HEAT EXCHANGER NETWORK SYNTHESIS WITH DETAILED DESIGN: REFORMULATION AS A SHORTEST PATH PROBLEM BY TEMPERATURE DISCRETIZATION

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ABSTRACT

HEAT EXCHANGER NETWORK SYNTHESIS WITH DETAILED DESIGN:
REFORMULATION AS A SHORTEST PATH PROBLEM BY TEMPERATURE
DISCRETIZATION

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This study presents an optimization approach to heat exchanger network synthesis (HENS). HENs are widely used in industry and bring several fluid streams into their desired temperatures by using available heat in the process for efficient usage of energy. Our aim is to provide a network design coupled with a detailed equipment design for heat exchangers. The suggested approach involves discretization of temperatures based on head load equalities and reformulation as a shortest-path problem, rather than dealing with a nonlinear model and a previously structured HEN, which are common methods in the literature.

We generate a shortest path network where every node corresponds to a heat exchanger alternative and each path represents a HEN design alternative. A mixed-integer nonlinear programming model is solved to design each exchanger alternative in detail, considering all thermo-physical and transport properties of streams at their temperatures and pressures. Our approach has modeling flexibility and successfully finds the required number of heat exchangers and their connections. In addition, one can control the solution quality by deciding on the heat load steps between stream inlet and outlets. Several HEN examples from the literature are solved to assess the performance of our approach and comparable results are obtained.

Keywords: Heat exchanger network synthesis, detailed heat exchanger design, mathematical modeling

ÖZ

EKİPMANLARI AYRINTILI TASARLANMIŞ ISI DEĞİŞTİRİCİ AĞI SENTEZİ: KESİKLİ SICAKLIKLARA DAYALI EN KISA YOL PROBLEMİNİN FORMÜLASYONU

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Bu çalışmada ısı değiştirici ağı sentezi problemine bir eniyileştirme yaklaşımı sunulmuştur. Isı değiştirici ağları, endüstride yaygınlıkla kullanılan ve farklı sıcaklıklardaki akımları bir araya getirerek enerjinin verimli kullanımını sağlayan sistemlerdir. Önerilen çözüm yaklaşımı, literatürde sıkça kullanılan bir yöntem olan doğrusal olmayan matematiksel modeller ve önceden belirlenmiş ısı değiştirici ağ yapısını kullanmak yerine, ısı eşitliğine dayalı kesikli sıcaklıkları kullanan ve problemin en kısa yol problemi olarak yeniden formüle edilmesini içerir.

Oluşturulan en kısa yol ağında, düğümler ısı değiştiricileri, her yol ise bir ısı değiştirici ağını temsil eder. Isı değiştiricilerin ayrıntılı tasarımı, akışkanların fiziksel ve aktarım özellikleri, bulundukları sıcaklık ve basınç koşulları göz önüne alınarak, karışık tamsayılı doğrusal olmayan bir matematiksel modelin çözümü ile elde edilir. Önerilen çözüm yaklaşımıyla gerekli ısı değiştirici sayısı ve bağlantıları bulunur. Modelleme açısından esnek bir yaklaşım sunulmuştur. Giriş ve çıkıştaki ısı farkı belirlenerek çözümün kalitesi kontrol edilir. Çözüm yöntemini test etmek için literatürden seçilen ısı değiştirici problemleri çözülmüş ve karşılaştırmalı sonuçlar elde edilmiştir.

Anahtar Kelimeler: Isı değiştirici ağı sentezi, ayrıntılı ekipman tasarımı, matematiksel modelleme

To my beloved family

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TABLE OF CONTENTS

ABSTRACT iv

ÖZ vi

ACKNOWLEDGEMENTS ix

TABLE OF CONTENTS xi

LIST OF TABLES xiii

LIST OF FIGURES xvi

CHAPTERS

1 INTRODUCTION 1

2 LITERATURE REVIEW 5

2.1 Detailed Heat Exchanger Design 5

2.2 Heat Exchanger Network Synthesis 11

2.2.1 Pinch Analysis Based Methods 15

2.2.2 Superstructure Based Methods 16

2.2.3 Elusive Methods 18

2.3 Heat Exchanger Network Synthesis with Detailed Equipment Design 19

2.4 Remarks 21

3 PROBLEM FORMULATION 22

3.1 Heat Exchanger Design 22

3.1.1 Heat Transfer Mechanisms 22

3.1.2 Shell-and-Tube Heat Exchanger Design Model 23

3.2 Heat Exchanger Network Synthesis 37

3.2.1 Problem Formulation 38

3.2.2 Mathematical Formulation 39

4 SOLUTION APPROACH 50
4.1 Solution Approach 50
4.2 Results and Discussion 67
4.2.1 Test instances from Yee and Grossmann (1990) 70
4.2.2 Test instances from Mizutani et al. (2003b) 74
4.2.3 Test instances from Ponce-Ortega et al. (2007) 74
4.2.4 Test instances from Turton et al. (2007) 78
4.2.5 Test instances from Gupta and Ghosh (2010) 78
4.2.6 Test instances from Ponce-Ortega et al. (2010) 78
4.2.7 Test instances from Huang and Chang (2012) 83
4.2.8 Second Best Solutions 83
4.3 Remarks 88
5 CONCLUSION 90
REFERENCES 92
APPENDICES
A TERMINOLOGY 98
B PINCH ANALYSIS METHOD 99
C SOLUTION OF DME EXAMPLE 102
D TEST PROBLEMS 106
E DESCRIPTION OF SOME TECHNICAL TERMS 153

LIST OF TABLES

TABLES

Table 4.1 Data of Example 52

Table 4.2 Q-discretization example - Example-1 of Yee and Grossmann (1990) 57

Table 4.3 The discretized inputs of the model for the illustrative example 58

Table 4.4 The number of test instances presented in some recent studies 67

Table 4.5 Test instances 68

Table 4.6 Results of instance YG-E1 from Yee and Grossmann (1990) 71

Table 4.7 Results of instance YG-E2 from Yee and Grossmann (1990) 72

Table 4.8 Results of instance YG-E3 from Yee and Grossmann (1990) 73

Table 4.9 Results of instance MG-E1 from Mizutani et al. (2003b) 75

Table 4.10 Results of instance MG-E2 from Mizutani et al. (2003b) 76

Table 4.11 Results of instance 4S1 from Ponce-Ortega et al. (2007) 77

Table 4.12 Results of instance Chapter 13-E2 from Turton et al. (2007) 79

Table 4.13 Results of instance 5SP from Gupta and Ghosh (2010) 80

Table 4.14 Results of instance PO-E2 from Ponce-Ortega et al. (2010) 81

Table 4.15 Results of instance PO-E3 from Ponce-Ortega et al. (2010) 82

Table 4.16 Results of instance HC-E1 from Huang and Chang (2012) 84

Table 4.17 Results of instance HC-E2 from Huang and Chang (2012) 85

Table 4.18 Results of instance HC-E3 from Huang and Chang (2012) 86

Table 4.19 Second best solutions for instance YG-E1 from Yee and Grossmann (1990) 87

Table 4.20 Second best solutions for instance MG-E2 from Mizutani et al. (2003b) . . 87

Table 4.21 Second best solutions for instance HC-E2 from Huang and Chang (2012) . . 88

Table 4.22 Problem sizes for instances 89

Table D.1 Process data for instance YG-E1 106

Table D.2 Process data for instance YG-E2 106

Table D.3 Process data for instance YG-E3 107

Table D.4 Process data for instance MG-E1 107

Table D.5 Process data for instance MG-E2 108

Table D.6 Process data for instance PO-E2 108

Table D.7 Process data for instance PO-E3 109

Table D.8 Process data for instance 5SP 109

Table D.9 Process data for instance HC-E1 110

Table D.10 Process data for instance HC-E2 110

Table D.11 Process data for instance HC-E3 110

Table D.12 Process data for instance 4S1 111

Table D.13 Process data for instance CH13-E2 112

Table D.14 Problem setups for instance YG-E1 from Yee and Grossmann (1990) 113

Table D.15 Problem setups for instance YG-E2 from Yee and Grossmann (1990) 114

Table D.16 Problem setups for instance YG-E3 from Yee and Grossmann (1990) 115

Table D.17 Problem setup for instance MG-E1 from Mizutani et al. (2003b) 116

Table D.18 Problem setup for instance MG-E2 from Mizutani et al. (2003b) 117

Table D.19 Problem setups for instance PO-E2 from Ponce-Ortega et al. (2010) 118

Table D.20 Problem setups for instance PO-E3 from Ponce-Ortega et al. (2010) 119

Table D.21 Problem setup for instance HC-E1 from Huang and Chang (2012) 120

Table D.22 Problem setups for instance HC-E2 from Huang and Chang (2012) 121

Table D.23 Problem setups for instance HC-E3 from Huang and Chang (2012) 122

Table D.24 Problem setup for instance 4S1 from Ponce-Ortega et al. (2007) 123

Table D.25 Problem setup for instance CH13-E2 from Turton et al. (2007) 124

Table D.26 Problem setups for instance 5SP from Gupta and Ghosh (2010) 125

Table D.27 Result of Experiment 1 of Instance YG-E1 from Yee and Grossmann (1990) 126

Table D.28 Result of Experiment 2 of Instance YG-E1 from Yee and Grossmann (1990) 127

Table D.29 Result of Experiment 1 of Instance YG-E2 from Yee and Grossmann (1990) 127

Table D.30 Result of Experiment 2 of Instance YG-E2 from Yee and Grossmann (1990) 128

Table D.31 Result of Experiment 3 of Instance PO-E2 from Ponce-Ortega et al. (2010) . 128

Table D.32 Result of Experiment 1 of Instance YG-E3 from Yee and Grossmann (1990) 129

Table D.33 Result of Experiment 2 of Instance YG-E3 from Yee and Grossmann (1990) 130

Table D.34 Result of Experiment 1 of Instance MG-E1 from Mizutani et al. (2003b) . . 131

Table D.35 Detailed Design Parameters for Experiment 1 of 4S1 131

Table D.36 Result of Experiment 1 of Instance MG-E2 from Mizutani et al. (2003b) . . 132

Table D.37 Result of Experiment 1 of Instance PO-E2 from Ponce-Ortega et al. (2010) . 133

Table D.38 Result of Experiment 2 of Instance PO-E2 from Ponce-Ortega et al. (2010) . 133

Table D.39 Result of Experiment 1 of Instance PO-E3 from Ponce-Ortega et al. (2010) . 134

Table D.40 Result of Experiment 2 of Instance PO-E3 from Ponce-Ortega et al. (2010) . 135

Table D.41 Result of Experiment 1 of Instance HC-E1 from Huang and Chang (2012) . 136

Table D.42 Result of Experiment 1 of Instance HC-E2 from Huang and Chang (2012) . 136

Table D.43 Result of Experiment 2 of Instance HC-E2 from Huang and Chang (2012) . 137

Table D.44 Result of Experiment 1 of Instance HC-E3 from Huang and Chang (2012) . 137

Table D.45 Result of Experiment 2 of Instance HC-E3 from Huang and Chang (2012) . 138

Table D.46 Result of Experiment 1 of Instance 4S1 from Ponce-Ortega et al. (2007) . . 138

Table D.47 Result of Experiment 1 of Instance CH13-E2 from Turton et al. (2007) . . . 139

Table D.48 Result of Experiment 1 of Instance 5SP from Gupta and Ghosh (2010) . . . 140

Table D.49 Result of Experiment 2 of Instance 5SP from Gupta and Ghosh (2010) . . . 140

Table D.50 Detailed Design Parameters for Experiment 1 of MG-E2 141

Table D.51 Detailed Design Parameters for Experiment 1 of MG-E1 141

LIST OF FIGURES

FIGURES

Figure 2.1 Some examples of heat exchangers (Shah and Sekulic 2003) 6

Figure 2.2 Heads and shell types of TEMA (Perry and Green 1997) 8

Figure 2.3 Shell and tube passes, tube layouts, and baffles in a heat exchanger (a. Perry and Green 1997, b. Mukherjee 1998) 9

Figure 2.4 Arrangement of battery heat exchangers (Broeck 1944) 12

Figure 2.5 Two stage HEN superstructure for two hot and two cold streams (Yee et al. 1990) 17

Figure 3.1 Examples of heat transfer mechanisms (CReSIS in the Field 2010) 24

Figure 3.2 Temperature profile in a counter-current heat exchanger 30

Figure 3.3 An example network for the HENS problem 39

Figure 3.4 Representation of a node 45

Figure 3.5 Costs on arcs 48

Figure 4.1 Main Steps of the HEN Synthesis Algorithm 51

Figure 4.2 Scaling of the illustrative example 56

Figure 4.3 Network of the illustrative example 66

Figure D.1 The resulting HEN of Experiment 1 of instance YG-E1 142

Figure D.2 The resulting HEN of Experiment 2 of instance YG-E1 142

Figure D.3 The resulting HEN of Experiment 1 of instance YG-E2 143

Figure D.4 The resulting HEN of Experiment 2 of instance YG-E2 143

Figure D.5 The resulting HEN of Experiment 1 of instance YG-E3 144

Figure D.6 The resulting HEN of Experiment 2 of instance YG-E3 145

Figure D.7 The resulting HEN of Experiment 1 of instance MG-E1 146

Figure D.8 The resulting HEN of Experiment 1 of instance MG-E2 146

Figure D.9 The resulting HEN of Experiment 2 of instance PO-E2 147

Figure D.10 The resulting HEN of Experiment 3 of instance PO-E2 147

Figure D.11 The resulting HEN of Experiment 1 of instance PO-E3 148

Figure D.12 The resulting HEN of Experiment 2 of instance PO-E3 148

Figure D.13 The resulting HEN of Experiment 1 of instance HC-E1 149

Figure D.14 The resulting HEN of Experiment 1 of instance HC-E2 149

Figure D.15 The resulting HEN of Experiment 2 of instance HC-E2 150

Figure D.16 The resulting HEN of Experiment 1 of instance HC-E3 150

Figure D.17 The resulting HEN of Experiment 2 of instance HC-E3 150

Figure D.18 The resulting HEN of Experiment 1 of instance 4S1 151

Figure D.19 The resulting HEN of Experiment 1 of instance CH13-E2 151

Figure D.20 The resulting HEN of Experiment 1 of instance 5SP 152

Figure D.21 The resulting HEN of Experiment 2 of instance 5SP 152

CHAPTER 1

INTRODUCTION

A heat exchanger (HE) is an equipment which is used to facilitate heat transfer efficiently between hot and cold mediums. HEs are widely used in process industries like power plants, chemical and petrochemical plants, and petroleum refineries plus in refrigeration, air conditioning and space heating. In industry, heat exchangers are needed at various stages of a production process to ensure that streams are at the desired temperatures for a chemical or physical transition. For example, in a phthalic anhydride production process, the raw materials, *o*-xylene and air, should be heated to 150°C from ambient temperature before they enter to the reactor, so that the reaction can take place. Since *o*-xylene oxidation is an exothermic (energy/heat producing) reaction, the outflow product stream at 385°C from the reactor, should be cooled to 130°C for further steps for purification operations. Another example is, in a dimethyl ether production process, the waste water formed at the end of the process should be cooled from 167°C to 50°C before sent to the waste water treatment. As it is seen from the examples, heat exchangers are binding fundamental equipment for industrial processes.

Heat addition or removal demands in a process are mostly met by using superheated steam and cooling water. These are called *utility streams*. Generally, industrial facilities are located close to a natural water resource like a lake, river or sea and the utilities are provided to the system from the nature. Superheated steam is produced heating source water with a fuel, where cooling water is produced by refrigerating source water, or source water is directly used for cooling. After they are used within the system for cooling/heating, they are disposed to the nature (into the water resource) and this causes a temperature increase in the water resource which affects ecosystems. Producing utility streams has negative impacts on environment and results in economical and environmental costs.

When operations in a process are considered separately, these utility streams become a necessity and one may try to improve the performance as considering just one equipment at a time. But, when the entire process is examined, it can be realized that there are potential beneficial interactions between different units and equipment. Let us reconsider *o*-xylene oxidation example. There is a need of energy before the reaction starts. After the reaction, excess energy should be taken out from the system. However, instead of using heat exchangers with hot and cold utilities, these two streams can be processed together in a heat exchanger where the cold stream can obtain necessary energy from the hot stream. The same is also applicable for the waste water in dimethyl ether process. It can be processed with a cold stream within the process. By this way, overall energy, utility consumption, and relevant costs are minimized. Such an approach where the output of a stream from an HE becomes the input to the other HE is called *heat integration*.

Succeeding heat integration in a process is not a straightforward issue. Heat should be balanced in the overall process. When overall generated and emitted heat in the unit operations is considered, the heat balance is generally not obtained due to the properties of chemical and physical transitions throughout the process. That is why utility streams are being used to ensure the system-wide heat balance. In heat integration, heat exchangers with utility streams are undesirable, but sometimes unavoidable for operating in steady-state.

When heat integration point of view is applied to a whole process, the following questions should be answered:

- What are the heat loads of streams?
- Which streams should be processed in an HE?
- How many HEs should be needed?
- Is there a need of hot or cold utility stream?
- If needed, how many HEs for utilities should be installed?

Answers of these questions result in a *heat exchanger network (HEN)* synthesis. HEN is an overall system that combines the heat release and neediness points in a process for efficient utilization of energy. At the same time, HENs are minimizing the usage of utility streams, hence the environmental damages.

Before proceeding further, a distinction should be made about HEN related terminologies used in operations research/industrial engineering and chemical engineering. The problem of coming up with an integrated heat exchanger network is called HEN *synthesis* in chemical engineering literature because synthesis means creating and structuring of component into a whole usually for a new system (non-existing system) in systems engineering. After the creation, a system is designed and thus the choices and an arrangement for specific functions are made. When we consider the problem from the industrial engineering point of view, the problem can be called HEN *design*. Because, in this view, design actually includes synthesis, and design should be made using analysis and synthesis together. Nevertheless, we use the title of "heat exchanger network synthesis (HENS)" as the problem title to be consistent with the large (mainly chemical engineering) literature. Further explanation about these terminological differences and its possible roots can be found in Appendix A.

The simple problem definition of the HENS as given in Furman and Sahinidis (2002) is:

"Given

- *a set of hot process streams to be cooled from the system inlet temperatures to the target temperatures,*
- *a set of cold process streams to be heated from the system inlet temperatures to the target temperatures,*
- *heat capacities and flow rates of the hot and cold process streams,*
- *the utilities available and the temperatures or temperature ranges and the costs for these utilities, and*
- *heat exchanger cost data,*

develop a network of heat exchangers with minimum annual investment and operating costs."

Although the definition is simple, the HENS is a complicated and challenging problem because of many decisions to be made and integrated that cause increase in complexity. Besides, detailed equipment design for each HE in the network can also be considered. This also brings more complexity to the problem. The studies in the literature which consider the HENS without detailed design use an overall heat transfer coefficient for calculation of heat exchanger areas, whereas it is calculated by considering the heat exchanger geometry and stream physical and thermal properties in detailed design. Therefore, the solutions with detailed heat exchanger design are more realistic.

There are numerous studies in the literature for solving the HENS. Mainly two approaches are widely be used. Chapter 2 gives an insight about these approaches and recent studies.

In this study, we propose a new solution method. We formulate the HENS as a shortest path problem, while designing every HE in the network. The formulation is explained in Chapter 3 and the solution methodology is given in Chapter 4.

The results are presented, compared to their competitors in the literature, and discussed also in Chapter 4. The strength of our method is that it succeeds in more realistic solutions in terms of easiness regarding implementation of these solutions into practice, and the method is highly flexible for constructing an HEN. A general insight about the performance of our formulation and future work directions are given in Chapter 5.

CHAPTER 2

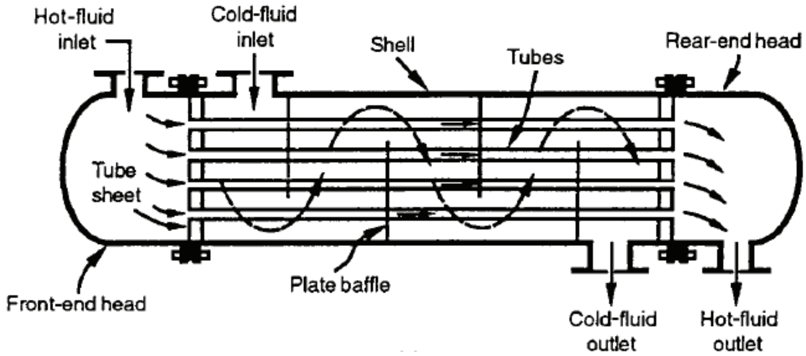
LITERATURE REVIEW

This thesis deals with the heat exchanger network synthesis (HENS) with detailed equipment design. Therefore we restrict ourselves to the literature on the problems for detailed heat exchanger design and HENS. Basically there are two literature surveys available about the HENS problem: Furman and Sahinidis (2002) and Morar and Agachi (2010), covering the studies published until 2008. Our purpose in this section is to summarize the literature until 2008 from these two surveys and to discuss the studies published since 2009 in detail. The following sections include brief definitions of the problems and solution methodologies in the literature. We also give brief information about heat exchangers (HEs), their types and usage. After that, we mention the shell and tube exchangers, their design aspects, and development. Some of the studies in detailed shell and tube HE design literature are summarized.

