200;

for (n = 1 to 1,

        qhs.lo = 11200;
        qhs.up = 44008;

        Display n, qhs.lo, qhs.up ;
        Solve EX7Local using minlp minimizing ZZ ;

        Display n, z.l, zcu.l, zhu.l, ZZ.l,qcs.l,qhs.l, q.l ;
        display qhu.l, qcu.l,ti.l, tj.l, A.l, Acu.l, Ahu.l  ;

        If ( ZZ.l le globminZZ,
              globminZZ = ZZ.l   ;
            );

        Display n, globminZZ ;
        f = qhs.lo ;
     );
```

Global optimization

```
*------------global optimization------------------
scalar n ;
scalar globminZZ  Global minimum cost, f  to Range qhs lower bound (E=11200 to 44000 kw) ;
globminZZ = inf ;
f = 9200;

for (n = 1 to 33,

        qhs.lo = f + 1000;
        qhs.up = qhs.lo + 999.9999;

        Display n, qhs.lo, qhs.up ;
        Solve EX7Local using minlp minimizing ZZ ;

        Display n, z.l, zcu.l, zhu.l, ZZ.l,qcs.l,qhs.l, q.l ;
        display qhu.l, qcu.l,ti.l, tj.l, A.l, TA.l, Acost.l, AUcost.l  ;

        If ( ZZ.l le globminZZ,
              globminZZ = ZZ.l   ;
            );

        Display n, globminZZ ;
        f = qhs.lo ;
     );
```

Global optimization with extension 1

```
*------------global optimization------------------
scalar n ;
scalar globminZZ  Global minimum cost, f  to Range qhs lower bound (E=17200 to 23200 kw) ;
globminZZ = inf ;
f = 17000;

for (n = 1 to 31,

        qhs.lo = f + 200;
        qhs.up = qhs.lo + 199.9999;

        Display n, qhs.lo, qhs.up ;
        Solve EX7Local using minlp minimizing ZZ ;

        Display n, z.l, zcu.l, zhu.l, ZZ.l,qcs.l,qhs.l, q.l ;
        display qhu.l, qcu.l,ti.l, tj.l, A.l, TA.l, Acost.l, AUcost.l  ;

        If ( ZZ.l le globminZZ,
             globminZZ = ZZ.l   ;
           );

        Display n, globminZZ ;
        f = qhs.lo ;
     );
```

Base case results

```
----    268 VARIABLE z.L  exchanger matching between hot I and cold J at stage K

                 K1          K2          K3          K4

H1.C1                                 1.000
H2.C3                     1.000
H3.C2                     1.000
H3.C4       1.000                                 1.000
H4.C4                                 1.000
H5.C1       1.000
H5.C2                     1.000
H6.C3       1.000         1.000


----    268 VARIABLE zcu.L  cold utility matching with hot I

H2 1.000,    H4 1.000


----    268 VARIABLE zhu.L  hot utility matching with cold J

C3 1.000,    C4 1.000


----    268 VARIABLE ZZ.L                  =  6365879.230  TAC when fixed E
            VARIABLE qcs.L                 =    13236.678  Vary sum cold utility
            VARIABLE qhs.L                 =    18842.178  Range sum Hot utility
```

```
----    268 VARIABLE q.L  heat exchanged between hot I and cold J

               K1          K2          K3          K4

H1.C1                               6252.000
H2.C3                   1412.893
H3.C2                    748.500
H3.C4     554.609                               847.891
H4.C4                               1850.429
H5.C1     748.500
H5.C2                   5251.500
H6.C3    4450.940       3049.060


----    269 VARIABLE qhu.L  heat exchanged between hot utility and cold J

C3 9087.107,    C4 9755.071


----    269 VARIABLE qcu.L  heat exchanged between cold utility and hot I

H2  2587.107,    H4 10649.571
```

Global optimization with extension 1 results

```
----    268 PARAMETER n                   =        7.000

----    268 VARIABLE z.L  exchanger matching between hot I and cold J at stage K

               K1          K2          K3          K4

H1.C1                               1.000
H1.C4                   1.000                   1.000
H2.C1       1.000
H3.C4       1.000       1.000
H4.C4                               1.000
H5.C2                               1.000
H6.C3                   1.000       1.000
H6.C4       1.000


----    268 VARIABLE zcu.L  cold utility matching with hot I

H2 1.000,    H3 1.000,    H4 1.000


----    268 VARIABLE zhu.L  hot utility matching with cold J

C3 1.000,    C4 1.000


----    268 VARIABLE ZZ.L                 =  5960899.830  TAC when fixed E
            VARIABLE qcs.L                =    12994.500  Vary sum cold utility
            VARIABLE qhs.L                =    18600.000  Range sum Hot utility
```

```
----    268 VARIABLE q.L  heat exchanged between hot I and cold J

              K1          K2          K3          K4

H1.C1                             4050.171
H1.C4                  664.508                1537.321
H2.C1     2950.329
H3.C4                 1637.341
H4.C4                             1068.830
H5.C2                             6000.000
H6.C3                             3232.369
H6.C4     4267.631


----    269 VARIABLE qhu.L  heat exchanged between hot utility and cold J

C3 14767.631,    C4  3832.369


----    269 VARIABLE qcu.L  heat exchanged between cold utility and hot I

H2  1049.671,    H3   513.659,    H4 11431.170
```

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