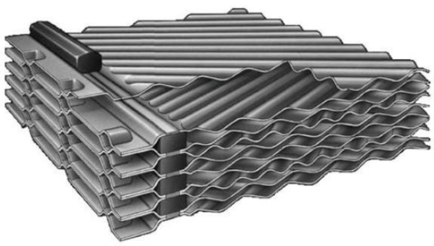
2.1 Detailed Heat Exchanger Design

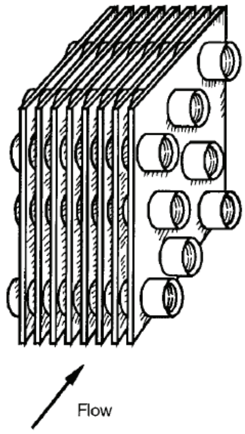
Heat exchangers (HEs) are essential for the process industries. They are used to transfer heat between two fluids. Most commonly, hot and cold fluids are not directly contacted with each other and separated by a tube wall or a flat surface, so that the energy transfer can occur through it. There are many different types of heat exchangers. Based on their construction technology, there are mainly four types of heat exchangers: Tubular, plate-type, extended surface, and regenerative (Shah and Sekulic 2003). In Figure 2.1, some of the examples of these types are shown. For more detailed aspects of classification and types of HEs, we refer the reader to Shah and Sekulic (2003).

Most widely-used type is shell-and-tube heat exchangers due to their superior features of

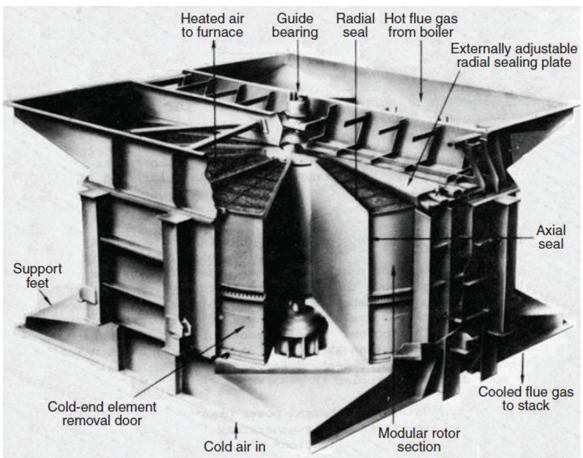


(a) Shell-and-tube HE (Tubular type)





(b) Welded plate HE (Plate type) ***(c) Tube-fin HE (Extended surface type)***



(d) Rotary regenerator

Figure 2.1: Some examples of heat exchangers (Shah and Sekulic 2003)

resistance in manufacturing environments, facilitating effective heat transfer and flexibility in design. This type of heat exchangers consists of a shell that covers a bundle of tubes. A fluid flows inside the tubes, while the other fluid flows over the tubes in the shell. By this way, the different streams transfer heat to each other.

Shell-and-tube heat exchangers were introduced in early 1900s in order to satisfy extended heat exchange needs in power plants. The mechanical design and manufacturing technology of these exchangers were developed in 1920s and 1930s. In 1930s, the water-water and water-steam shell and tube heat exchangers were designed as good as today, because of their superior fouling (accumulation of unwanted biological and material dirt) resistant feature. In 1941, TEMA (Tubular Exchanger Manufacturers Association) provided standards for mechanical design for safety, and quality control, and they are still being used. The increasing demand on shell and tube exchangers resulted great increase in the research activities in 1940s and 1950s. Although it appears that all the developments in thermohydraulic as well as mechanical design of HEs used in practice are originated from U.S. resources, they are influenced heavily from the German research (Taborek 1983).

The correlations for the design of shell and tube HEs are reviewed in Emerson (1963). Most of the techniques reviewed in Emerson (1963) are still being used today for simpler designs. These standards for the design of shell-and-tube heat exchangers are given according to their types, shell dimensions, and number of tubes. Figure 2.2 shows head types and shell types of shell and tube heat exchangers by TEMA. Appropriate designs are selected among these. Also, ASME (American Society of Chemical Engineers) has standards for tubes inside the HEs. These standards have been specified in a wide range to cover various sizes of HEs and they are more economical than those with special design.

Design of heat exchangers is based on basic heat transfer mechanisms and the laws of thermodynamics. The mathematical representation of these mechanisms depends on some empirical equations. Detailed design aims to determine shell and tube diameters, the number of tubes, tube layout, the number of shell and tube passes, baffle spacing, baffle cuts. These features are shown in Figure 2.3. Baffles are parts of HE and they are placed in the shell side. They maintain the stream to be mixed during its flow on the tubes for an efficient heat transfer. The objective is to minimize the total heat exchange area where the total capital cost of an HE consists of installation and operation (e.g., maintenance, pumping) costs. Due to fluid friction,

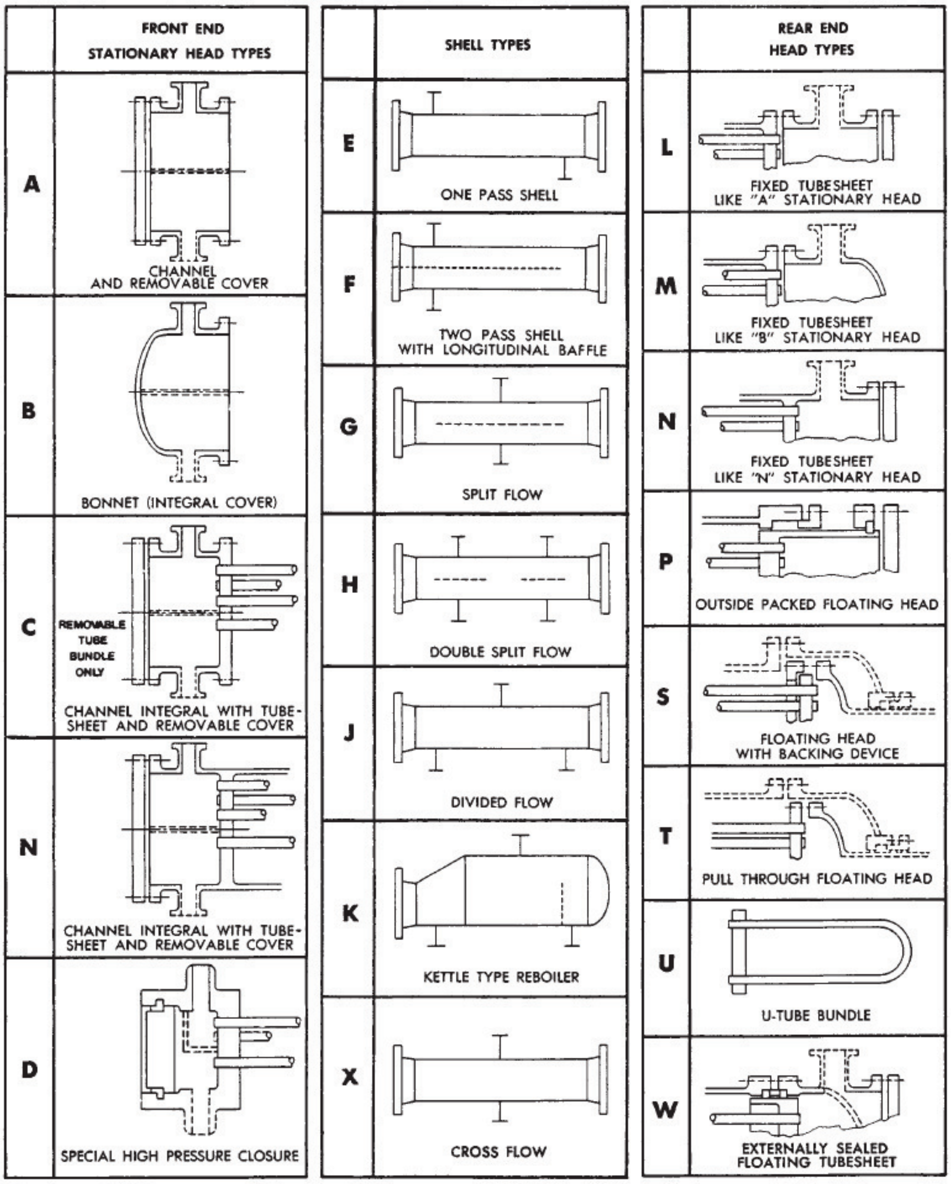


Figure 2.2: Heads and shell types of TEMA (Perry and Green 1997)

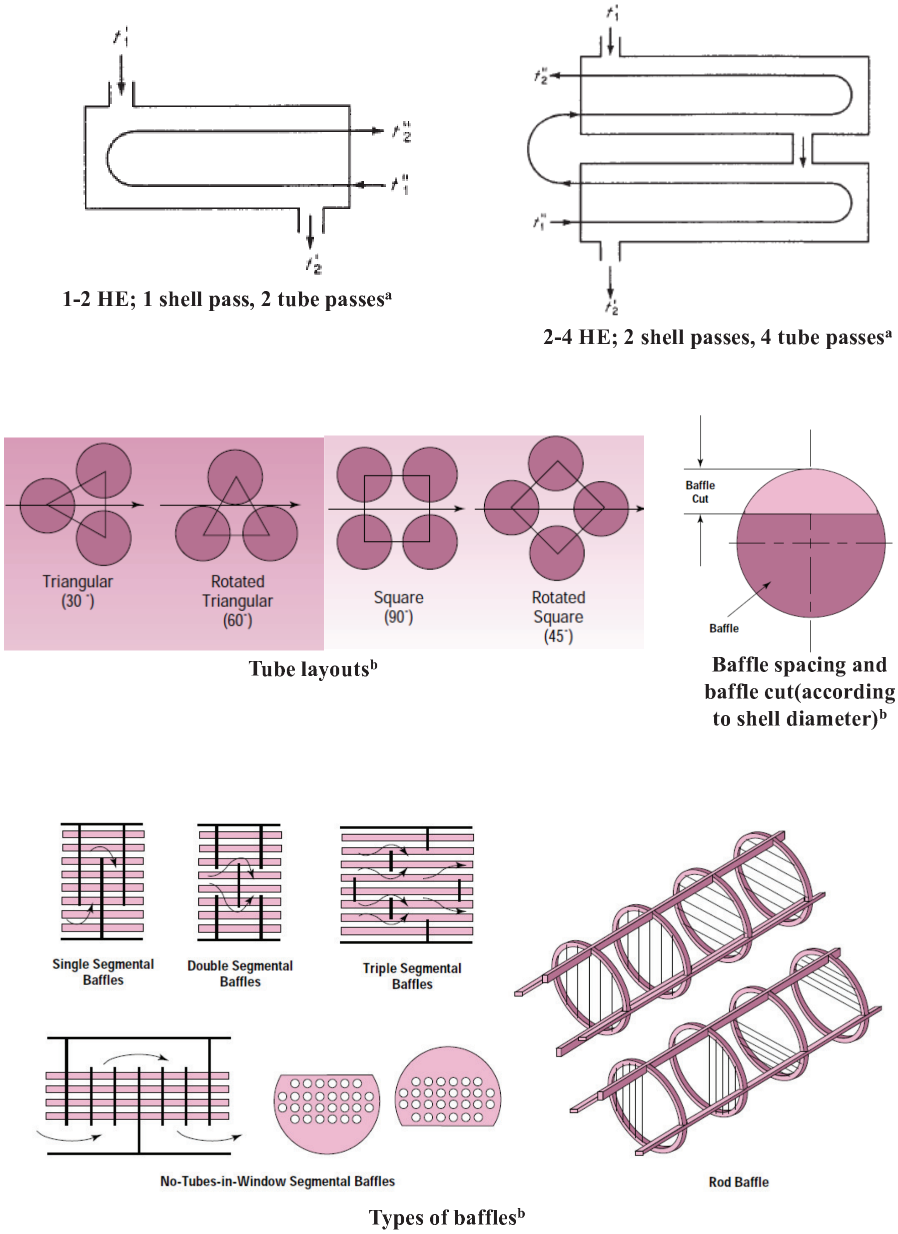


Figure 2.3: Shell and tube passes, tube layouts, and baffles in a heat exchanger (a. Perry and Green 1997, b. Mukherjee 1998)

pressure drop occurs in a HE. Mechanical characteristics (tube bendings, baffles, etc.) and flow regime are important factors for pressure drop. In order to maintain a steady pressure in the equipment, the fluids are needed to be pumped. The required pumping power and its operating cost are directly proportional to the amount of pressure drop in a HE. Fouling is another factor for design and operation of HEs. Fouling means an accumulation of undesirable materials, like crystals, corrosion products, and biological growth, on the heat exchange surface of a HE. It may lead to pressure increase, inefficient heat transfer, and even failure of the equipment. In most of the studies, pressure drop and fouling factors are considered in the model as constraints.

TEMA has developed its own software for the detailed design of shell and tube HEs. Also, there are some other commercially developed simulation based software for design of processes that includes HE design, such as CHEMCAD and Aspen.

Although there are some more detailed formulations for the same purpose in the literature; among all, Bell Delaware method is the most accurate but most complex method for designing shell and tube HEs. In this method, effects of mechanical design, mostly baffles, on the flow are extensively included into the calculations. Here, some of the recent works will be presented. Serna and Jimenez (2004) suggest a step-wise algorithm and use the Bell Delaware method for the design of HE. Later, Serna and Jimenez (2005) suggest an analytical expression that relates the pressure drop, exchanger area, and shell-side film transfer coefficient. The equation is based on the Bell Delaware method. They use a similar iterative stage-wise algorithm in order to find a minimum cost solution. Their results show that detailed calculations are better for representing the real situations, therefore these formulations can also be used along with the heat exchanger network synthesis.

Babu and Munawar (2007) apply genetic algorithm and differential evolution method for the solution of the HE design problem. Compared to traditional design methods like Serna and Jimenez (2005) both perform well. The differential evolution is faster and its likeliness of finding global optimum in wide range of parameters is better compared to the genetic algorithm. Selbas et al. (2006) also use genetic algorithm and their solutions are comparable to the traditional methods. Besides, multiple solutions with the same quality can be found and this gives flexibility to the decision maker. The objective of all studies is to minimize the heat exchange area. Ravagnani et al. (2009) use particle swarm optimization for the detailed design of shell and tube HEs. They use two different objectives; minimization of heat exchange area and minimization of total costs of area and pumping operations. The results show that particle swarm optimization performs well in the detailed design problem of shell and tube HEs.

Our study uses a simpler HE design model, which is less detailed compared to these studies. However, for a more realistic approach, all the physical and transport properties of the streams are determined at their specified temperatures contrary to using average values for these properties as were used above mentioned studies.

2.2 Heat Exchanger Network Synthesis

Heat integration within processes has become an important issue due to continuous increase of energy costs and environmental considerations for the past fifty years. Therefore, the heat exchanger network synthesis(HENS) problem takes a significant place in the process optimization literature.

The HENS problem is first introduced by Broeck (1944). Broeck (1944)'s problem definition is:

"The aim is to determine the minimum cost heat exchanger sizes in system, which is called battery, that a main stream, W, interacts with set of side streams, w_1, w_2, w_3, in heat exchangers, $1, 2, 3$, and there are coolers, a, b, c, for each side stream. The inlet and target temperatures of streams are given. The representation of the battery HE system is given in Figure 2.4. Here, T's represent the temperature of main stream, t's are temperatures of side streams, and t_i, t_w are inlet and outlet temperatures of water in the coolers, respectively."

The major development in the area started after Linnhoff and Flower (1978) redefined the problem as given below (Linnhoff and Flower 1978, Papoulias and Grossmann 1983):

"A set of z streams, of known mass flow rates and constant specific heat capacities, are to be brought from given supply temperatures T_S to given target temperatures T_T. For $T_S > T_T$, the stream is called hot stream and for $T_T > T_S$, it is called cold stream. Apart from heat exchange between the streams, cooling with a cooling water and heating with steam are considered for the streams that are not reached their target temperatures. The objective is to

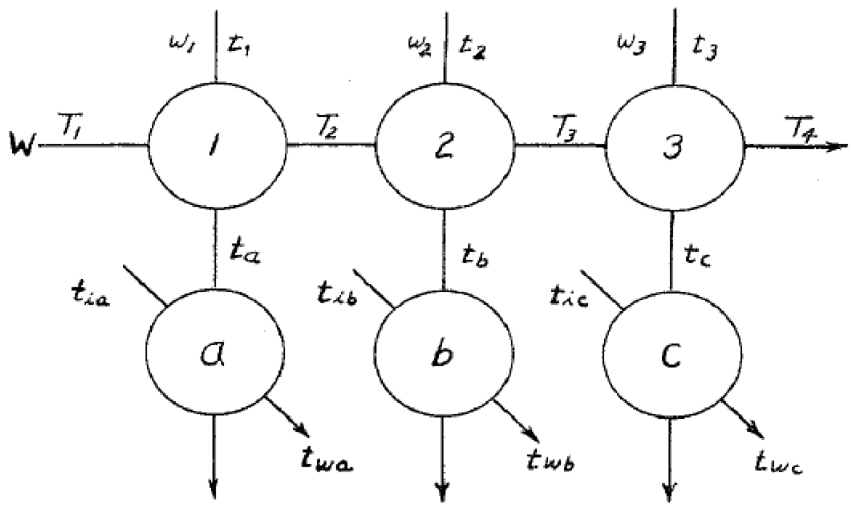


Figure 2.4: Arrangement of battery heat exchangers (Broeck 1944)

develop a network of heat exchangers that satisfies the specifications at minimum investment and operating cost, which are in annualized form."

This definition is still used for the HENS problem. The main difference between these two definitions is that the structured form of the Broeck (1944)'s definition. The problem is extended in the Linnhoff and Flower (1978)'s definition. In this definition, heaters are used as well as coolers and every stream can match with each other in a HE. It is seen that the current definition increases the complexity and the difficulty of the problem.

Linnhoff and Hindmarsh (1983) suggest a new mathematical method, called pinch analysis. Highest energy recovery with a given number or capital units is targetted in this method. There are a few significant studies that appeared in the literature during that four decades between studies of Broeck (1944) and Linnhoff and Flower (1978). Interested reader is referred to Furman and Sahinidis (2002) for a detailed reading about the subject.

Cerda et al. (1983) and Cerda and Westerburg (1983) suggest a transportation model, and Papoulias and Grossmann (1983) extended this formulation to the transshipment model. The transportation model by Cerda et al. (1983) minimizes the utility usage by penalizing it in the objective function. For every stream in the system, temperature versus enthalpy flow diagram is drawn and by merging them, the minimum hot and cold utility needs of the overall system are found. Also by determining some points on the graph, depending on an inequality for generated/absorbed heat, the alternative temperature differences are generated. The heat loads for utilities and process HEs (stream pairs) are continuous variables and if these are greater than zero, it means that the heat exchanger is included in the constructed HEN. Cerda and Westerburg (1983) use the same formulation, but the utilities are restricted and the objective is to minimize the number of stream/stream matches, i.e., the number of HEs in the network. The same approach for partitioning temperature intervals is valid in the transshipment model in Papoulias and Grossmann (1983). In the model, heat is regarded as the commodity that is shipped from hot streams to cold streams subject to thermodynamical constraints. Depending on the objectives, a number of formulations are presented in Papoulias and Grossmann (1983). The objectives are minimum utility cost with and without stream matching restrictions, minimum number of heat exchangers (stream matches) and also a combination of these. The advantage of these approaches is that they reduce the complexity of the problem. However, individual HEs are not considered in these formulations. The heat exchange area is also an important performance measure for the HENS problem. These formulations are superior compared to pinch analysis method, but the formulations that consider heat exchange areas as well as utility and number of HEs perform better than them. The *superstructure* proposed by Yee and Grossmann (1990) and their formulation of the problem as mixed integer nonlinear program (MINLP) dominates the HEN literature together with the *pinch analysis method* of Linnhoff and Hindmarsh (1983).

There are two extended reviews for the HENS problem by Furman and Sahinidis (2002) and Morar and Agachi (2010). Furman and Sahinidis (2002) cover over 450 studies about the HENS problem from 1994 to 2001 and present the milestones about development of the field. Classifications are made according to the HENS problem solution methods and the topics of the HENS problem. It is a detailed survey where the features of every work that is referred are explained separately. Morar and Agachi (2010) provide a selective and more condensed review. They give a selection of studies about the heat integration and heat exchanger network synthesis. An evaluation in the development of heat integration is investigated through years 1975 to 2008. The relationships between authors, journals, and domains are presented. According to this analysis, Linnhoff and co-workers are dominating the literature with pinch analysis technique. Yee and Grossmann (1990)'s mathematical model formulation with superstructure follows the pinch analysis. The most cited journals about heat integration are

Computers and Chemical Engineering, Industrial & Engineering Chemistry Research, Chemical Engineering Research and Design, AIChE Journal, Chemical Engineering Science, and Applied Thermal Engineering. In this section, further development of the problem will be summarized to give an insight and recent works will be discussed.

Mainly there are two aspects of the HENS problem in the literature. These are the HEN synthesis from scratch and the retrofit analysis. Definition of retrofit is to improve an existing structure, thus the HEN retrofit corresponds to the analysis and redesign of a given HEN to improve its effectiveness. In retrofit of HEN, some limitations are introduced to the problem. Usage of existing HEs, considering topological constraints are important constraints for the problem and since the solution space is tightened, the complexity of the problem is reduced compared to the HENS from scratch. Smith et al. (2010), Feng et al. (2011) and Pan et al. (2012) are based on the retrofit analysis. Since we are interested in the HEN design from scratch, we will provide a brief review about these related studies. Smith et al. (2010) modified the pinch analysis method to retrofit design. The modified method includes stream splitting and mixing and unit operations while considering temperature dependencies of thermal properties. The usage of existing heat exchangers and number of modifications are constrainted and the cost is incurred whenever a larger heat exchanger is needed. Feng et al. (2011) applied a step-wise algorithm with pinch analysis for heat integration retrofit analysis. Two examples from petrochemical complexes are solved. The results show that a significant amount of utility saving can be achieved without changing the existing HEN structure. Pan et al. (2012) suggest a MINLP model with two iteration loops. Their objective is to increase the energy recovery without changing network topology. The difficulty of solving NLP model is resolved with this formulation.

Furman and Sahinidis (2002) and Morar and Agachi (2010) suggest that there are two major classes in the HENS literature, sequential synthesis and mathematical modeling in addition to a group of studies that cannot be included into these two classes and be described a single group in terms of commonalities. Sequential synthesis methods mainly consist of variations of pinch analysis technique and some evolutionary methods in solving the problem. Based on the formulation of the problems, we classify the study done in literature in three groups which are *pinch analysis based methods*, *superstructure based methods*, and *elusive methods*.

2.2.1 Pinch Analysis Based Methods

The pinch analysis method is introduced by Linnhoff and Hindmarsh (1983). It is a graphical procedure. Firstly, energy targets are identified by using composite curves and then by establishing the minimum temperature difference, the pinch point is identified for the design. The heat exchangers are specified around the pinch point to minimize the need of hot and cold utilities. An explanation of the procedure is given in Appendix B. It is effective and easy to apply, even if there are some disadvantages like overestimation of the number of heat exchangers. It is still in use with various extensions and some of the recent ones are discussed below.

The dynamic behavior of the physical properties with changing temperature is usually disregarded in the HENS literature. This negligence sometimes leads unrealistic solutions, especially if there is a phase change in the process. Castier and Queiroz (2002) take this into account and use the nonlinear behavior of heat capacities in the formulation of the problem. They also adapt phase change to pinch analysis method in their study. In our study, all the physical properties are considered to change with temperature and phase change.

With a similar approach of pinch analysis, a graphical method is suggested by Wan Alwi and Manan (2010) for the HENS. In this approach, instead of using two different diagrams, composite curves and grid diagrams, separately, a composite stream temperature vs. enthalpy plot is proposed for the solution of the problem. The advantage of this study is that the solutions obtained are more realistic for targeting multiple utilities and minimum heat exchange area. Also, pinch points, energy targets, and maximum heat allocation are seen in a single graph by this method.

Pinch analysis method requires many calculations and it is hard to solve bigger problems. Since it is based on a heuristic approach, the solutions generally have large optimality gaps. With this method, the configuration of HEN is defined, and if overall heat transfer coefficients are provided, heat exchanger areas can also be found. However, the detailed designs of HEs are not considered and the heat exchange areas found by using the assumed overall heat transfer coefficients cause the model to be not realistic.

2.2.2 Superstructure Based Methods

The superstructure proposed by Yee et al. (1990) is generated by fixing the number of stages with the maximum number of hot or cold streams. At each stage all the streams are split into the number of streams which they will be processed. Each hot stream is matched with each cold stream in every stage and, by this way, the heat exchangers are formed. At the end of every stage, the outlet streams from every exchanger are mixed for each stream and they are headed to the other stage at that temperature. It is assumed that outlet temperatures of a stream from the HEs in a stage are the same. Here, the temperatures between stages are taken as variables. Even though the stream splitting is defined in the superstructure, it can be restricted by the constraints and, similarly, some restrictions on hot and cold stream matches can be input to the problem. A representation of superstructure for a process which has two hot and two cold streams is shown in Figure 2.5. In the figure, W's correspond to cooling water (cold utility) and S's correspond to superheated steam (hot utility). The temperatures at the end of each stage is shown with $t_{i,k}$. Each stage, every hot stream is split into two and processed with both cold streams. The inverse is also true for every cold stream. The number of stages is fixed at the beginning and the outlet temperatures of every HE should be equal to each other at each stage. Numerous works use the superstructure as it is or with some modifications. Also, there are some attempts to use different restrictions on the formulation and somehow create a structure for HEN.

Lotfi and Boozarjomehry (2010) aim to minimize the total annual cost by using the superstructure approach. They develop a genetic algorithm to find an initial HEN design and then a simulator calculates heat loads and temperatures. The model evolves until the output of simulation is close to the target temperature. Toffolo (2009)'s hybrid optimization method consists of two levels where the topology of HEN is also considered. An evolutionary algorithm and sequential quadratic programming are used for minimizing the total annual cost while using the superstructure formulation.

Similar to our study, Ponce-Ortega et al. (2008b) consider multipass (multiple shell and tube passes) HEs within the HEN structure. They use a genetic algorithm to solve the extended version of the problem whose mathematical model is from Yee and Grossmann (1990). Ponce-Ortega et al. (2008a) revise the superstructure model of Yee and Grossmann (1990) by taking phase changes and stream splitting into consideration and minimizing the total annual cost.

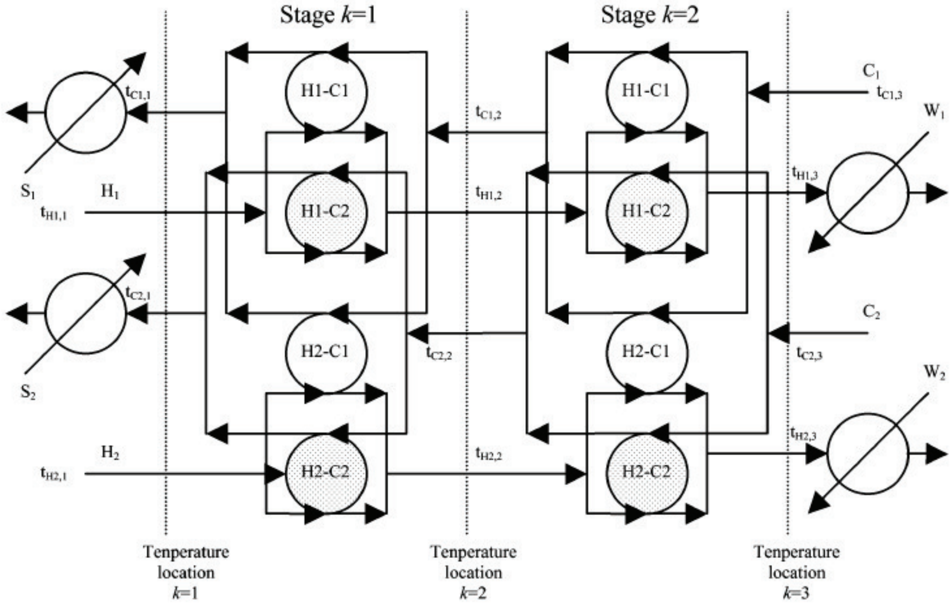


Figure 2.5: Two stage HEN superstructure for two hot and two cold streams (Yee et al. 1990)

Ponce-Ortega et al. (2010) give multiple utility options, instead of one hot and one cold utility, to the model so that the costs can be reduced by selecting the most appropriate one. They formulate the problem by using the superstructure and as an MINLP model. Huang and Chang (2012) improve the performance of the mathematical model by Yee and Grossmann (1990) by introducing heat exchanger efficiency and variation of the heat transfer coefficients to the problem.

Bogataj and Bagajewicz (2008) represent a new superstructure model and solve both HEN and water network problem together with an MINLP model. The mixing units are added to the superstructure to track the isothermal and non-isothermal (i.e., constant and variating temperature) mixing points for the water networks. Bogataj and Kravanja (2012) use another alternative superstructure for the problem and global optimization methods to solve the mathematical model (i.e., MINLP). Their superstructure has an aggregated substructure in addition to Yee et al. (1990), which also allows bypasses in the process. Every existing match of streams in the Yee et al. (1990)'s superstructure is mapped to a HE in the aggregated substructure. From the mathematical description of this substructure, the complexity emerged from nonconvexity is reduced.

Laukkanen and Fogelholm (2011) suggest a bilevel optimization method by dividing the problem to four subproblems. It involves grouping the process streams and optimizing each group for HENS. The solution method comprises solving NLP and MINLP mathematical models in subproblems. Similarly, Khorasany and Fesanghary (2009) solve the problem in two levels. In the first level, structures of HENs are generated. The number of heat exchangers and stream branches are decided in the second level. Both levels are modeled as NLPs and a meta-heuristic method based on harmony search and sequential quadratic programming method are applied for solving the NLPs. In both studies, the superstructure method is not directly applied but similar structures are fixed at the first steps of the problems. Laukkanen and Fogelholm (2011) do not take stream splitting into consideration whereas Khorasany and Fesanghary (2009) allow it in their model.

Laukkanen et al. (2010) propose a multiobjective approach to the HENS problem based on the superstructure model of Yee and Grossmann (1990). The objectives are minimizing hot and cold utility costs, fixed cost per unit exchanger, and area costs. The model is solved by using an interactive NIMBUS weighing method. Lopez-Maldonado et al. (2011) use goal programming for the same problem with two minimizing objectives: total annual cost and environmental impact. Stream splitting is not allowed in either of these studies.

Using superstructure based methods can cause overestimation on the number of heat exchangers in the resulting network. Since a stage number is prespecified, the flexibility of the method is low. Generally, these methods are focused on finding the HEN structure and they do not consider the individual HE design. Our method covers the HE design along with the HENS, and it is flexible compared to the superstructure based methods.

2.2.3 Elusive Methods

Other than the methods discussed above, there are some other methods based on heuristic and meta-heuristic techniques to solve the HENS problem. Some of these methods are briefly summarized below.

Anantharaman et al. (2010) divide the HENS problem into sub-problems and suggest a sequential framework which includes solving several LP, MILP, and NLP problems. The solution methodology has a sequential and iterative framework. The computational complexity of the HENS problem due to MINLP modeling is reduced by using NLP and MILP instead.

Thus, the solution of industrial sized problems becomes easier to find with this methodology.

Gupta and Ghosh (2010) use a randomized algorithm for finding HEN with the minimum cost. Limits on the number of heat exchangers are applied for randomizing possible HENs and stream splitting is allowed in the process.

Salama (2012) uses the minimum rule in its mathematical model for the HENS problem. With this rule, some constraints are eliminated from the model. The problem is solved with and without stream splitting.

Yerramsetty and Murty (2008) apply a differential evolutionary algorithm for optimization of the HENS problem by taking stream splitting into consideration. Dipama et al. (2008) use a genetic algorithm for the same purpose. The HEN structure is initialized by defining the number of stages at the beginning in both studies.

2.3 Heat Exchanger Network Synthesis with Detailed Equipment Design

All the solution methods discussed in the previous section are concentrated in the synthesis of a heat exchanger network for the given system. The conceptual design of HEs is taken into account and heat exchange areas are calculated in these studies, but the mechanical design of heat exchangers in the network is not considered. There are a few studies in the HEN literature that solve the HENS problem and the detailed HE design problem simultaneously.

Serna-Gonzalez and Ponce-Ortega (2011) consider both pressure drop and area effects while targeting to reach a minimal total cost for the resulting HEN design. They use the pinch analysis approach in their MINLP mathematical model. The main idea is to improve the consistency between conceptual design and detailed design of heat exchangers. They include Bell Delaware method calculations to their MINLP formulation for pressure drop effects, but the specifications of HEs are defined prior to the solution of MINLP model. There is no optimization for HE design, but it is included in the calculations.

Roque and Lona (2000) use the pinch analysis for the HENS problem and Bell Delaware method for the detailed design of heat exchangers. The results are obtained for those with and without stream splitting cases. Ravagnani et al. (2003) use the same method except they add pressure drop and fouling factor calculations into the formulation, and the heat exchangers are designed in TEMA standards.

Mizutani et al. (2003a) give an MINLP formulation for the detailed design of shell-and-tube heat exchangers. In their consecutive study, Mizutani et al. (2003b) combine the superstructure formulation of Yee and Grossmann (1990) with the detailed equipment design. Since the overall heat transfer coefficients are not assumed, the results are better compared to the results in the previous studies. However, the effect of temperature change on the physical properties are not taken into account in that formulation either. An average value is used for these properties instead.

Ravagnani and Caballero (2007) and Silva et al. (2008) propose models similar to the ones by Mizutani et al. (2003b). Ravagnani and Caballero (2007) solve the superstructured HEN problem with a stage-wise approach and use a MINLP model for the detailed heat exchanger design with TEMA standards. Silva et al. (2008) use a particle swarm optimization heuristic for solving the MINLP made of two distinct submodels. Ponce-Ortega et al. (2007) suggest a genetic algorithm for the solution of the same model.

Garcia et al. (2006) use a hybrid method. Similarly, Roque and Lona (2000) apply the pinch analysis for the HENS problem and use a mathematical model for the detailed equipment design. An evolutionary algorithm with an IP model is used for the HE design. This provides easiness for large-scale problems.

Allen et al. (2009) use the pinch analysis for the HENS problem and a genetic algorithm for the detailed design. They allow partial or complete condensation of hot utility and design the condensers accordingly.

These studies consider the same problem as our study. It is observed that superstructure based methods dominates the HENS literature. Heuristic approaches are usually used for the solution of mathematical models. As it is mentioned previously, our method provides a flexible structure for HEN and optimality is guaranteed for the HEN structure depending on the sensitivity parameters. Unlike these studies, the overall heat transfer coefficients for every HE in the network are calculated depending on the physical and transport properties of the streams, and the heat exchanger design configuration. This leads to more realistic solutions for the problem.

2.4 Remarks

The HE design and the HENS are both highly complicated problems to solve. In the chemical engineering literature, there are many aspects of problem descriptions, different formulations, and numerous solution approaches to the HEN problem. An optimal solution cannot be guaranteed with these approaches because of the problem nature. The superstructure of Yee and Grossmann (1990) and the pinch analysis of Linnhoff and Hindmarsh (1983) are somehow dominating the literature from the formulation point of view. The heuristic approaches, mathematical modeling based algorithms, and stage-wise algorithms are the mostly used as solution methods. The studies that combine the HENS with the detailed HE design generally use both approaches. What we see in the literature is that there are two basic approaches. In the first approach, the HEN to be designed is restricted at the beginning of a model formulation, then the model is solved according to this prespecified structure. The second approach is based on randomizing. The HEN structure is randomized by some heuristic method, then either a model is solved to find the design or feasibility checks are done to finalize the randomized design. As these approaches tighten the solution space, they may ignore some better solutions at the feasible solution set of the problem. In this study, we suggest a method that numerous possible HEN alternatives to be generated and all HEs in the generated network will be designed. The dynamic nature of the physical properties are also being considered, which give a more realistic feature to the model compared to its competitors. Because of the complexity of the problem and increase in the solution times as the problem size grow, a simpler design method is used for the detailed design of HEs.

CHAPTER 3

PROBLEM FORMULATION

Main motivation of this study is to propose a realistic approach to the solution of heat exchanger network synthesis (HENS) problem. We formulate the HENS as *a shortest path problem*, which aims to find the least costly path on the network of HEN configuration alternatives. We generate a network that is able to include all possible alternatives of a HEN for a given system of various hot and cold streams. The *nodes*, *v*, represent individual heat exchangers (HEs) and the *arcs*, *u*, between nodes represent annual costs due to installation and operation of equipments. Two dummy nodes are placed at both ends of the network. The arcs from and to these nodes include the costs of utility usage and utility HEs. The *shortest path* on the network gives the HEN configuration with the minimum total annual cost. The detailed design of every heat exchanger (i.e., every node) on the network is achieved by formulating a design problem with mixed integer nonlinear programming (MINLP) model.

In this chapter, we formulate the HENS with detailed equipment design in detail. The problem formulation of detailed HE design with a brief introduction to heat transfer mechanisms and equipments are given in Section 3.1. Formulation of the HENS is defined in Section 3.2.

3.1 Heat Exchanger Design

3.1.1 Heat Transfer Mechanisms

'Heat transfer' is energy in transit due to a temperature difference which is the driving force of energy flow. There are three basic mechanisms of heat transfer: Conduction, convection and radiation (Figure 3.1).

Conduction occurs by the interaction of adjacent molecules while transferring some of their energy to each other. Heat can be conducted inside of an object or between objects that are in physical contact. Conduction of heat occurs through solids, liquids, and gases when a temperature gradient exists. Heat transfer through walls of a refrigerator or a furnace, freezing of the ground during the winter are some examples of conduction mechanism.

When the energy transfer happens due to motion of fluid through a surface (mostly solid), the mechanism is called *convection*. A distinction should be made depending on how the convection takes place. *Natural convection* occurs when there are circulation motions, which is the result of buoyancy forces caused by the density differences due to temperature differences in the fluid. On the other hand, it is called *forced convection* when the fluid is forced to flow on a solid surface by external means (e.g., pumps, fans, stirrers). Cooling of a hot cup of coffee occurs with convection. If one blows over coffee's surface, it is called forced convection. Otherwise, after a while, there will be a density difference in the air over coffee's surface and heat transfer will occur. This is called natural convection.

Radiation differs from conduction and convection in a way that no physical medium is needed for its transmission. Radiation is the energy transfer through the space by electromagnetic waves. Transport of the heat to the earth from the sun is the most relevant example for radiation. Heat transfer may occur by any mechanism or any of these three mechanisms (Geankoplis 2003).

3.1.2 Shell-and-Tube Heat Exchanger Design Model

Heat exchangers are equipments that enable two fluids (one hot and one cold) to interact and transfer excess heat of hot fluid to cold fluid. There are different types of HEs, but in this study, we use shell-and-tube heat exchangers in the process (refer to Section 2.1). In shell-and-tube heat exchangers, out of three basic mechanisms, conduction and convection take place. In the equipment design conductive and convective heat effects are reflected to the model with theoretical and empirical expressions.

Mizutani et al. (2003a) formulate the problem of detailed design of shell-and-tube exchangers as follows:

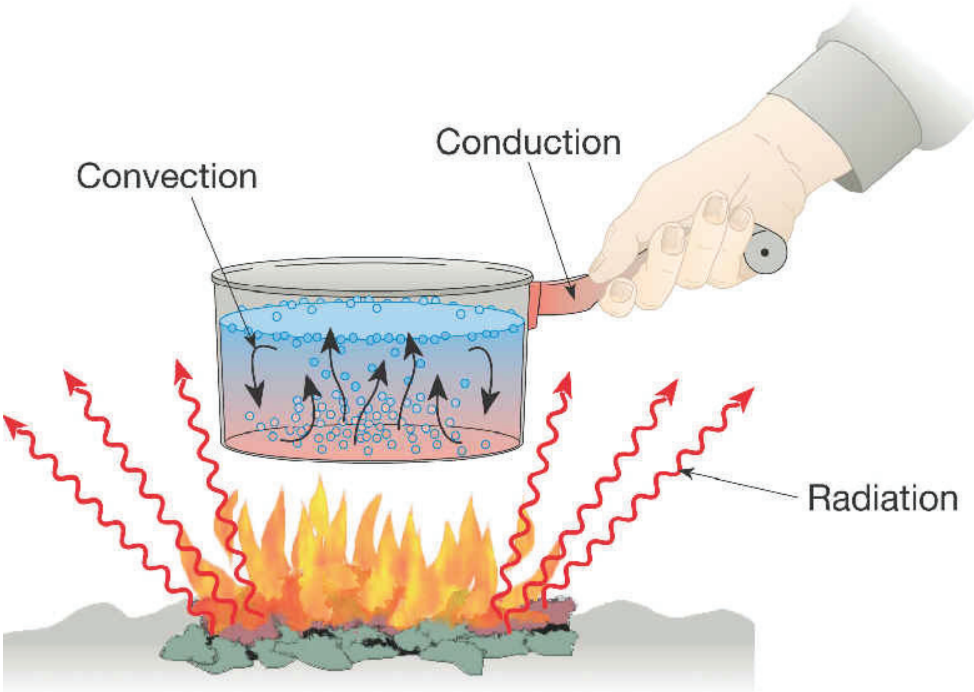


Figure 3.1: Examples of heat transfer mechanisms (CReSIS in the Field 2010)

"Given are hot and cold streams for heat exchange with their specified supply and target temperatures, as well as their fluid flow rates. Also given for each stream are its physical properties: viscosity, density, thermal conductivity, and thermal capacity. The problem then consists of determining the optimal shell-and-tube heat exchanger design options: number of tubes, number of tube passes, internal and external tube diameters, tube arrangement pattern, number of baffles, head type, and fluid allocation. The objective is to minimize the total annual investment and operating costs."

Our problem formulation is the same with slight differences. The physical and thermal properties are not taken as constant and they are calculated at their specified temperatures. Thus, instead of fluid flow rates of streams, the compositions and molar flow rates of each component in the streams are inputs to the model. In order to identify the phase change, the pressures of streams are also needed as inputs. The fluid allocation is assumed and the number of baffles are not decided in our model. Accordingly, our problem formulation is:

A hot stream and a cold stream are given; where their inlet and outlet temperatures, pressures, and composition of each stream is known. The molar flow rate of each substance in each stream composition is also known. The problem seeks to determine the design parameters *of the shell-and-tube heat exchanger: number of tubes, number of shell and tube passes, inner and outer diameters of tubes, inner diameter of shell, tube arrangement, head type, and length of tubes. The objective is to minimize the total annual cost. The components of the cost function are cost of investment due to installation of heat exchangers in the network and operating cost due to pumping against pressure drop.*

A mixed integer nonlinear programming (MINLP) model is formulated with a basic method for determining design of the shell-and-tube heat exchanger options. Here are the assumptions made for the sake of simplification:

- All exchangers are countercurrent exchangers. This means that hot and cold streams flow in the heat exchanger in opposite directions. The heat exchange process is more effective in this type of HEs.

- Material of construction for the tube-side is taken as carbon steel (which is a widely used material).

- In all HEs, the cold stream flows from the tube-side, where the hot stream flows from the shell-side.

- Phase change (condensation for hot streams and vaporization for cold streams), if applicable, is taken into account while calculating overall heat load of the heat exchanger. Special design equations are not used for phase changing conditions in the detailed design.

- The alternatives considered for shell and tube passes are 1-1 (1 shell, 1 tube pass), 1-2, 2-4, and 3-6.

- The logarithmic mean temperature difference (LMTD) is used for calculating the overall temperature difference throughout a HE. The correction factor, F of LMTD (which is dependent on the shell and tube passes), is assumed to be 1 for all alternatives of passes. Also, when the temperature differences equal to each other, the logarithmic mean temperature difference cannot be calculated (e.g., it results in division by zero error). In this case, the arithmetic mean temperature difference is used.

- The pressure drop and fouling effects are assumed to be negligible in a HE.

The reason to simplify the model is that the solution time of a more detailed design will be much longer. Of course, there is a trade-off in eliminating features from the model and long computation times for solving the model. With every assumption the model is drawing away from the reality, but it is needed to get solutions in reasonable times and to have an insight. It is important to know the limitations of the model and interpret the solutions accordingly.

Individual detailed design of a shell-and-tube HE is done by using the necessary design equations which represent the flow characteristics of both fluids and heat transfer properties in HE. For given inlet (*in*) and outlet (*out*) temperatures of both hot (*h*) and cold (*c*) streams, $T^{h(in)}$, $T^{h(out)}$, $T^{c(in)}$, $T^{c(out)}$, and mass flow rates of these, m^h, m^c, the detailed design of HE can be found with the MINLP model which is explained throughout this section. Since it is assumed that the cold stream (hot stream) flows in the shell-side (s) (tube-side (t)), the inlet and outlet temperatures of the shell-side (tube-side), $T^{s(in)}$, $T^{s(out)}$ ($T^{t(in)}$, $T^{t(out)}$) are equal to the inlet and outlet temperatures of cold stream (hot stream), $T^{c(in)}$, $T^{c(out)}$ ($T^{h(in)}$, $T^{h(out)}$). Similarly, the mass flow rate of cold stream (hot stream) is equal to the mass flow rate of shell-side (tube-side), m^s (m^t).

We generate a design configuration data set according to the TEMA standards. Each HE design alternative (*al*), l, in the data set corresponds to a design configuration for HE. This configuration includes:

- inner and outer diameter of tubes, $d_l^{in(al)}$, $d_l^{out(al)}$,
- pitch arrangement of tubes (also called configuration of tubes), $conf_l^{al}$, as triangular or square (see Figure 2.3),
- pitch length, which is the distance between centers of adjoining tubes, $pitch_l^{al}$,
- TEMA style, $TEMA_l^{al}$, as L, M, P, S or U (see Figure 2.2),
- number of shell and tube passes, $n_l^{s(al)}$, $n_l^{t(al)}$, as 1-1, 1-2, 2-4, or 3-6,
- number of tubes, N_l^{al}, and
- inner diameter of shell, $D_l^{s(al)}$.

There are two coefficients, δ and θ, which are used for calculating the shell-side heat transfer coefficient. They are dependent to the outer diameter of the tubes, the pitch length, and the pitch arrangement. In addition to the mechanical configuration parameters, these, δ_l^{al}, θ_l^{al}, are also added to the data set.

The decision variable a_l indicates which configuration is selected among the set of standards, where

$$a_l = \begin{cases} 1, & \text{if standard } l \text{ is selected in data set,} \\ 0, & \text{otherwise.} \end{cases} \tag{3.1}$$

f_{design} is a set of linear and nonlinear functions that are dependent on the design configuration of a HE and the physical and transport properties of the fluid streams. These properties are density, ρ, heat capacity, Cp, thermal conductivity, k, and viscosity, μ and they are combination of tube-side and shell-side properties, i.e., $\widetilde{\rho} = (\rho^t, \rho^s)$, $\widetilde{Cp} = (Cp^t, Cp^s)$, $\widetilde{k} = (k^t, k^s)$, and $\widetilde{\mu} = (\mu^t, \mu^s)$. Here, ρ^t, Cp^t, k^t and μ^t are tube-side properties at bulk temperature where ρ^s, Cp^s, k^s and μ^s are shell-side properties at film temperature. All these are functions of T which represents the inlet and outlet of both streams. Note that $\widetilde{\bullet}(T)$ denotes the function of $\widetilde{\bullet}(\cdot,\cdot)$ in terms of T parameters for any property $\bullet$. For example, the thermal conductivity k of liquid phase o-xylene is computed as $\left(0.1783 - 9.4 \times 10^{-5}T - 2 \times 10^{-5}T^2\right)$. $Area$ is the solution which indicates the heat exchange area and it is dependent on the set of design equations defined in f_{design}. The condensed form of the model that finds the heat exchanger configuration that minimizes the heat exchanger area by searching available specified standards:

$$EA= \quad \text{Min} \quad Area \tag{3.2}$$

$$\text{s. to:} \quad Area = f_{design}\left(a_l, \widetilde{\rho}(T), \widetilde{Cp}(T), \widetilde{k}(T), \widetilde{\mu}(T)\right) \tag{3.3}$$

$$\sum_{l=1}^{L} a_l = 1 \tag{3.4}$$

$$a_l \in \{0, 1\} \qquad \forall l = 1, ..., L \tag{3.5}$$

$$\text{where} \qquad T = (T^{h(in)}, T^{h(out)}, T^{c(in)}, T^{c(out)})$$

Additional Notation

Before giving the complete mathematical model, here are the additional parameters and decision variables which are not explained before:

Parameters

m^s : mass flow rate of shell-side fluid in kilogram per second

m^t : mass flow rate of tube-side fluid in kilogram per second

k^{tube} : thermal conductivity of tube material in Watt per meter Kelvin at wall temperature

y^{gas} : 1 if the fluid inside the tubes is gas, 0 otherwise

y^{liq} : 1 if the fluid inside the tubes is liquid, 0 otherwise

y^{wat} : 1 if the fluid inside the tubes is water, 0 otherwise

Tlm : logarithmic mean temperature difference in Kelvin

Q^s : shell-side heat load in Joule per second

μ^{avg} : ratio of μ^t and $\mu^{t(w)}$ where $\mu^{t(w)}$ is viscosity of tube-side fluid at wall temperature

NPr^s : Prandtl number of shell-side fluid

NPr^t : Prandtl number of tube-side fluid

$upper$: upper bound for variables

$lower$: lower bound for variables

Decision Variables

d^{in} : inner diameter of tubes in meter

d^{out} : outer diameter of tubes in meter

D^s : inner diameter of shell in meter

$conf$: configuration of tubes, 1 if square, 2 if triangular

$pitch$: pitch length of tubes in meter

$TEMA$: TEMA type of HE, 1 if F or S, 2 if U, 3 if L or M

n^t : number of tube passes, 1, 2, 4, or 6

n^s : number of shell passes, 1, 2, or 3

N : number of tubes

δ : constant δ for calculating shell-side heat transfer coefficient

θ : constant θ for calculating shell-side heat transfer coefficient

A^{ics} : inside cross-sectional area of tubes in m^2

A^{ocs} : outside cross-sectional area of tubes in m^2

Alm : logarithmic mean area in meter square

A^{log} : variable for calculating Alm

A^s	: cross-sectional area of shell in meter square
v^{in}	: velocity of flow inside tubes meter per second
v^{out}	: velocity of flow outside tubes meter per second
NRe^s	: shell-side Reynolds number
NRe^t	: tube-side Reynolds number
NNu^s	: shell-side Nusselt number
NNu^t	: tube-side Nusselt number
ch^t	: convective heat transfer coefficient inside tubes in Watt per meter square Kelvin
ch^s	: convective heat transfer coefficient outside tubes in Watt per meter square Kelvin
U^{over}	: overall heat transfer coefficient based on outside area of tube in Watt per meter square Kelvin
$Length$	: length of heat exchanger in meter

Preliminary Calculations

For some parameters, preliminary calculations should be done as explained below.

Bulk temperature, T^{bulk}, and wall temperature, T^{wall}, are average temperatures of tube-side and shell-side in Kelvin, respectively.

$$T^{bulk} = \frac{T^{t(in)} + T^{t(out)}}{2} \tag{3.6}$$

$$T^{wall} = \frac{T^{s(in)} + T^{s(out)}}{2} \tag{3.7}$$

Film temperature, T^{film}, is temperature of the fluid film formed on the tubes in the shell-side and it is defined as the average of bulk and wall temperatures in Kelvin.

$$T^{film} = \frac{T^{bulk} + T^{wall}}{2} \tag{3.8}$$

Log-mean temperature difference is average temperature difference in a HE in Kelvin. The temperature differences through HE are shown in Figure 3.2.

$$\Delta T^1 = T^{h(in)} - T^{c(out)} \tag{3.9}$$

$$\Delta T^2 = T^{h(out)} - T^{c(in)} \tag{3.10}$$

$$Tlm = \frac{\Delta T^2 - \Delta T^1}{\ln(\Delta T^2/\Delta T^1)} \tag{3.11}$$

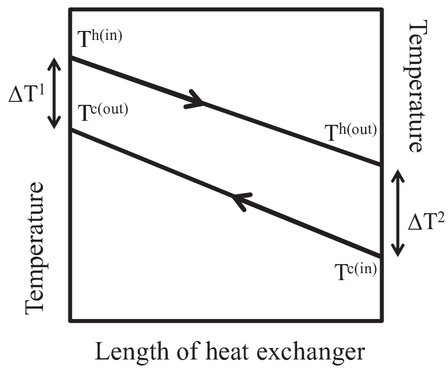


Figure 3.2: Temperature profile in a counter-current heat exchanger

If a stream consists of g components and mass flow rates of each component g are given as m_g^t for tube-side fluid and m_g^s for shell-side fluid where $m^t = \sum_{\forall g} m_g^t$ and $m^s = \sum_{\forall g} m_g^s$, the physical properties are calculated as follows:

$$\rho^t = \sum_{\forall g} \rho_g^t \left(\frac{m_g^t}{m^t} \right) \tag{3.12}$$

$$\rho^s = \sum_{\forall g} \rho_c^s \left(\frac{m_g^s}{m^s} \right) \tag{3.13}$$

where ρ_g^t and ρ_g^s are densities of pure component g in tube-side and shell-side in kilogram per cubic meter, respectively.

$$Cp^t = \sum_{\forall g} Cp_g^t \left(\frac{m_g^t}{m^t} \right) \tag{3.14}$$

$$Cp^s = \sum_{\forall g} Cp_g^s \left(\frac{m_g^s}{m^s} \right) \tag{3.15}$$

where Cp_g^t and Cp_g^s are heat capacities of pure component g in tube-side and shell-side in Joule per kilogram Kelvin, respectively.

$$k^t = \sum_{\forall g} k_g^t \left(\frac{m_g^t}{m^t} \right) \tag{3.16}$$

$$k^s = \sum_{\forall g} k_g^s \left(\frac{m_g^s}{m^s} \right) \tag{3.17}$$

where k_g^t and k_g^s are thermal conductivities of pure component g in tube-side and shell-side Watt per meter Kelvin, respectively.

$$\mu^t = \sum_{\forall g} \mu_g^t \left(\frac{m_g^t}{m^t}\right) \tag{3.18}$$

$$\mu^s = \sum_{\forall g} \mu_g^s \left(\frac{m_g^s}{m^s}\right) \tag{3.19}$$

where μ_g^t and μ_g^s are viscosities of pure component g in tube-side and shell-side Pascal second, respectively.

Heat loads for shell and tube sides, Q^s, Q^t, are the heat absorbed/generated by the fluids in Watt. From the first law of thermodynamics of conservation of energy, the generated heat by hot stream should be equal to the heat emitted by cold stream in the system, i.e., $Q^s = Q^t$. If there is a phase change in the equipment, the relevant heat, heat of vaporization, ΔH^{vap}, or condensation, ΔH^{cond}, should be added to the heat loads.

$$Q^s = m^s \cdot Cp^s \cdot (T^{s(in)} - T^{s(out)}) + m^s \cdot \Delta H^{vap} \tag{3.20}$$

$$Q^t = m^t \cdot Cp^t \cdot (T^{t(in)} - T^{t(out)}) + m^t \cdot \Delta H^{cond} \tag{3.21}$$

Viscosity fraction is the fraction of tube-side viscosities at bulk temperature and at wall temperature.

$$\mu^{avg} = \frac{\mu^t}{\mu^{t(w)}} \tag{3.22}$$

Prandtl number is a dimensionless number, which is the ratio of viscous and thermal diffusion rates. Physically, it relates the relative thickness of the hydrodynamic layer and the thermal boundary layer.

$$NPr^s = \frac{Cp^s \cdot \mu^s}{k^s} \tag{3.23}$$

$$NPr^t = \frac{Cp^t \cdot \mu^t}{k^t} \tag{3.24}$$

The Complete Model (CM)

The following constraints from 3.27 to 3.56 are given for the condensed form of the model. These design equations are taken from Geankoplis (2003) and one may refer to the same book for more detailed explanation of heat transfer mechanisms and the HE design.

$$EA = \text{Min} \quad Area \tag{3.25}$$

$$\text{s. to:} \tag{3.26}$$

Among all the alternative configurations of HEs, only one is selected.

$$\sum_{\forall l} a_l = 1 \tag{3.27}$$

The outer diameter of tubes is specified among l alternative configurations.

$$d^{out} = \sum_{\forall l} a_l \cdot d_l^{out(al)} \tag{3.28}$$

The inner diameter of tubes is specified among l alternative configurations.

$$d^{in} = \sum_{\forall l} a_l \cdot d_l^{in(al)} \tag{3.29}$$

The outer diameter of shell is specified among l alternative configurations.

$$D^{s} = \sum_{\forall l} a_l \cdot D_l^{s(al)} \tag{3.30}$$

The tube arrangement is specified among l alternative configurations.

$$conf = \sum_{\forall l} a_l \cdot conf_l^{al} \tag{3.31}$$

The number of shell passes is specified among l alternative configurations.

$$n^{s} = \sum_{\forall l} a_l \cdot n_l^{s(al)} \tag{3.32}$$

The number of tube passes is specified among l alternative configurations.

$$n^{t} = \sum_{\forall l} a_l \cdot n_l^{t(al)} \tag{3.33}$$

The TEMA type is specified among l alternative configurations.

$$TEMA = \sum_{\forall l} a_l \cdot TEMA_l^{al} \tag{3.34}$$

The pitch length is specified among l alternative configurations.

$$pitch = \sum_{\forall l} a_l \cdot pitch_l^{al} \tag{3.35}$$

The number of tubes is specified among l alternative configurations.

$$N = \sum_{\forall l} a_l \cdot N_l^{al} \tag{3.36}$$

The constant δ is specified among l alternative configurations.

$$\delta = \sum_{\forall l} a_l \cdot \delta_l^{al} \tag{3.37}$$

The constant θ is specified among l alternative configurations.

$$\theta = \sum_{\forall l} a_l \cdot \theta_l^{al} \tag{3.38}$$

Inner cross-sectional area of tubes is calculated.

$$A^{ics} = \frac{\pi \cdot \left(d^{in}\right)^2}{4} \tag{3.39}$$

Outer cross-sectional area of tubes is calculated.

$$A^{ocs} = \frac{\pi \cdot (d^{out})^2}{4} \tag{3.40}$$

Ratio of inner and outer cross-sectional area of tubes is calculated.

$$A^{log} = \frac{A^{ocs}}{A^{ics}} \tag{3.41}$$

Logarithmic mean area of tubes is calculated.

$$Alm = \frac{A^{ocs} - A^{ics}}{\ln(A^{log})} \tag{3.42}$$

Cross-sectional area of shell is calculated.

$$A^s = \frac{\pi \cdot (D^s)^2}{4} - (N \cdot A^{ocs}) \tag{3.43}$$

Velocity of flow inside the tubes is calculated.

$$v^{in} = \frac{m^t}{\rho^t \cdot N \cdot A^{ics}} \tag{3.44}$$

Velocity of flow outside the tubes is calculated.

$$v^{out} = \frac{m^s}{\rho^s \cdot A^s} \tag{3.45}$$

Reynolds number is a dimensionless number, which indicates the regime characteristic of the flow. If the fluid flow is at low velocities, it is called laminar flow; whereas, at high velocities, it is called turbulent flow. Reynolds number for both shell and tube sides, NRe^s and NRe^t, are calculated.

$$NRe^s = \frac{d^{out} \cdot v^{out} \cdot \rho^s}{\mu^s} \tag{3.46}$$

$$NRe^t = \frac{d^{in} \cdot v^{in} \cdot \rho^t}{\mu^t} \tag{3.47}$$

Nusselt number is used to relate the data for the heat transfer coefficient to the thermal conductivity of a fluid and a characteristic dimension, e.g., diameter of the tube. For the turbulent flow inside a pipe, an empirical formula is used to calculate the tube-side Nusselt number, NNu^t, (Geankoplis 2003).

$$NNu^t = 0.027 \left(NRe^t\right)^{0.8} \cdot \left(NPr^t\right)^{1/3} \cdot (\mu^{avg})^{0.14} \tag{3.48}$$

For the flow past over bank of tubes, also an empirical formula is used to calculate the shell-side Nusselt number, NNu^s, (Geankoplis 2003).

$$NNu^s = C \cdot (NRe^s)^m \cdot (NPr^s)^{1/3} \tag{3.49}$$

The heat transfer coefficient is a function of the geometry, fluid properties, flow velocity, and temperature difference. Since it cannot often be predicted theoretically, empirical correlations are available to predict this coefficient. The tube-side heat transfer coefficient, ch^t, can be calculated with three different equations. If the stream is in the gas state, the first equation is activated and by the definition of Nusselt number, ch^t is calculated. The second or third equations are applicable when the stream is liquid or water, respectively. The second and third equations depend on the approximations (Geankoplis 2003).

$$\begin{aligned} ch^t = & y^{gas} \cdot \left[\frac{NNu^t \cdot k^t}{d^{in}}\right] + y^{liq} \cdot \left[423 \frac{\left(v^{in}\right)^{0.8}}{\left(d^{in}\right)^{0.2}}\right] \\ & + y^{wat} \cdot \left[1429 \left(1 + 0.0146 \left(\frac{(T^{t(in)} - T^{t(out)})}{2} - 273.15\right) \left(\frac{\left(v^{in}\right)^{0.8}}{\left(d^{in}\right)^{0.2}}\right)\right)\right] \end{aligned} \tag{3.50}$$

The shell-side heat transfer coefficient, ch^s, is calculated by the definition of Nusselt number.

$$ch^s = \frac{NNu^s \cdot k^s}{d^{out}} \tag{3.51}$$

The overall heat transfer coefficient is the measure of the overall ability of series of conductive and convective heat transfer barriers.

$$U^{over} = \frac{1}{\dfrac{A^{ocs}}{A^{ics} \cdot ch^t} + \dfrac{A^{ocs} \cdot (d^{out} - d^{in})}{2k^{tube} \cdot Alm} + \dfrac{1}{ch^s}} \tag{3.52}$$

The heat exchanger area is calculated.

$$Area = \frac{Q^s}{U^{over} \cdot Tlm} \tag{3.53}$$

HE length is calculated.

$$Length = \frac{Area}{N \cdot \pi \cdot d^{out} \cdot n^t} \tag{3.54}$$

The lower and upper bounds are set to the same value for all variables.

$$lower \leq \text{All variables (except } a_l\text{'s)} \leq upper \tag{3.55}$$

Alternatives are restricted to binary variables.

$$a_l \in \{0, 1\} \qquad \forall l = 1, ..., L \tag{3.56}$$

The solution of the model CM gives the heat exchanger configuration with the minimum heat exchange area. This complete model can also be defined as a complete enumeration scheme of possible heat exchanger alternatives and selecting the best solution (minimum heat exchanger area) among them.

When the pressure drops inside the tubes and across the tube bank are considered, the construction and solution of a mathematical model like CM is necessary for the design of HEs. The problem actually becomes an optimization problem in this case. According to the calculations given by Chopey (2004), the constraints for pressure drop are as follows:

Pressure drop inside tubes:

$$\Delta P^t \leq \frac{4 f^t {m^t}^2 n^t \, Length}{2(144) gc \rho^t d^{in}} \tag{3.57}$$

Pressure drop across tube bank:

$$\Delta P^s \leq \frac{4f^s m^{s2} Nr(Nb-1)R_1 R_b \mu^{sw}/\mu^{sb}}{2(144)gc\rho^s} \tag{3.58}$$

The parameters in these constraints are as follows:

ΔP^t : upper bound for pressure drop in tube-side

ΔP^s : upper bound for pressure drop in shell-side

μ^{sw} : viscisity of shell-side fluid at wall temperature

μ^{sb} : viscisity of shell-side fluid at bulk temperature

gc : the gravitational constant

Friction factor is a function of tube dimensions and flow characteristic of the stream. Baffle window ratio and number of baffles are also dependent to the tube configuration and dimensions. Thus, these are the variables of the constraints.

f^t : friction factor for tube side

f^s : friction factor for shell side

Nr : baffle window ratio (different for square and triangular pitch)

Nb : number of baffles

These calculations can also be performed in a more detailed level by considering the pressure drops at inlet-outlet nozzles and entry-exit of tubes.

As explained before, the problem without pressure drop constraints (3.57) and (3.58) can be solved with total enumeration, for example, by using an Excel spreadsheet. However, enumeration gets complicated when these constraints are added, because in that case, some trade-offs between constraints arise. Minimizing the area may lead to high pressure drops and vice versa: low pressure drops may result in higher area. Therefore we refer to the mathematical model instead of conducting total enumeration for solving the problem.

3.2 Heat Exchanger Network Synthesis

In this section, we define our problem in detail (Section 3.2.1) and represent our formulation (Section 3.2.2). In general, we create HE alternatives by discretizing the temperatures of streams. Then we solve the detailed HE model for every HE alternative. Every HE is represented as a node in a network and the shortest path of the network gives us the HEN configuration of the system.

3.2.1 Problem Formulation

The heat exchanger network synthesis (HENS) problem with detailed equipment design is formulated by Mizutani et al. (2003b). According to the best of our knowledge, since then studies in the literature use the same problem formulation.

"Given are a set of hot and cold streams with their supply and target temperatures as well as their corresponding flow rates. Given are also hot and cold utility temperatures and their corresponding costs. For each stream, the following physical properties are known: viscosity, density, thermal conductivity, and thermal capacity. The problem consists of determining the optimal heat exchanger network structure, the hot and cold utilities that are required, the heat loads of each heat-exchanger unit and its design variables: number of tubes, number of tube passes, internal and external tube diameters, tube arrangement pattern, number of baffles, head type, and fluid allocation. The objective is to minimize the total annual investment and operating costs."

Our problem formulation is mainly the same, as that of Mizutani et al. (2003b), but there are several different aspects on the detailed HE design. As described in Section 3.1, the physical and thermal properties are not taken as constants, and pressures of streams, compositions, and molar flow rates of each component in the streams are taken as inputs to the formulation. However, the fluid allocation is assumed and the number of baffles are not decided. Our problem formulation is:

A set consisting of I hot and J cold streams is given, where their system inlet and target temperatures, pressures, and composition of each stream are known. The molar flow rate of each substance in each stream composition is also known. In addition, hot and cold utility temperatures and their corresponding costs are given. The problem seeks to determine the heat exchanger network configuration by deciding how many heat exchangers should be installed; how their arrangements should be; which hot and cold streams should be processed in which HE; what the inlet and outlet temperatures of each HE in the network should be; whether there is any need for hot and cold utilities; what the heat load for each HE should be; how many heat exchangers should be installed for utilities; the design parameters that should be used for each HE: number of tubes, number of shell and tube passes, inner and outer diameters of tubes, inner diameter of shell, tube arrangement, head type, and length of tubes. The *objective is to minimize the total annual cost. The components of the cost function are cost of investment due to installation of heat exchangers in the network and operating costs due to hot and cold utility usage.*

3.2.2 Mathematical Formulation

We formulate the HENS problem as the shortest path problem. We generate the network, called *GRAPH* consisting of HEN alternatives. Every node v on *GRAPH* represents a HE design alternative and $cost_{v,w}$ is the installation and operation cost associated with each arc (v, w). Two dummy nodes are also placed at the start and at the end of the network in order to maintain the desired temperature changes through HEN. The shortest (minimum cost) path gives the optimal HEN configuration on *GRAPH*. Consider the network given in Figure 3.3. The dummy nodes, 'start' and 'end', are connected to every node, which will be explained later in detail. The numbered nodes represent HE candidates. The shortest path (i.e., HEN configuration with minimum total cost) is illustrated in bold and corresponds to the path of Start-1-10-7-3-End.

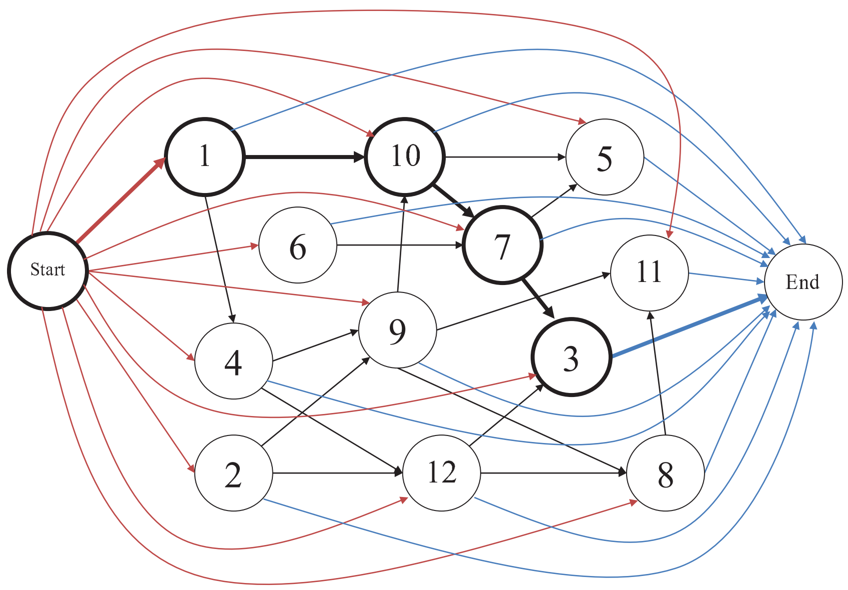


Figure 3.3: An example network for the HENS problem

A. HE Design Alternative Generation

We need to generate nodes for the formulation of the shortest path model. Every node in the network correspond to a HE. Let us define some indices and parameters for the representation of a node (i.e., HE):

Indices

i : hot streams, $i = \{1, ..., I\}$

j : cold streams, $j = \{1, ..., J\}$

Parameters

$T_i^{h(system)}$: system inlet temperature of hot stream i

$T_i^{h(target)}$: target temperature of hot stream i

$T_j^{c(system)}$: system inlet temperature of cold stream j

$T_j^{c(target)}$: target temperature of cold stream j

A HE processes one hot and one cold stream. Accordingly, a HE can be described with these hot i and cold j streams, including their inlet and outlet temperatures. Let us redefine T as $(T_i^{h(in)}, T_i^{h(out)}, T_j^{c(in)}, T_j^{c(out)})$ where $T_i^{h(in)}$, $T_j^{c(in)}$ and $T_i^{h(out)}$, $T_j^{c(out)}$ are inlet and outlet temperatures of hot i and cold j streams of the HE, respectively. Now, we can generate all possible heat exchanger candidates by considering all possible temperature values. In order to determine all possible temperature values, the temperatures for all given streams are discretized between their given system inlet and target temperature values. Let TH_i be a set of discretized temperatures of hot stream i and TC_j be a set of discretized temperatures of cold stream j where $T_i^{h(in)}, T_i^{h(out)} \in TH_i$ and $T_j^{c(in)}, T_j^{c(out)} \in TC_j$. Second, we form a grand set R to generate all possible HE design alternatives, using the sets of discretized temperatures of hot and cold streams, as follows:

$$R = \bigcup_{i=1}^{I} \bigcup_{j=1}^{J} \left(TH_i \times TH_i \times TC_j \times TC_j \right) \tag{3.59}$$

$$\text{where } T = (T_i^{h(in)}, T_i^{h(out)}, T_j^{c(in)}, T_j^{c(out)}). \tag{3.60}$$

Let r be an index that shows the number of a HE alternative where $r = \{1, ..., |R|\}$.

Of course, not all alternatives in R are feasible since the cartesian product of four sets generates $\left|TH_i \cdot TC_j\right|^2$ many of 4-tuples of T without checking thermal feasibilities of (discretized) temperatures. In order for an alternative r to be feasible, it should satisfy two conditions that are represented by variables $pair_r$ and A_r^R. $pair_r$ shows whether temperatures (i.e., inlet and outlet temperatures) are properly defined and heat is balanced for a HE alternative r with streams i and j and temperature profile T_r. A_r^R denotes whether individual HE design alternative r is feasible or not. How $pair_r$ and A_r^R are computed is explained in detail below.

Let $N' \subseteq R$ and N' includes all feasible HE design alternatives which is defined as:

$$N' = \left\{ \left(T_i^{h(in)}, T_i^{h(out)}, T_j^{c(in)}, T_j^{c(out)} \right) \in R \parallel pair_r = 1, A_r^R \text{ is feasible.} \right\}, \tag{3.61}$$

where the variable A_r^R can be defined as follows:

$$A_r^R = \begin{cases} EA, & \text{if the model CM returns a feasible solution (Area > 0) for HE alternative } r \in R \\ \text{infeasible}, & \text{otherwise} \end{cases} \tag{3.62}$$

Temperature Feasibility and Heat Balance Check: Calculating $pair_r$

For a HE, heat generated by hot stream should be equal to the heat absorbed by cold stream. In order to control that, heat loads of each stream should be calculated. Phase changes and temperature difference should be taken into account for calculating the heat loads. Below we explain how to determine the phase change.

Phase Change:

$phase_i^h$ and $phase_j^c$ are binary variables that indicate whether the hot steam i or cold stream j changes phase during the heat exchange process, respectively. The vapor pressure is a measure to understand whether a phase change occurs or not. The vapor pressure of a mixture can be calculated by using *the Raoult's Law*. Multiplying the molar fraction of a component in the mixture with the vapor pressure of the pure substance gives the partial vapor pressure of the mixture caused by that component. The relevant definitions that are needed for determining the phase change are as follows:

g	: number of components in a stream, $g = \{1, ..., G\}$
P_g	: vapor pressure of component g
$P_g^\circ(T)$	: vapor pressure of component g as pure liquid which is a function of temperature
mol_g	: molar fraction of component g in the process stream

Partial vapor pressure of mixture (stream) due to vapor pressure of component g is:

$$P_g = mol_g \cdot P_g^{\circ}(T) \tag{3.63}$$

Total vapor pressure of mixture (stream) is:

$$P_{total} = \sum_{g=1}^{G} P_g \tag{3.64}$$

Boiling takes place when the vapor pressure of the liquid is equal to the environment pressure. According to this, for a cold stream, if the vapor pressure at the inlet temperature is lower than the environment pressure and the vapor pressure at the outlet temperature is equal or higher than the environment pressure, then it is said that phase change occurs. So, for cold streams:

$$phase_j^c = \begin{cases} 1, \text{ if } P_{total,in} < P_{environment} \; \& \; P_{total,out} \geq P_{environment}, \\ 0, \text{ otherwise.} \end{cases} \tag{3.65}$$

On the contrary, a hot stream is condensed if the vapor pressure at inlet temperature is higher than the environment temperature and the vapor pressure at outlet temperature is equal to or lower than the environment pressure:

$$phase_i^h = \begin{cases} 1, \text{ if } P_{total,in} > P_{environment} \; \& \; P_{total,out} \leq P_{environment}, \\ 0, \text{ otherwise.} \end{cases} \tag{3.66}$$

Now, we explain how heat is balanced below.

Heat Balance:

Q_i^h : heat emitted by hot stream i

Q_j^c : heat absorbed by cold stream j

m_i^h : mass flow rate of hot stream i

m_j^c : mass flow rate of cold stream j

Cp_i^h : heat capacity of hot stream i

Cp_j^c : heat capacity of cold stream j

$\Delta H_{g,i}^{cond}$: heat of condensation of component g of hot stream i

$\Delta H_{g,j}^{vap}$: heat of vaporization of component g of cold stream j

The heat of phase changes is calculated:

$$\Delta H_i^{cond} = \sum_{g=1}^{G} mol_{g,i} \cdot \Delta H_{g,i}^{cond} \tag{3.67}$$

$$\Delta H_j^{vap} = \sum_{g=1}^{G} mol_{g,j} \cdot \Delta H_{g,j}^{vap} \tag{3.68}$$

The overall heat load of hot stream i and cold stream j are:

$$Q_i^h = m_i^h \cdot Cp_i^h \cdot (T_i^{h(in)} - T_i^{h(out)}) + phase_i^h \cdot \Delta H_i^{cond} \tag{3.69}$$

$$Q_j^c = m_j^c \cdot Cp_j^c \cdot (T_j^{c(in)} - T_j^{c(out)}) + phase_j^c \cdot \Delta H_j^{vap} \tag{3.70}$$

The parameter $pair_r$ depends on two conditions:

1. Recall Figure 3.2. In a counter-current heat exchanger, the streams are entering to it from opposite sides and the inlet temperature of hot stream should be higher than the outlet temperature of cold stream in order to let heat transfer to occur. At the same time, the outlet temperature of hot stream should also be higher than the inlet temperature of cold stream.
2. According to the first law of thermodynamics, i.e., law of conservation of energy, in an isolated system, the total amount of energy should remain the same over time. So, for a HE, energy generated by the hot stream should be equal to the energy absorbed by cold stream.

Mathematically, $pair_r$ is defined as:

$$pair_r = \begin{cases} 1, & \text{if } T_i^{h(in)} > T_i^{h(out)}, T_j^{c(in)} < T_j^{c(out)}, T_i^{h(out)} > T_j^{c(in)}, T_i^{h(in)} > T_j^{c(out)} \\ & \text{and } Q_i^h = Q_j^c \text{ for alternative } r \\ 0, & \text{otherwise} \end{cases} \tag{3.71}$$

B. Node Generation

Nodes are generated from the feasible HE set N'. Every node corresponds to a feasible HE and consists of necessary information (i.e., inlet and outlet temperatures). All streams' inlet and outlet temperatures are kept in the node. Here, a distinction should be made between streams. A stream is called processed stream if it undergoes a heat exchange in that node (HE), on the other hand, a stream is called unprocessed stream if it is not processed in that HE. For processed streams, inlet and outlet temperatures are different from each other where these temperatures are equal for unprocessed streams.

In a HE, as we mentioned above, two streams (one hot and one cold stream) are processed and in set N', every array defines the inlet and outlet temperatures of processed streams. Although, the other streams' (unprocessed streams for a specific HE) temperatures are unknown in that case and they are needed to relate the HEs with each other. Therefore, to be able to trace every stream's temperature through the network, we create copies of the feasible HEs and for every temperature of every unprocessed stream. In Figure 3.4, a generic representation of a node and an example node are given where there are four hot and three cold streams in a system. It shows that hot stream 2 and cold stream 3 are processed in the HE. Hot stream is cooled down to 175°C from 250°C and cold stream is heated from 52°C to 125°C. The inlet and outlet temperatures of unprocessed streams are the same.

Recall the definition of set N'. Here, i and j are processed streams. Then, i' and j' are used to represent unprocessed streams. The set of nodes, N, can be defined as follows:

$$N = N' \times \left[\bigcup_{i' \neq i} TH_{i'} \right] \times \left[\bigcup_{j' \neq j} TC_{j'} \right] \tag{3.72}$$

Consider a given system in which there are three hot streams and two cold streams. For a feasible HE alternative, let us say that hot stream 2 and cold stream 1 are processed with specified inlet and outlet temperatures. To generate nodes, this alternative is copied for every temperature alternative of hot streams 1 and 3 and cold stream 2. Then, the array which defines a node becomes: $(T_2^{h(in)}, T_2^{h(out)}, T_1^{c(in)}, T_1^{c(out)}, T_1^{h(in)} = T_1^{h(out)}, T_3^{h(in)} = T_3^{h(out)}, T_2^{c(in)} = T_2^{c(out)}) \in N$.

v, w are indices for nodes where $v = w = \{1, ..., |N|\} = \{1, ..., V\}$.

	Inlet temperatures of hot streams					Outlet temperatures of hot streams						Inlet temperatures of cold streams					Outlet temperatures of cold streams					Node v
Hot	$T_1^{h(in)}$	…	$T_i^{h(in)}$	…	$T_I^{h(in)}$	$T_1^{h(out)}$	…	$T_i^{h(out)}$	…	$T_I^{h(out)}$	Cold	$T_1^{c(in)}$	…	$T_j^{c(in)}$	…	$T_J^{c(in)}$	$T_1^{c(out)}$	…	$T_j^{c(out)}$	…	$T_J^{c(out)}$	
i											j											

a. Hot i and cold j streams are processed in a node (i.e., a HE). Highlighted columns are inlet and outlet temperatures of these streams.

	Inlet temperatures of hot streams				Outlet temperatures of hot streams					Inlet temperatures of cold streams			Outlet temperatures of cold streams			Node v=87
Hot	$T_1^{h(in)}$	$T_2^{h(in)}$	$T_3^{h(in)}$	$T_4^{h(in)}$	$T_1^{h(out)}$	$T_2^{h(out)}$	$T_3^{h(out)}$	$T_4^{h(out)}$	Cold	$T_1^{c(in)}$	$T_2^{c(in)}$	$T_3^{c(in)}$	$T_1^{c(out)}$	$T_2^{c(out)}$	$T_3^{c(out)}$	
2	100°C	250°C	398°C	156°C	100°C	175°C	398°C	156°C	3	30°C	16°C	52°C	30°C	16°C	125°C	

b. An example of a node . Hot stream 2 and cold stream 3 are processed in the HE (in node 87). Hot streams 1, 3, 4 and cold streams 1, 2 are unprocessed streams.

Figure 3.4: Representation of a node

C. Arc Generation

The temperature information for all processed and unprocessed streams are kept in a node in set N. In our HE alternative network, node v is connected to node w if the outlet temperatures of all streams in v is equal to the inlet temperatures of all streams in w. Besides, v is connected to the dummy node *V+1* (called start) and the dummy node *V+2* (called end). The arc from *V+1* to v contains utility heat exchangers for the streams that are not at their system inlet temperatures. Similarly, the arc from v to *V+2* contains utility heat exchangers for the streams that are not reached their target temperatures. The sets defining these connections are N_v^+ and N_v^-, where N_v^+ is a set of nodes immediately connected to node v plus $V+1$ and N_v^- is a set of nodes immediately connected from node v plus $V+2$.

For example, let us consider Figure 3.3. For node 7, we have $N_7^+ = \{\text{Start}, 6, 10\}$ and $N_7^- = \{\text{End}, 3, 5\}$.

The costs associated with the arc (v, w) are indicated by $cost_{v,w}$ and calculated as follows. Recall the previous example with three hot and two cold streams. If two hot streams and one cold stream of v are at their target temperatures, then it needs two utility HEs, hot and cold utilities to make the connection to the end node $V + 2$. The cost of arc $(v, V + 2)$ is the total of utility usage cost and cost of installed HEs for utility. If only one cold stream is not at its system inlet temperature and the other streams of v are at their corresponding temperatures, then the cost associated with arc $(V + 1, v)$ is the total cost of installation of HE (of node v), one utility HE, and utility usage. The cost of connecting v to w, i.e., (v, w) is the cost of installation of HE in w. Figure 3.5 shows the arcs and their associated costs.

For the calculation of utilities and costs, we introduce the following additional notation:

$CU_{V+1,v,i}$:	amount of cold utility for hot stream i of node v from the start node $V + 1$ in Watt
$CU_{v,V+2,i}$:	amount of cold utility for hot stream i of node v to the end node $V + 2$ in Watt
$HU_{V+1,v,j}$:	amount of hot utility for cold stream j of node v from the start node $V + 1$ in Watt
$HU_{v,V+2,j}$:	amount of hot utility for cold stream j of node v to the end node $V + 2$ in Watt
$ACU_{V+1,v,i}$:	area of cold utility HE for hot stream i of node v from the start node $V + 1$

in meter square

$ACU_{v,V+2,i}$: area of cold utility HE for hot stream i of node v to the end node $V+2$ in meter square

$AHU_{V+1,v,j}$: area of hot utility HE for cold stream j of node v from the start node $V+1$ in meter square

$AHU_{v,V+2,j}$: area of hot utility HE for cold stream j of node to the end node $V+2$ v in meter square

U^{cu} : overall heat transfer coefficient for cold utility HEs in Watt per meter Kelvin

U^{hu} : overall heat transfer coefficient for hot utility HEs in Watt per meter Kelvin

The heat balances are provided by using Equations (3.69) and (3.70). The phase change enthalpies should be added to the equation if a phase change occurs in the HE at node v. Equation (3.53) gives the heat exchange area of HEs for utilities. The logarithmic mean temperature difference is calculated by using Equation (3.11).

For the arc $(V+1, v)$ from the start dummy node to v we have:

$$CU_{V+1,v,i}=m_i^h \cdot Cp_i^h \cdot (T_i^{h(system)} - T_{i,v}^{h(in)}) + phase_{i,v}^h \cdot \Delta H_i^{cond} \tag{3.73}$$

$$HU_{V+1,v,j}=m_j^c \cdot Cp_j^c \cdot (T_{j,v}^{c(in)} - T_j^{c(system)}) + phase_{j,v}^c \cdot \Delta H_j^{vap} \tag{3.74}$$

$$ACU_{V+1,v,i}=\frac{CU_{V+1,v,i}}{U^{cu} \cdot Tlm} \tag{3.75}$$

$$AHU_{V+1,v,j}=\frac{HU_{V+1,v,j}}{U^{hu} \cdot Tlm} \tag{3.76}$$

For the arc $(v, V+2)$ from v to the end dummy node we have:

$$CU_{v,V+2,i}=m_i^h \cdot Cp_i^h \cdot (T_{i,v}^{h(out)} - T_i^{h(target)}) + phase_{i,v}^h \cdot \Delta H_i^{cond} \tag{3.77}$$

$$HU_{v,V+2,j}=m_j^c \cdot Cp_j^c \cdot (T_j^{c(target)} - T_{j,v}^{c(out)}) + phase_{j,v}^c \cdot \Delta H_j^{vap} \tag{3.78}$$

$$ACU_{v,V+2,i}=\frac{CU_{v,V+2,i}}{U^{cu} \cdot Tlm} \tag{3.79}$$

$$AHU_{v,V+2,j}=\frac{HU_{v,V+2,j}}{U^{hu} \cdot Tlm} \tag{3.80}$$

$$\tag{3.81}$$

Let CHU and CCU be unit costs of hot and cold utilities in \$/W.year, respectively, A_v^N be the area of v in meter square, and $f_{capital}$ be the cost function of investment of HEs dependent on

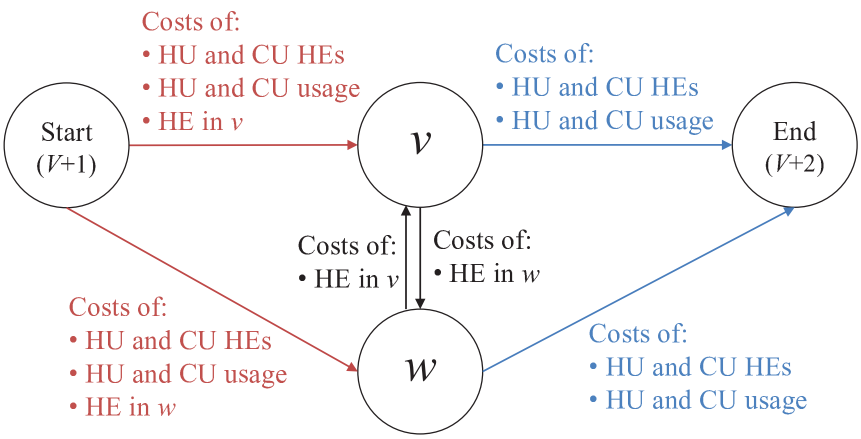


Figure 3.5: Costs on arcs

the HE area where $f_{capital}$ is generally given in the following form, $f_{capital} = \overline{a} + \overline{b}\, Area^{\overline{c}}$ where $\overline{a}$, $\overline{b}$, and $\overline{c}$ are constants. The cost associated with the arc (v, w) can be defined as follows:

$$cost_{v,w} = \begin{cases} f_{capital}(A_w^N), & \text{if } v \neq V+1 \text{ or } V+2 \\ f_{capital}(A_w^N) + \sum_{\forall i} f_{capital}(ACU_{V+1,w,i}) + \sum_{\forall j} f_{capital}(AHU_{V+1,w,j}) & \\ \qquad +CCU \cdot \sum_{\forall i} CU_{V+1,w,i} + CHU \cdot \sum_{\forall i} HU_{V+1,w,j}, & \text{if } v = V+1 \\ \sum_{\forall i} f_{capital}(ACU_{v,V+2,i}) + \sum_{\forall j} f_{capital}(AHU_{v,V+2,j}) & \\ \qquad +CCU \cdot \sum_{\forall i} CU_{v,V+2,i} + CHU \cdot \sum_{\forall i} HU_{v,V+2,j}, & \text{if } w = V+2 \end{cases} \tag{3.82}$$

D. The Shortest Path Model

A network *GRAPH* is generated with the nodes in set N plus two dummy nodes, $V+1$ and $V+2$, and the arcs with their associated costs.

Defining $x_{v,w}$ as:

$$x_{v,w} = \begin{cases} 1, & \text{if arc } (v, w) \text{ is on the path,} \\ 0, & \text{otherwise,} \end{cases} \tag{3.83}$$

the shortest path representation of the heat exchanger network synthesis problem is given below:

$$\text{Min} \sum_{v=1}^{V+2} \sum_{w=1}^{V+2} cost_{v,w} x_{v,w} \tag{3.84}$$

$$\text{s.to}$$

$$\sum_{w=1}^{|N_{V+1}^-|} x_{V+1,w} - \sum_{p=1}^{|N_{V+1}^+|} x_{p,V+1} = 1 \tag{3.85}$$

$$\sum_{w=1}^{|N_v^-|} x_{v,w} - \sum_{p=1}^{|N_v^+|} x_{p,v} = 0 \qquad \forall v = \{1, ..., V\} \tag{3.86}$$

$$\sum_{w=1}^{|N_{V+2}^-|} x_{V+2,w} - \sum_{p=1}^{|N_{V+2}^+|} x_{p,V+2} = -1 \tag{3.87}$$

$$x_{v,w} \in \{0, 1\} \qquad \forall v, w = \{1, ..., V, V+1, V+2\} \tag{3.88}$$

Constraints (3.85), (3.86) and (3.87) are flow conservation constraints where a single unit flow is sent through the nodes on the network from node $V + 1$ to node $V + 2$ on $GRAPH$. In all nodes except start and end dummy nodes, the sum of incoming flows should be equal to the sum of outgoing flows so that the flow is balanced through the network.

The shortest path obtained from the solution of the model is the optimal HEN configuration with detailed equipment design of HEs on the network.

CHAPTER 4

SOLUTION APPROACH

In this chapter, we present our solution approach to the heat exchanger network synthesis (HENS) problem with detailed heat exchanger (HE) design and our computational results. In solution approach, the aim is to explore a large set of possible HEN structures and select the minimum-cost configuration among them. For this purpose, we create HE alternatives that cover all possible pairings of hot and cold streams and place them in a network. As defined in Chapter 3, a HEN alternative network is generated by representing every HE as a node. Every path in the alternative network corresponds to a HEN configuration alternative.

In the second part, computational results obtained by solving the test instances in the literature are presented. 13 different test instances are solved for testing the suggested solution approach.

4.1 Solution Approach

Our solution approach can be represented as an algorithm, which mainly consists of two steps. First, a network of alternatives is created, then, the shortest path is found on this network. The algorithm is summarized shortly in Figure 4.1.

In Steps 1 and 2, while determining the inlet and outlet temperatures of the streams for each HE, we discretize the temperatures of the streams and consider HE designs where the temperatures are selected from this set of discrete temperature levels. Discretization is achieved by dividing the temperature range between the initial and target temperatures of a stream into β equal parts, with α degrees in between. Of course, not all these alternatives turn out to correspond to physically feasible HE designs; therefore, an elimination is made in Step 2.2 by

A. Generating network of alternative heat exchanger networks	
Step 1	Discretization of stream inlet and outlet temperatures
Step 2	Construction of HE alternatives
Step 2.1	Selecting stream pairs and temperatures for each HE
Step 2.2	Elimination of HEs with infeasible stream inlet and outlet temperature pairings
Step 2.3	Conducting detailed HE design for the remaining feasible HEs, using mathematical modeling
Step 3	Developing the alternative network
Step 3.1	Generation of nodes by HE copying, allowing to keep track of the inlet and outlet temperatures of all streams
Step 3.2	Connecting nodes on the network (creating arcs)
Step 3.3	Placing utilities and calculating costs of arcs
B. Solving shortest path problem on the generated network	

Figure 4.1: Main Steps of the HEN Synthesis Algorithm

checking inlet and outlet temperature feasibilities for each HE. Then, in Step 2.3, a detailed design model is solved with the objective of area minimization for every remaining feasible HE.

In Step 3, the alternatives are arranged into the form of a network, where each node corresponds to a HE alternative. Here, note that two nodes might correspond to the exact same HE, however they are multiplied into different nodes in Step 3.1 in order to be able to keep track of the different inlet and outlet temperatures of other streams that do not exchange heat in the HE. In Step 3.2, the nodes are connected to each other by means of arcs, where the outlet temperatures of the streams in the node that the arc originates is equal to the inlet temperatures of the streams in the node that the arc ends. In Step 3.3, the cost of each arc is calculated, where the cost has three components: cost of the corresponding HE, cost of the corresponding utility HEs (if needed), and cost of the utilities (again, if needed). Finally, the shortest path problem is solved on the generated network; finding the minimum-cost solution and the corresponding HEN alternative with detailed HE design.

Every step is explained in detail throughout this chapter. For a better understanding, an illustrative example is used. The problem in the example is extracted from the preliminary design of a dimethylether (DME) production process which is given by Turton et al. (2012). Detailed solution with every step of the algorithm are given in Appendix C.

Illustrative Example:

This example is developed from the preliminary design of a dimethylether (DME) production process. For the sake of simplicity, we do not consider all streams in the process, rather, just take 1 cold and 2 hot streams into consideration. There is no phase change in the selected streams. Here, note that the streams H1 and C1 are actually different stages of the same flow; where C1 enters a reactor and its composition is changed, becoming H1. The objective is to find a HEN configuration with a minimum annual cost for the given set of hot and cold streams. The problem inputs, i.e., system inlet and target temperatures, pressures, and compositions of hot and cold streams, are given in Table 4.1. Also, temperatures and unit costs of hot and cold utilities, overall heat transfer coefficients for utility HEs, and cost functions for HEs are specified.

Table 4.1: Data of Example

	System Inlet (°C)	Target (°C)	Pressure (bar)	Component molar flow (kmol/h)		
				DME	Water	Methanol
H1	364	100	13.9	130.5	132.9	64.9
H2	167	50	7.6	0.0	131.6	0.7
C1	154	250	15.2	1.5	3.8	323.0
HU*	254	234	42	-	-	-
CU**	30	40	5	-	-	-

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for utility HEs:
U = 1140 W/m^2.K if HE is a reboiler,
U = 850 W/m^2.K if HE is a condenser or water to liquid heat transfer occurs in the HE,
U = 60 W/m^2.K if liquid to gas heat transfer occurs in the HE,
U = 30 W/m^2.K if gas to gas heat transfer occurs in the HE.
Cost of heaters: $Cost = 1200 + 60A^{0.6}$ where A is heat exchange area in m^2.
Cost of coolers and process HEs: $Cost = 1000 + 60A^{0.6}$ where A is heat exchange area in m^2.
Cost of hot utility: 60 $/kW.yr
Cost of cold utility: 6 $/kW.yr

A. Generating network of alternative heat exchanger networks

Our aim is to represent the HENS problem in a network structure so that the problem is reduced to a shortest path problem. The shortest path on that network gives us the optimal HEN configuration with detailed equipment design. Nodes on the alternative network represents alternative HE designs, thus every path on network corresponds to a candidate HEN configuration. Accordingly, generation of these alternatives is a major part of our solution approach. How temperatures are discretized, how HE alternatives are created by checking the thermal feasibility conditions, and how the alternative network is formed are presented in the following steps.

Step 1: Discretization of stream inlet and outlet temperatures

As explained before, we select the stream inlet and outlet temperatures from a set of discrete alternatives we construct. An alternative approach would be treating the temperatures as continuous variables and solving HENS as one large nonlinear model (see Mizutani et al. (2003b) for an example of this approach). Instead, we restrict ourselves into a fairly accurate set of temperature levels and explore all alternatives that correspond to these levels, finding the best solution among them.

This step is very important for us, as it determines the accuracy level of our model. The accuracy level increases as the number of temperature alternatives we create for each stream increases. However, this also results in a rapid increase of solution time and space. Therefore, it is a fine balance to determine the level of accuracy in the discretization versus the solution time and space needed. We use parameters α and β to determine this accuracy level.

We choose β temperature levels that are equally spaced from each other with a temperature difference of α degrees, in the interval $\left[T_i^{h(target)}, T_i^{h(system)}\right]$ for hot streams, and $\left[T_j^{c(system)}, T_j^{c(target)}\right]$ for cold streams. The relation between these parameters is given in Equations 4.1 and 4.2.

$$\alpha_i^h \cdot \beta_i^h = \left|T_i^{h(target)} - T_i^{h(system)}\right| \tag{4.1}$$

$$\alpha_j^c \cdot \beta_j^c = \left|T_j^{c(target)} - T_j^{c(system)}\right| \tag{4.2}$$

where:

α_i^h : temperature difference at each step for hot stream i

α_j^c : temperature difference at each step for cold stream j

β_i^h : number of steps needed to reach target temperature for hot stream i

β_j^c : number of steps needed to reach target temperature for cold stream j

Let us consider the stream C1 in the example. The difference between its system inlet and target temperatures, $\left|T_j^{c(target)} - T_j^{c(system)}\right|$, is 205°C. If β_1^c is set to 10 steps, then α_1^c is 20.5°C. Similarly, α_1^c becomes 5°C when β_1^c is set to 41 steps.

During this study, we identified two different discretization methods: *T-discretization* and *Q-discretization*. T-discretization method is based on setting the temperature difference α, which is equal to an (almost) constant value for all streams. On the other hand, Q-discretization aims to specify a different α for each stream so that the amount of heat transfer is equal at each step of different streams. Our initial approach was to use T-discretization. However, we identified several major drawbacks regarding this method. For a physically feasible HE design, according to the first law of thermodynamics, the amount of heat released from a hot stream should be equal to the amount of heat absorbed by a cold stream. In T-discretization, the temperature levels that are explored do not necessarily correspond to equal heat loads. One can introduce a tolerance level in order to determine which differences are acceptable and which are not. Tight levels of tolerance result in the elimination of numerous HE alternatives, whereas loose levels of tolerance decrease the accuracy of the model. To overcome this, one needs to decrease α (i.e., increase β) in order to increase the number of alternatives that satisfy the tolerance level. This means increasing solution time and space, although we know in advance that most of the alternatives we are going to explore will actually turn out to be infeasible.

Due to the reasons stated above, Q-discretization method is used throughout this study. This approach ensures that all created alternatives are feasible with respect to the heat balance constraint. Let us consider an example from Yee and Grossmann (1990) which is shown in Table 4.2. The system has 2 hot and 2 cold streams. Total heat amounts that are needed for every stream are calculated (shown in Total Q Diff. column).

While determining the relevant α and β levels, the main purpose is to find the close ΔQ values for every stream so that the accuracy level of the solution is similar for all streams and for every HE, where β is an integer value. We take the ΔQ of the stream that has the biggest heat load difference as our reference point and arrange the other streams' ΔQ values accordingly. Let ΔQ^{max} be our reference point. It is seen from Table 4.2 that C2 has the biggest difference of heat loads. Suppose that β_2^c is decided to be 16 steps which makes ΔQ_2^c and accordingly $\Delta Q^{max} = 150$ kW.

The other streams' β values are then adjusted so that the difference between their ΔQ and the reference point, ΔQ^{max}, is minimum. This is achieved by dividing the total heat load difference of the related stream by ΔQ^{max} and rounding it to the nearest integer. For example, for determining β_1^c of C1, we divide $m_1^c \cdot Cp_1^c \cdot \left| T_1^{c(target)} - T_1^{c(system)} \right| = 2300$ by $\Delta Q^{max} = 150$, which results in a value of 15.333. We then round this value to the nearest integer, setting $\beta_1^c = 15$. The same calculation is repeated for all remaining streams, namely H1 and H2. It is resulted to set β_1^h and β_2^h to 22 and 12 steps, respectively. The ΔQ values for H1 and H2 are equal to that of C2, 150 kW, as it is desired whereas ΔQ of C1 becomes 153.33 kW. Correspondingly, by using the Equation 4.3, the α_1^h, α_2^h, α_1^c, and α_2^c are 5°C, 10°C, 7.67°C, and 3.75°C, respectively.

$$\alpha = \frac{\Delta Q}{m \cdot Cp} = \frac{\Delta Q}{Fcp} \tag{4.3}$$

What we see here is that even if we try to equate heat load differences (ΔQ) for each stream, we may not achieve a desirable discretization for every system of streams. The ideal condition is to set the Q differences (ΔQ) to the greatest common divisor of the total heat loads of each stream. By this way, heat balances are perfectly established for every stream and in every HE alternative. However, if doing this results in large number of steps, due to technical limitations (solution time and space), the model can not be solved. Consequently, the number of steps for each stream should be arranged by taking this trade-off into account. For every pair of hot and cold streams (i.e., alternative HE), we define a design error scale, γ. Recall the example explained above. Every step for C1 corresponds to 153.33 kW where other streams' steps are 150 kW. For a HE alternative of H1 and C1 with one step change, the design error will be $\gamma = (153.33 - 150)/150 = 2.22\%$.

These heat load differences are tolerated within the algorithm while doing the individual design for every HE. The temperature differences that occur due to heat load differences are reflected to the outlet temperatures of the related stream for the calculations of individual HE. Let these temperature differences be λ_i^h and λ_j^c and recall the equations (3.69) and (3.70) for heat load calculations of the hot and cold streams, respectively. The temperature differences are calculated as follows:

$$\lambda = \begin{cases} \lambda_i^h = \frac{Q_j^c - Q_i^h}{m_i^h \cdot Cp_i^h}, \lambda_j^c = 0, & \text{if } Q_i^h < Q_j^c, \\ \lambda_j^c = \frac{Q_i^h - Q_j^c}{m_j^c \cdot Cp_j^c}, \lambda_i^h = 0, & \text{if } Q_i^h > Q_j^c, \\ \lambda_i^h = \lambda_j^c = 0, & \text{if } Q_i^h = Q_j^c. \end{cases} \tag{4.4}$$

Back to discretization, Table 4.3 shows the discretization results of the illustrative example.

System inlet and target temperatures, differences between them and Q differences, ΔQ, α, and β values and the differences between ΔQ and ΔQ^{max} are stated for each stream. To make the size of the illustrative example small, we divide the stream H1 into 9 steps where every step corresponds to 168.059 kW of heat transfer. The other streams' values are decided accordingly.

By discretization, we actually define a scale for our problem, which makes us able to represent a stream's distance from its target temperature without the need for stating the corresponding temperature levels. Taking the target temperature as level 0, the number of steps, β, represent the distance from the target temperature of a stream at its inlet temperature. Therefore, a stream needs to take β steps to reach its target temperature. For example, H2 stream can reach its target temperature with 2 steps. Its temperature change per step is 58.5°C, so it will reach to 167°C - (1)58.5°C = 108.5°C after taking one step. Similarly, if stream C1 is 2 steps away from its target temperature, then its current temperature can be calculated as 250°C - (2)32°C = 186°C. Scales for every stream of the example are given in Figure 4.2.

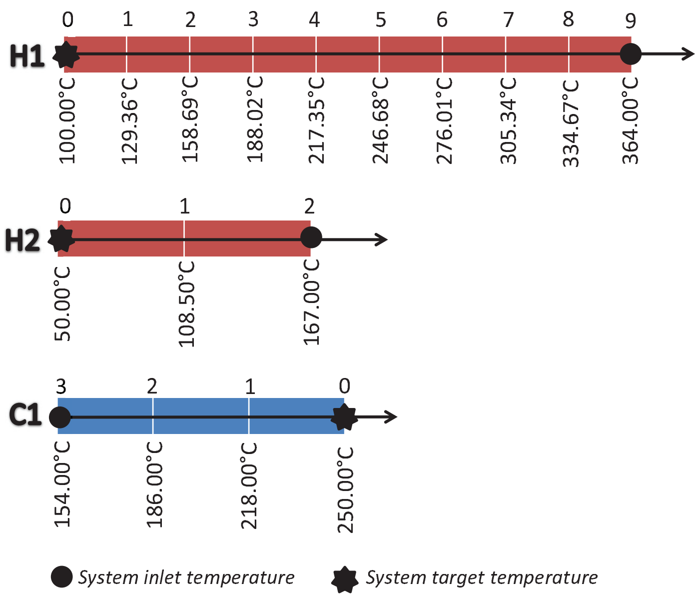


Figure 4.2: Scaling of the illustrative example

Suppose that H1 and C1 are processed in a HE. H1's inlet and outlet temperatures are 276.01°C

Table 4.2: Q-discretization example - Example-1 of Yee and Grossmann (1990)

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/°C)	Total T Diff. (°C)	Total Q Diff. (kW)	ΔQ (kW)	α (°C)	β	ΔQ - ΔQ^{max} (kW)
H1	170	60	30	110	3300	150	5	22	0
H2	150	30	15	120	1800	150	10	12	0
C1	20	135	20	115	2300	153.33	7.67	15	3.33
C2	80	140	40	60	2400	150	3.75	16	0

Table 4.3: The discretized inputs of the model for the illustrative example

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/°C)	Total T Diff. (°C)	Total Q Diff. (kW)	ΔQ (kW)	α (°C)	β	ΔQ - ΔQ^{max} (kW)
H1	364	100	5.729	264	1512.535	168.059	29.33	9	0.000
H2	167	50	2.818	117	329.659	164.830	58.50	2	-3.230
C1	154	250	5.191	96	498.336	166.112	32.00	3	-1.947

(level 6) and 217.35°C (level 4); whereas C1 enters to the HE at 154°C (level 3) and leaves at 218°C (level 1). The temperature changes can then be represented as 6-4 for H1 and 3-1 for C1. Throughout this chapter, for simplicity, the temperatures are stated using this kind of scale.

Step 2: Construction of HE alternatives

Each heat exchanger processes one hot stream and one cold stream. Accordingly, a HE can be represented by the two processed streams and their inlet and outlet temperatures. Thus, to create HE alternatives, we pair hot and cold streams and determine their inlet and outlet temperatures from their corresponding set of discretized temperatures.

Step 2.1: Selecting stream pairs and temperatures for each HE

In our algorithm, every hot stream is paired with every cold stream in the problem to create all possible HE alternatives. The discretized temperatures from Step 1 are used to assign inlet and outlet temperatures of every stream pair for generating HEs. While assigning the temperatures, the differences of inlet and outlet streams should be considered. In a HE, outlet temperature should be higher than inlet temperature for a cold stream; whereas the contrary is true for a hot stream. Since our scale automatically satisfies this condition, temperature levels should be decreased through an HE for both streams. Another important part is that, since in every step all streams exchange the same amount of energy, the energy balance within the HE is also obtained. Thus, in a HE, a cold stream and a hot stream should change the same number of steps. Accordingly, our scaling satisfies heat balance condition in advance, too.

Let us consider the streams of the illustrative example. Their alternative inlet and outlet temperature combinations are:

H1 : 9-8, 9-7, 9-6, 9-5, 9-4, 9-3, 9-2, 9-1, 9-0, 8-8, 8-7, 8-6, 8-5, 8-4, 8-3, 8-2, 8-1, 8-0, 7-6, 7-5, 7-4, 7-3, 7-2, 7-1, 7-0, 6-5, 6-4, 6-3, 6-2, 6-1, 6-0, 5-4, 5-3, 5-2, 5-1, 5-0, 4-3, 4-2, 4-1, 4-0, 3-2, 3-1, 3-0, 2-1, 2-0, 1-0,

H2 : 2-1, 2-0, 1-0,

C1 : 3-2, 3-1, 3-0, 2-1, 2-0, 1-0.

It is seen that 44 alternatives for H1 stream, 3 alternatives for H2 stream, and 6 alternatives for inlet-outlet temperature combinations are available. Since there are one cold and two hot streams in the example, two different stream pairs exist for HE alternatives, which are H1-C1 and H2-C1. As stated above, the number of step changes should be the same for both streams in a HE, so that the heat balance is satisfied. Depending on this, let us calculate the number of candidate HE alternatives for H1-C1 pair. H1 has 9 steps and C1 has 3 steps. Thus, the maximum number of step change that can occur in a H1-C1 pair is 3 steps. There can be 3, 2 or 1 step changes. If there is 2 step change, for C1 there are 2 alternatives (i.e., 3-1 and 2-0) and for H1 there are 8 alternatives (i.e., 9-7, 8-6, 7-5, 6-4, 5-3, 4-2, 3-1, and 2-0). As a result, there can be $2 \times 8 = 16$ alternatives for a 2-step change H1-C1 HE alternative. Calculating in the same manner, there are $(1 \times 7) + (2 \times 8) + (3 \times 9) = 50$ unique HE alternatives for the H1-C1 pair and $(1 \times 3) = 3$ unique HE alternatives for the H2-C1 pair. The total number of unique HE alternatives is 53 for the given example. Some of the HE alternatives are:

H1: 9-6 & C1: 3-0,
H1: 3-2 & C1: 2-1,
H1: 7-5 & C1: 3-1,
H2: 2-1 & C1: 2-1,
H2: 2-0 & C1: 3-1,
H2: 1-0 & C1: 1-0, etc.

Recall β_i^h and β_j^c, which are the number of steps needed to reach target temperature for hot stream i and cold stream j, respectively. The total number of unique HE alternatives, *Unique*, are given by Equation (4.5).

$$Unique = \sum_{\forall i} \sum_{\forall j} \sum_{z=1}^{\min\left(\beta_i^h, \beta_j^c\right)} z \cdot \left(z + \max\left(\beta_i^h, \beta_j^c\right) - \min\left(\beta_i^h, \beta_j^c\right)\right) \tag{4.5}$$

Note that, if phase change occurs, Equation 4.5 cannot be used for finding an upper bound of number of unique HE alternatives. Because in this equation only equal number of step changes for hot and cold streams IS considered. When phase change occurs, depending on which stream is in transition, step change of a stream should be greater than that of other stream in the HE. For example, if a cold stream changes phase from liquid to vapor and its temperature change is 3 steps, then the corresponding hot stream's temperature change should be greater than 3. Let us say it is 5, then the difference of 2 step changes corresponds to the heat of vaporization of the cold stream.

Step 2.2: Elimination of HEs with infeasible stream inlet and outlet temperature pairings

For an HE alternative to be valid, the inlet and outlet temperatures of streams should hold two conditions:

1. Inlet temperature of hot stream should be higher than the outlet temperature, where the opposite is true for cold stream. This condition is satisfied while pairing the streams and the corresponding temperatures in Step 2.1. Therefore, this condition is automatically satisfied by the time we reach this step.

2. In a countercurrent HE, the inlet temperature of hot stream should be higher than the outlet temperature of cold stream, and the outlet temperature of hot stream should be higher than the inlet temperature of cold stream (Recall Figure 3.2).

Recall that we introduce the temperature differences due to heat load differences in step changes, λ, in Step 1, then, the outlet temperatures are recalculated based on the greater overall heat load, in order to obtain more accurate results in the detailed HE design step. With the introduction of λ, the inlet and outlet temperatures become:

$$\widehat{T}_i^{h(in)} = T^{h(target)_i} + \beta_i^{h(in)} \cdot \alpha_i^h \tag{4.6}$$

$$\widehat{T}_i^{h(out)} = T^{h(target)_i} + \beta_i^{h(out)} \cdot \alpha_i^h - \lambda_i^h \tag{4.7}$$

$$\widehat{T}_j^{c(in)} = T^{c(target)_j} - \beta_j^{c(in)} \cdot \alpha_j^c \tag{4.8}$$

$$\widehat{T}_j^{c(out)} = T^{c(target)_j} - \beta_j^{c(out)} \cdot \alpha_j^c + \lambda_j^c \tag{4.9}$$

where β's are the inlet and outlet step temperatures for streams i and j which are determined in Step 2.1.

Accordingly, if $\widehat{T}_i^{h(in)} > \widehat{T}_j^{c(out)}$ and $\widehat{T}_i^{h(out)} > \widehat{T}_j^{c(in)}$, the HE alternative is feasible.

Step 2.3: Conducting detailed HE design for the remaining feasible HEs, using mathematical modeling

After Steps 1 and 2.2 are concluded, we are left with physically feasible HE alternatives. In this step, we solve the model CM (given in Section 3.1) for every HE alternative, in order to obtain the detailed mechanical design for each HE. This model selects the appropriate design configuration among approximately 17000 design standards. These standards are obtained from the tubing characteristics and tube-hole count tables given in Perry and Chilton (1973). Model is solved by using the GAMS/BARON solver.

The objective of the model is to minimize the total HE area. In industry applications, design of HEs that have an area smaller than 10 m^2 are not favored. Therefore, we select the minimum-area HE that has a total area larger than 10 m^2. However, if we end up having areas smaller than 10 m^2, in sake of not losing generality, we accept that HE too, but we try to select a value that is closest to 10 m^2.

We partition the design standard set into 17, so that each standard set contains 1000 data point. We solve the same MINLP model 17 times, every time with different standard set that we partitioned. The reason behind this is to obtain solutions within a reasonable time. The objective is to find the minimum area. The minimum of the results of 17 models are taken as the design of the HE alternative. As stated above, there is a restriction in industry that design of HE that has an area greater than 10 m^2 is more economical and should be favored. So, the design of a HE alternative is determined by the criteria given in Equation 4.10. The solution returns 0 if all of the models do not return a solution, i.e., the HE alternative is infeasible. We take the lower bound *lower* as 1×10^{-9} and the upper bound *upper* as 1×10^{9} to introduce a bound to the variables in the model.

q: number of data sets of standards for the HE design problem, $q = \{1, ..., 17\}$

$$A_r^R = \begin{cases} \min\,(A_{1r}^R, A_{2r}^R, ..., A_{17r}^R)\text{ , if all } A_{qr}^R \geq 10\text{ m}^2, \\ \max\,(A_{1r}^R, A_{2r}^R, ..., A_{17r}^R)\text{ , if all } A_{qr}^R < 10\text{ m}^2, \\ \min_{A_{qr}^R \geq 10}\,(A_{1r}^R, A_{2r}^R, ..., A_{17r}^R)\text{ , if some of } A_{qr}^R \geq 10\text{ m}^2 \text{ and some of } A_{qr}^R < 10\text{ m}^2, \\ 0\text{ , otherwise.} \end{cases} \tag{4.10}$$

Step 3: Developing the alternative network

After generating a set of HE alternatives in Step 2, in this step, we place HEs in the network. Thus, all possible HEN configurations are represented in the network of alternatives.

Step 3.1: Generation of nodes by HE copying, allowing to keep track of the inlet and outlet temperatures of all streams

The HEs generated in the previous step are represented in the network as nodes. We need to trace every stream's temperature through the network, but in a HE alternative, only two of the streams' temperature information is known since they are processed in that HE. For example, in our example, there are two types of HEs, H1-C1 pairs and H2-C1 pairs. Assume that in the final design of HEN, there are 3 HEs with a sequence of H2-C1, H1-C1, and again H2-C1. To be able to know the temperature of H2 at second HE, we need to keep that information in that node. Otherwise we become unable to connect these nodes with each other. Therefore, in a node, all streams' temperature information should be kept (see Figure 3.4). In the node, the streams that go under a heat exchange process are called processed streams where the other streams are called unprocessed streams. The inlet and outlet temperatures should be equal to each other for unprocessed streams.

To generate nodes, the unique HEs that are created before are copied for every discretized temperature of every unprocessed stream. In other words, for combination of temperature alternatives for unprocessed streams, we generate a node for the same HE. For example, let us consider the feasible HE alternative of H1: 9-4 C1: 5-0. Three copies of this HE are created due to the temperatures of unprocessed stream H2. The multiplied nodes are:

- Node 37: H1: 7-5 C1: 2-0 and H2: 1-1,
- Node 38: H1: 7-5 C1: 2-0 and H2: 2-2,
- Node 39: H1: 7-5 C1: 2-0 and H2: 0-0.

Recall that i and j are processed streams whereas i' and j' are unprocessed. The maximum number of nodes without eliminating due to feasibilities is given as follows:

$$\text{max. number of nodes} = \sum_{\forall i,j}\left[unique_{i,j} \prod_{\forall i' \neq i}\left(\beta_i^h + 1\right) \prod_{\forall j' \neq j}\left(\beta_j^c + 1\right)\right] \tag{4.11}$$

$$\text{where, } unique_{i,j} = \sum_{z=1}^{\min\left(\beta_i^h, \beta_j^c\right)} z \cdot \left(z + \max\left(\beta_i^h, \beta_j^c\right) - \min\left(\beta_i^h, \beta_j^c\right)\right)$$

For our example, the maximum number of nodes are 149. With feasibility checks, the number of nodes in the network is 87. Note that the gap between these two values and the number of nodes are even more for a larger system of streams like 3 hot and 3 cold stream systems.

Step 3.2: Connecting nodes on the network (creating arcs)

In this step, the nodes are connected with each other to create a directed alternative network that represents the HEN configuration alternatives as paths. There are two kinds of connections in the network: dummy node connections and connections between nodes which are explained below.

i) Dummy node connections: We define two dummy nodes in the network, one is called the start node and the other is called the end node. Every node v should be connected to the start and end dummy nodes. Utility HEs are placed between node v and the dummy nodes for every stream if needed.

ii) Connections between nodes (Forming network): For all nodes which are not equal to each other (i.e., $v \neq w$), node v and node w should be connected if outlet temperatures of all streams of node v are equal to the inlet temperatures of all streams of node w.

Considering our example,

- Node 23: H1: 6-5 C1: 2-1 and H2: 2-2,
- Node 41: H1: 7-6 C1: 2-1 and H2: 2-2,
- Node 50: H1: 7-6 C1: 3-2 and H2: 2-2,
- Node 57: H1: 8-6 C1: 2-0 and H2: 0-0,
- Node 68: H1: 8-7 C1: 3-2 and H2: 2-2,
- Node 87: H1: 9-8 C1: 3-2 and H2: 0-0.

Since the condition of equality of temperatures holds, arcs (68,41), (87,57), and (50,23) are created.

The whole network of the illustrative example is shown in Figure 4.3. As we see, it is a directed network with a start (Node 88) and an end (Node 89) node. For a better visualization, all connections cannot be shown in the figure, but explained. All nodes are connected to both of the dummy nodes. The large rectangle is the set of displayed nodes and all are only connected to the start and end nodes.

Step 3.3: Placing utilities and calculating costs of arcs

As explained in section 3.2.2, utilities are needed to ensure that every stream enters to the system at their system inlet temperature (i.e., utilities between the start node and node v) and leave the system at their target temperature (i.e., the utilities between node v and the end node). Presence of utilities in the HEN is undesired yet necessary for the overall heat balance of the system. The costs associated with the arcs include annual investment and utility usage costs. In Figure 3.5 costs of the arcs are summarized. The calculations are done as explained in Section 3.2.

B. Solving shortest path problem on the generated network

In the generated alternative network, every path corresponds to a HEN configuration. Solving the shortest path model SM on that network gives us an optimal HEN configuration. Dijkstra's algorithm is used to solve the SM model.

For the illustrative example, the optimal HEN is 88-80-89, as shown in Figure 4.3. The cost of the path is 7539.9 \$/year. H1 and C1 are processed in the HE. Their inlet and outlet temperatures are 364°C to 276.01°C and 154°C to 250°C, respectively. Two utility HEs are placed for stream H1 and for stream H2 at the end of the system. These utility HEs need 221.13 kW and 325.02 kW cold utility and their areas are 26.98 m^2 and 6.61 m^2, for hot stream H1 and H2, respectively. The process HE has an area of 10.322 m^2. Its inner configuration is given as follows:

Inner diameter of tubes	: 0.0141 m	Number of tubes	: 55
Outer diameter of tubes	: 0.0159 m	Number of tube passes	: 1
Tube arrangement	: Square pitch	Number of shell passes	: 1
Pitch length	: 0.0206 m	Shell diameter	: 0.2032 m
TEMA type	: P or S	Length of HE	: 3.7631 m

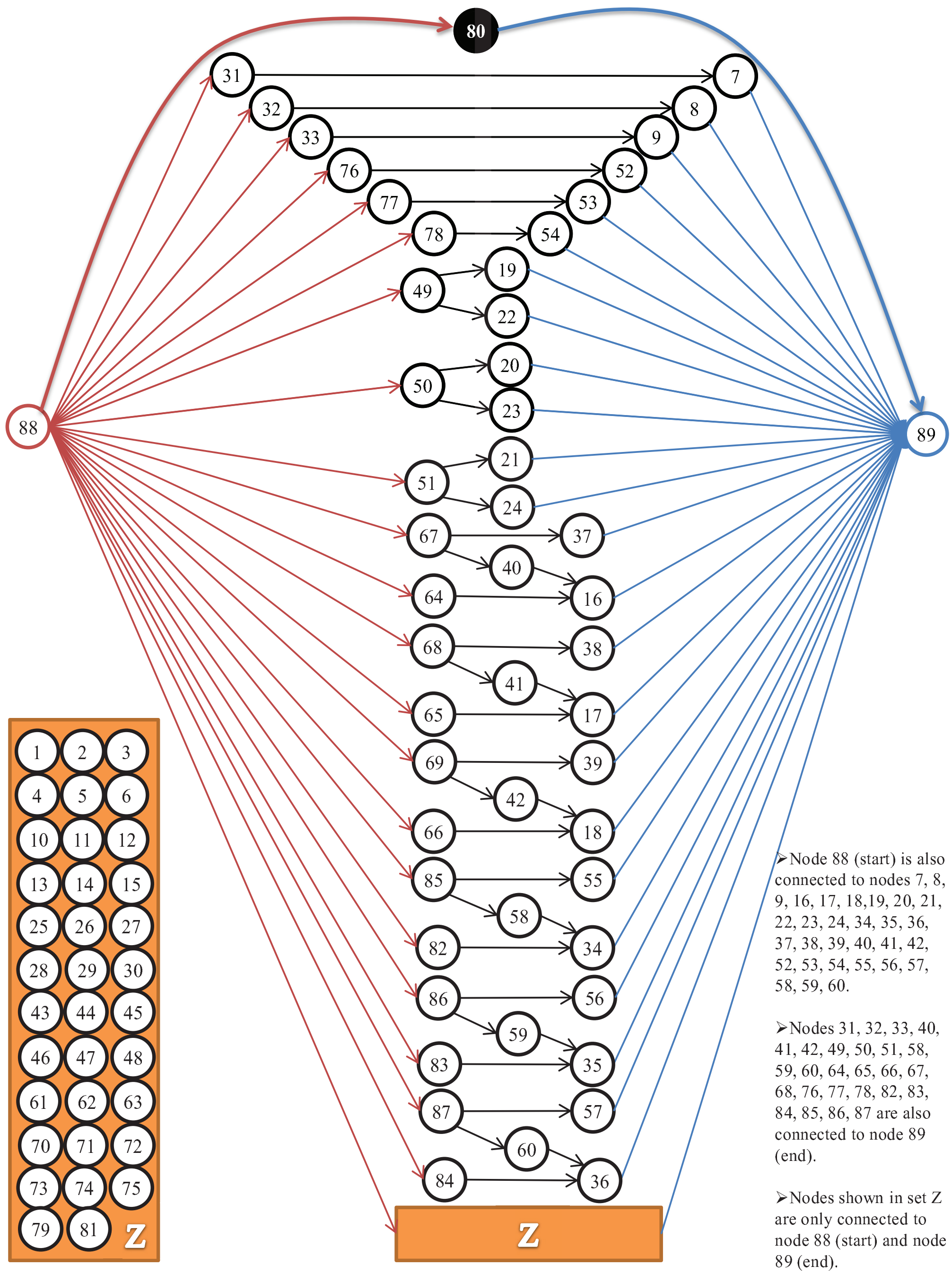


Figure 4.3: Network of the illustrative example

4.2 Results and Discussion

The computer implementation of our solution procedures was developed in MATLAB version 7.12.0.635 (R2011a) 32-bit (win32), in connection with GAMS Build 23.7.3 WIN 27723.27726 VS8 x86/MS Windows. The computations were carried out on two different PC settings: one with 3.50 GB of RAM and Intel® Core™2 Duo CPU processor of 3.00 GHz, another with 6.0 GB of RAM and Intel® Core™i5-2400 CPU processor of 3.10 GHz.

Although there are some test instances that are solved and compared across different studies in the literature, there is no predefined set of test instances widely used. In fact, as it can be seen from Table 4.4, the number of test instances considered in any studies in the literature is quite limited. One might think that the number of test instances are limited due to the complex nature of the problem.

Table 4.4: The number of test instances presented in some recent studies

Reference	Number of test instances
Huang and Chang (2012)	3
Brandt et al. (2011)	2
Laukkanen and Fogelholm (2011)	3
Gupta and Ghosh (2010)	3
Laukkanen et al. (2010)	2
Ponce-Ortega et al. (2010)	4
Allen et al. (2009)	2
Khorasany and Fesanghary (2009)	4
Luo et al. (2009)	4
Ponce-Ortega et al. (2008a)	1
Silva et al. (2008)	1
Yerramsetty and Murty (2008)	5
Ponce-Ortega et al. (2007)	6
Mizutani et al. (2003b)	3
Yee and Grossmann (1990)	5

In our study, the solution approach has been tested on 13 different examples, using 22 different discretization settings in total. The examples are summarized in Table 4.5. As discussed in sections 3.2.2 and 4.1, our solution approach includes detailed design for every HE in the network. However, the number of test instances available in literature that solve for detailed HE designs in a network setting are extremely limited. Therefore, we also tested our approach on problems without detailed design, as well.

Table 4.5: Test instances

Test instance name	Reference	Size	Number of discretization settings	Detailed design	Stream splitting	Multiutility
YG-E1	Yee and Grossmann (1990)	2H2C	2	No	No	No
YG-E2	Yee and Grossmann (1990)	2H2C	2	No	No	No
YG-E3	Yee and Grossmann (1990)	5H1C	2	No	Yes	No
MG-E1	Mizutani et al. (2003b)	2H2C	1	Yes	Yes	No
MG-E2	Mizutani et al. (2003b)	3H3C	1	Yes	Yes	No
4S1	Ponce-Ortega et al. (2007)	2H2C	1	Yes	Yes	No
CH13-E2	Turton et al. (2007)	3H3C	1	No	No	No
PO-E2	Ponce-Ortega et al. (2010)	2H1C	3	No	Yes	Yes
PO-E3	Ponce-Ortega et al. (2010)	2H3C	2	No	Yes	Yes
5SP	Gupta and Ghosh (2010)	3H2C	2	No	Yes	No
HC-E1	Huang and Chang (2012)	2H2C	1	No	Yes	No
HC-E2	Huang and Chang (2012)	1H2C	2	No	Yes	No
HC-E3	Huang and Chang (2012)	1H2C	2	No	Yes	No

The approach we suggest is designed to handle all the physical properties of all streams, namely, specific heats, thermal conductivities, viscosities, and densities at their environment temperature. In order to be able to identify and use all these properties at the substance's related temperature level, the composition of each stream (i.e., molar or mass fractions of substances within the stream) should be known. Unfortunately, the composition of the streams are not provided for the test instances used in the literature. Therefore, we use the average values given for the physical properties. In addition, for the case without detailed design, the overall heat transfer coefficients are also provided for the streams, which is used as an input to the model, rather than a decision variable.

In the following sections, the results obtained from the solution of instances are given and discussed. Problem inputs and details of resulting HEN configurations for each instance are given in Appendix D. Performance measure tables are provided for each instance. Performances are compared by giving percentage improvement values for costs, heat exchanger areas, and heat loads. The formula given in Equation 4.12. From the formula, positive values show that our solution outperformed whereas negative numbered performance measures show that the benchmark solution is better.

$$\text{\% improvement} = 100\times(\text{cost of benchmark soln. - cost of our soln.})/\text{cost of benchmark soln.} \tag{4.12}$$

Every instance has different cost figures (in terms of both capital investment and utility costs), overall heat transfer coefficient calculations (for the instances that do not consider detailed design of every HEs), and utility environments. Therefore, these changes are implemented on every instance to be able to compare the obtained results with literature. More than one experiment are done for some instances in order to find better solutions. Different experiments are developed by changing (decreasing) the heat load differences for each step (ΔQ's).

The results are compared with the study which the instance is taken from and the most recent study in the literature that solves the given instance with the same parameters and cost functions. As it can be observed in the sections below, in most cases these two studies are the same. There are a few number of studies that solve the instances in Yee and Grossmann (1990), especially for instances YG-E1 and YG-E2, all these studies use different cost functions and overall heat transfer coefficients. This prevents us to compare them with our approach. Therefore, the comparisons are only made with Yee and Grossmann (1990) for the instances YG-E1 and YG-E2.

4.2.1 Test instances from Yee and Grossmann (1990)

Three test instances are taken from Yee and Grossmann (1990). The results obtained in these instances are summarized in Tables 4.6, 4.7, and 4.8. In these tables, our results are given combined with the results of Yee and Grossmann (1990). Improvement compared to their results is shown in the comparison column. Different performance measures are compared to be able to understand our solution quality. These are number of process and utility HEs, amount of utility needed, HE areas, and operating, capital, and total annual costs are given. As it can be seen from the tables, we obtain 6.92% better results with respect to the total annual cost in YG-E2, whereas 8.13% and 10.36% worse results in Examples 1 and 3, respectively.

There are two major challenges regarding the test instances taken from Yee and Grossmann (1990): Some of them allow stream splitting and the large gap between the initial and target temperatures of the streams cause greater overall heat load. Stream splitting enlarges the feasible region of the problem. Therefore, better results can be found. However, no stream splitting is allowed in our model due to limiting system requirements in terms of memory and solution time.

In order to be able to find a fine-tuned solution, one needs to decrease the ΔQ level, which results in a rapid increase of the total number of nodes created in the model. It can be clearly seen from Table 4.7, as the heat load difference of a step is decreased better results are obtained. However, one may ask the reason of increase in the total annual cost in Table 4.8. This case may happen if the right heat load cuts (i.e., feasible heat loads for HEs) cannot be found and the model tries to ensure the heat balance by placing more utilities with higher costs, which results in a higher total cost for the HEN. In this case, the number of steps should be increased while decreasing the heat load differences. For YG-E1 and YG-E3, when the number of steps are increased, the better solutions could not be obtained, because the memory limitation has exceeded.

Table 4.6: Results of instance YG-E1 from Yee and Grossmann (1990)

YG-E1	Yee and Grossmann (1990)	Exp. 1 (ΔQ=150)	Exp. 2 (ΔQ=100)	Exp. 1 Comparison	Exp. 2 Comparison
Number of Process HEs	3	3	3	same	same
Number of Utility HEs	1	2	2	+1	+1
Total Process HE Area (m^2)	524.1	371.4	320.7	29.13%	38.80%
Total Utility HE Area (m^2)	38.3	44.0	44.8	-14.86%	-16.86%
Total Utility (kW)	400.0	753.3	800.0	-88.33%	-100.00%
Total Capital Cost ($/yr)	72909.0	63362.0	59489.2	13.09%	18.41%
Utility Operating Cost ($/yr)	8000.0	24267.0	28000.0	-203.34%	-250.00%
Total Annual Cost ($/yr)	80909.0	87629.0	87489.2	-8.31%	-8.13%

Table 4.7: Results of instance YG-E2 from Yee and Grossmann (1990)

YG-E2	Yee and Grossmann (1990)	Exp. 1 (ΔQ=300)	Exp. 2 (ΔQ=150)	Exp. 1 Comparison	Exp. 2 Comparison
Number of Process HEs	3	2	2	-1	-1
Number of Utility HEs	3	3	3	same	same
Total Process HE Area (m^2)	2610.1	1408.5	1409.2	46.03%	46.01%
Total Utility HE Area (m^2)	435.4	914.4	902.2	-110.04%	-107.24%
Total Utility (kW)	1475.0	3200.0	3108.3	-116.95%	-110.73%
Total Capital Cost ($/yr)	715970.0	582730.0	577270.0	18.61%	19.37%
Utility Operating Cost ($/yr)	94000.0	184000.0	176670.0	-95.74%	-87.95%
Total Annual Cost ($/yr)	809970.0	766730.0	753940.0	5.34%	6.92%

Table 4.8: Results of instance YG-E3 from Yee and Grossmann (1990)

YG-E3	Yee and Grossmann (1990)^a	Luo et al. (2009)^b	Exp. 1 (ΔQ=120)	Exp. 2 (ΔQ=100)	Exp. 1 Comparison with *a*	Exp. 2 Comparison with *a*	Exp. 1 Comparison with *b*	Exp. 2 Comparison with *b*
Number of Process HEs	5	6.0	5	5	same	same	-1	-1
Number of Utility HEs	2	2.0	3	4	+1	+2	+1	+2
Total Process HE Area (m^2)	160.4	Not reported	94.6	85.7	41.01%	46.56%	-	-
Total Utility HE Area (m^2)	40.5	Not reported	47.2	47.8	-16.61%	-18.08%	-	-
Total Utility (kW)	3892.8	3658.4	4717.1	4831.0	-21.17%	-24.10%	-28.94%	-32.05%
Total Capital Cost ($/yr)	59780.0	357550.8	51200.2	50250.6	14.35%	15.94%	85.68%	85.95%
Utility Operating Cost ($/yr)	516860.0	214147.2	582392.7	586155.8	-12.68%	-13.41%	-171.96%	-173.72%
Total Annual Cost ($/yr)	576640.0	571698.0	633592.9	636406.4	-9.88%	-10.36%	-10.83%	-11.32%

4.2.2 Test instances from Mizutani et al. (2003b)

These instances are those of the limited instances that consider the HEN problem with detailed design of equipments. The physical and thermal properties of the streams are given as an average value.

For MG-E1, as we see from the Table 4.9, when the results are compared with Mizutani et al. (2003b), the numbers of process and utility HEs are not changed in our solution. The utility requirement is the same as Mizutani et al. (2003b). There is a significant difference in the total area of process HEs. With our approach, it is reduced by 67.24%. The reflection of this reduction is not clear when the total annual cost is considered, because the cost of utility dominates the total annual cost figure. Thus, comparing the total capital costs can be seen more reasonable in this case. We see that the total capital cost is reduced by 10.12% with our approach. A similar result is obtained from the comparison of performance measures by Silva et al. (2008). Here, the improvement in total capital cost is 0.78%.

When the results of MG-E2, which are given in Table 4.10, are considered, it is seen that the total cost is reduced by 71.87% in our approach according to the comparison with Mizutani et al. (2003b). The numbers of both process and utility HEs are reduced as well. The drastic change in the total cost is mainly because the utility usage is reduced by 83.79%. Total process HE area is also decreased, which shows that more effective HEs (i.e., HEs with better temperature profile) are installed. Ponce-Ortega et al. (2007) also decrease the utility usage, but compared to them, a 5.80% better result for the total annual cost is obtained with our approach. It is seen that major difference is in process HE area by 70.88% and it reflects to the total capital cost and accordingly to the total annual cost.

4.2.3 Test instances from Ponce-Ortega et al. (2007)

For the instance 4S1 in Table 4.11, we outperform the solutions obtained by Ponce-Ortega et al. (2007) by 10.51%. The major driver of this improvement is the reduction in the total capital cost by 87.83%. It is seen that even the utility usage is increased, because of the improvement in number process HEs and their corresponding areas, the total annual cost is reduced.

Table 4.9: Results of instance MG-E1 from Mizutani et al. (2003b)

MG-E1	Mizutani et al. (2003b)[a]	Silva et al. (2008)[b]	Exp. 1 (ΔQ=100)	Exp. 1 Comparison with *a*	Exp. 1 Comparison with *b*
Number of Process HEs	2	2	2	same	same
Number of Utility HEs	2	2	2	same	same
Total Process HE Area (m^2)	89.5	100.2	29.3	67.24%	70.73%
Total Utility HE Area (m^2)	21.9	Not reported	21.9	0.00%	-
Total Utility (kW)	1500.0	1500.0	1500.0	0.00%	0.00%
Total Capital Cost ($/yr)	5608.0	5783.2	5040.2	10.12%	12.85%
Utility Operating Cost ($/yr)	90000.0	90000.0	90000.0	0.00%	0.00%
Total Annual Cost ($/yr)	95608.0	95783.2	95040.2	0.59%	0.78%

Table 4.10: Results of instance MG-E2 from Mizutani et al. (2003b)

MG-E2	Mizutani et al. (2003b)[a]	Ponce-Ortega et al. (2007)[b]	Exp. 1 (ΔQ=800)	Exp. 1 Comparison with *a*	Exp. 1 Comparison with *b*
Number of Process HEs	6	5	5	-1	-1
Number of Utility HEs	3	1	1	-2	-2
Total Process HE Area (m^2)	308.8	507.9	147.9	52.10%	70.88%
Total Utility HE Area (m^2)	Not reported	5.6	5.5	-	2.17%
Total Utility (kW)	4626.0	766.7	750.0	83.79%	2.17%
Total Capital Cost ($/yr)	12388.0	10572.5	8288.2	33.09%	21.61%
Utility Operating Cost ($/yr)	173456.0	45999.3	45000.0	74.06%	2.17%
Total Annual Cost ($/yr)	189456.0	56571.8	53288.2	71.87%	5.80%

Table 4.11: Results of instance 4S1 from Ponce-Ortega et al. (2007)

4S1	Ponce-Ortega et al. (2007)	Exp. 1 (ΔQ=300)	Exp. 1 Comparison
Number of Process HEs	5	2	-3
Number of Utility HEs	2	2	same
Total Process HE Area (m^2)	251.2	87.7	65.08%
Total Utility HE Area (m^2)	Not reported	8.7	-
Total Utility (kW)	1130.0	1500.0	-32.74%
Total Capital Cost ($/yr)	453404.0	55163.5	87.83%
Utility Operating Cost ($/yr)	71800.0	105000.0	-46.24%
Total Annual Cost ($/yr)	178971.4	160163.5	10.51%

4.2.4 Test instances from Turton et al. (2007)

The instance CH13-E2 is an example from Turton et al. (2007). This instance is solved by using the pinch analysis method. The comparison results are given in Table 4.12. It is seen that there is a significant decrease in process heat exchange area. Utility usage is slightly higher as compared to the results of Turton et al. (2007). Total annual cost is decreased by 13%.

4.2.5 Test instances from Gupta and Ghosh (2010)

Our results for the instance 5SP are 6.55% worse than those of Gupta and Ghosh (2010)'s. In our solution, we obtain an improvement of 7.74% in terms of capital cost, whereas we use 39.70% more utilities. This shows that the cost function for this instance is far less sensitive to the utility usage. Also, Gupta and Ghosh (2010) use stream splitting, which also explains their better results.

4.2.6 Test instances from Ponce-Ortega et al. (2010)

Two instances from Ponce-Ortega et al. (2010) are solved. The results and comparisons are given in Tables 4.14 and 4.15 for the instances PO-E2 and PO-E3, respectively. In these instances, multiple utilities are available and their associated costs are given. For example, the cost of middle pressure stream is lower than that of high pressure steam. Ponce-Ortega et al. (2010) allow placing utility HEs between process HEs. We change the model to handle multiple utilities, but in our approach, since utilities are unwanted because of environment and cost considerations, utility HEs can only be placed in the beginning and the end of the network. Because of the inlet and outlet temperature constraint (as it is explained in Step 2.2 of the algorithm) our model selects the most expensive utility for both instances. Let us consider that we are using one kind of each utility. The solution Experiment 1 of the instance PO-E2 shows that the utility usages are decreased by 14.72%. As a result, our total annual cost would be lower than that of the results of Ponce-Ortega et al. (2010).

Table 4.12: Results of instance Chapter 13-E2 from Turton et al. (2007)

CH13-E2	Turton et al. (2007)	Exp. 1 (ΔQ=60)	Exp. 1 Comparison
Number of Process HEs	7	5	-2
Number of Utility HEs	2	2	same
Total Process HE Area (m^2)	1063.0	941.7	11.41%
Total Utility HE Area (m^2)	24.7	25.9	-4.96%
Total Utility (kW)	150.0	190.0	-26.67%
Total Capital Cost ($/yr)	17231.0	13899.7	19.33%
Utility Operating Cost ($/yr)	6300.0	6540.0	-3.81%
Total Annual Cost ($/yr)	23531.0	20439.7	13.14%

Table 4.13: Results of instance 5SP from Gupta and Ghosh (2010)

5SP	Gupta and Ghosh (2010)	Exp. 1 (ΔQ=19)	Exp. 2 (ΔQ=12)	Exp. 1 Comparison	Exp. 2 Comparison
Number of Process HEs	3	1	1	-2	-2
Number of Utility HEs	2	4	4	+2	+2
Total Process HE Area (m^2)	Not reported	57.8	59.8	-	-
Total Utility HE Area (m^2)	Not reported	120.9	120.8	-	-
Total Utility (kW)	395.6	552.7	550.9	-39.70%	-39.26%
Total Capital Cost ($/yr)	55598.9	51293.0	51446.0	7.74%	7.47%
Utility Operating Cost ($/yr)	24780.1	34353.4	34335.8	-38.63%	-38.56%
Total Annual Cost ($/yr)	80379.0	85646.5	85781.8	-6.55%	-6.72%

Table 4.14: Results of instance PO-E2 from Ponce-Ortega et al. (2010)

PO-E2	Ponce-Ortega et al. (2010)	Exp. 1 (ΔQ=75)	Exp. 2 (ΔQ=37.5)	Exp. 3 (ΔQ=16)	Exp. 1 Comparison	Exp. 2 Comparison	Exp. 3 Comparison
Number of Process HEs	3	2	2	2	-1	-1	-1
Number of Utility HEs	4	3	3	3	-1	-1	-1
Total Process HE Area (m^2)	110.5	148.3	116.9	131.0	-34.21%	-5.80%	-18.57%
Total Utility HE Area (m^2)	73.6	54.1	56.8	55.2	26.55%	22.86%	24.96%
Total Utility (kW)	1130.0	963.6	1037.5	991.2	14.72%	8.19%	12.28%
Total Capital Cost ($/yr)	69944.0	46299.0	39740.0	42612.6	33.81%	43.18%	39.08%
Utility Operating Cost ($/yr)	27135.0	54636.0	61000.0	57912.3	-101.35%	-124.80%	-113.42%
Total Annual Cost ($/yr)	97079.0	100940.0	100740.0	100524.9	-3.98%	-3.77%	-3.55%

Table 4.15: Results of instance PO-E3 from Ponce-Ortega et al. (2010)

PO-E3	Ponce-Ortega et al. (2010)	Exp. 1 (ΔQ=1500)	Exp. 2 (ΔQ=1150)	Exp. 1 Comparison	Exp. 2 Comparison
Number of Process HEs	3	4	5	+1	+2
Number of Utility HEs	5	5	4	same	-1
Total Process HE Area (m^2)	3365.1	4065.7	3146.2	-20.82%	6.50%
Total Utility HE Area (m^2)	1558.4	1418.8	1522.4	8.96%	2.31%
Total Utility (kW)	16030.6	15980.1	17064.3	0.32%	-6.45%
Total Capital Cost ($/yr)	540457.0	607112.5	543167.2	-12.33%	-0.50%
Utility Operating Cost ($/yr)	580718.0	674334.3	707642.9	-16.12%	-21.86%
Total Annual Cost ($/yr)	1121175.0	1281446.8	1250810.1	-14.29%	-11.56%

4.2.7 Test instances from Huang and Chang (2012)

Huang and Chang (2012) use Yee and Grossmann (1990)'s methodology to pre-evaluate their instances' results. As it is mentioned before,Yee and Grossmann (1990)'s methodology does not allow stream splitting. Since this assumption is also valid for our approach, we also compare our results with these measures. The results for the instances HC-E1, HC-E2, and HC-E3 are given in Table 4.16, Table 4.17, and Table 4.18, respectively. For the instance HC-E1, it can be said that our solutions are comparable with Huang and Chang (2012)'s. There is only 2.25% difference with respect to the total annual cost between our solutions and their solutions. Our approach finds better total heat exchange area, consequently a better total capital cost. There is no difference in the number of heat exchangers to be installed. Our results are also comparable to the results obtained by Yee and Grossmann (1990)'s methodology.

When HC-E2 instance is considered, it can be seen that their results are significantly better (with 40.70%). The number of utility heat exchangers are increased, hence the total utility is also higher than that of Huang and Chang (2012). For this instance we see that their solution consists of streams that are splitted in the resulting HEN. This is, again, why they get better results. When we compare our results with no stream splitting case (i.e., with Yee and Grossmann (1990)'s methodology), it is seen that the results are very close.

For instance HC-E3, a similar situation with instance HC-E2 occurs.

4.2.8 Second Best Solutions

An important property of our approach is that our solution consists of many different HEN configurations. Since the HENS problem with detailed HE design is actually a multiobjective problem, a more costly solution may be better for implementation for an objective regarding reducing use of utilities. For example, let us consider an instance where the least cost HEN alternative has 2 process and 2 utility HEs. But for its second or third best solution, we see that this alternative has 3 process and 1 utility HEs. In this case, one may consider that the second best is favorable because the utility usage is decreased, accordingly the negative environmental impact is decreased.

To demonstrate this property, second best (least cost) solutions of our three test instances are

Table 4.16: Results of instance HC-E1 from Huang and Chang (2012)

HC-E1	Huang and Chang (2012) Result 1*	Huang and Chang (2012) Result 2**	Exp. 1 (ΔQ=200)	Exp. 1 Comparison with Result 1	Exp. 1 Comparison with Result 2
Number of Process HEs	3	3	3	same	same
Number of Utility HEs	2	3	2	same	-1
Total Process HE Area (m^2)	Not reported	Not reported	258.6	-	-
Total Utility HE Area (m^2)	Not reported	Not reported	55.7	-	-
Total Area (m^2)	345.0	345.0	314.3	8.90%	8.90%
Total Utility (kW)	2686.0	2702.0	2800.0	-4.24%	-3.63%
Total Capital Cost ($/yr)	78230.0	79284.0	74643.7	4.58%	5.85%
Utility Operating Cost ($/yr)	73990.0	74736.0	81000.0	-9.47%	-8.38%
Total Annual Cost ($/yr)	152220.0	154021.0	155643.7	-2.25%	-1.05%

*Best solution

**Solution via Yee and Grossmann (1990)'s methodology

Table 4.17: Results of instance HC-E2 from Huang and Chang (2012)

HC-E2	Huang and Chang (2012) Result 1*	Huang and Chang (2012) Result 2**	Exp. 1 (ΔQ=60)	Exp. 2[a] (ΔQ=30)	Exp. 1 Comparison with Result 1	Exp. 1 Comparison with Result 2
Number of Process HEs	2	2	2	2	same	same
Number of Utility HEs	1	2	2	2	+1	same
Total Process HE Area (m^2)	Not reported	Not reported	76.6	76.6	-	-
Total Utility HE Area (m^2)	Not reported	Not reported	13.4	13.4	-	-
Total Area (m^2)	104.0	92.0	90.0	90.0	13.46%	2.18%
Total Utility (kW)	120.0	464.0	480.0	480.0	-300.00%	-3.45%
Total Capital Cost ($/yr)	45905.0	52869.0	47564.6	47564.6	-3.62%	10.03%
Utility Operating Cost ($/yr)	2400.0	19632.0	20400.0	20400.0	-750.00%	-3.91%
Total Annual Cost ($/yr)	48305.0	72502.0	67964.6	67964.6	-40.70%	6.26%

*Best solution

**Solution via Yee and Grossmann (1990)'s methodology

[a]Exp. 2 Comparisons with Results 1 and 2 are not given here because they are completely same the same as the figures of Exp.1 Comparisons with Results 1 and 2.

Table 4.18: Results of instance HC-E3 from Huang and Chang (2012)

HC-E3	Huang and Chang (2012) Result 1*	Huang and Chang (2012) Result 2**	Exp. 1 (ΔQ=180)	Exp. 2 (ΔQ=90)	Exp. 1 Comparison with Result 1	Exp. 1 Comparison with Result 2	Exp. 2 Comparison with Result 1	Exp. 2 Comparison with Result 2
Number of Process HEs	2	2	2	2	same	same	same	same
Number of Utility HEs	0	2	2	2	+2	same	+2	same
Total Process HE Area (m^2)	Not reported	Not reported	166.6	166.6	-	-	-	-
Total Utility HE Area (m^2)	Not reported	Not reported	2.5	2.5	-	-	-	-
Total Area (m^2)	204.0	165.0	169.1	169.1	17.10%	-2.49%	17.11%	-2.48%
Total Utility (kW)	0.0	104.0	90.0	90.0	-	13.46%	-	13.46%
Total Capital Cost ($/yr)	73295.0	80468.0	79818.3	79814.5	-8.90%	0.81%	-8.89%	0.81%
Utility Operating Cost ($/yr)	0.0	7334.0	6300.0	6300.0	-	14.10%	-	14.10%
Total Annual Cost ($/yr)	73295.0	87802.0	86118.3	86114.5	-17.50%	1.92%	-17.49%	1.92%

*Best solution

**Solution via Yee and Grossmann (1990)'s methodology

Table 4.19: Second best solutions for instance YG-E1 from Yee and Grossmann (1990)

YG-E1	Best	1^{st} arc	2^{nd} or 3^{rd} arc	4^{th} arc
# of Process HEs	3	3	4	3
# of Utility HEs	2	2	2	2
Total Process HE Area (m^2)	371.4	360.8	391.5	266.4
Total Utility HE Area (m^2)	44.0	28.2	44.0	48.5
Total Area (m^2)	415.4	389.1	435.5	314.9
Total Utility (kW)	753.3	1050.0	753.3	1056.7
Total Capital Cost ($/yr)	63362.0	58522.3	68819.4	55105.9
Utility Operating Cost ($/yr)	24267.0	39000.0	24266.7	39533.3
Total Annual Cost ($/yr)	87629.0	97522.3	93086.0	94639.2

Table 4.20: Second best solutions for instance MG-E2 from Mizutani et al. (2003b)

MG-E2	Best	1^{st} arc	2^{nd}, 3^{rd}, 4^{th}, 5^{th} or 6^{th} arc
# of Process HEs	5	5	same with best solution
# of Utility HEs	1	1	
Total Process HE Area (m^2)	147.9	184.6	
Total Utility HE Area (m^2)	5.5	5.5	
Total Area (m^2)	153.4	190.1	
Total Utility (kW)	750.0	750.0	
Total Capital Cost ($/yr)	8288.2	8635.2	
Utility Operating Cost ($/yr)	45000.0	45000.0	
Total Annual Cost ($/yr)	53288.2	53635.2	

obtained and given in Tables 4.19, 4.20, and 4.21. These solutions are found by individually fathoming arcs on the best solution path and solving the shortest path model again every time. In Tables 4.19 and 4.21, it is seen that the results obtained when the first and fourth arc are deleted for YG-E1 and the second (or third) arc is deleted for HC-E2 have smaller process HE area, smaller capital cost, and even smaller utility HE area (for first arc only), smaller utility usage and smaller utility operating costs as compared to their best solutions, respectively. Such solutions can be preferred when the environmental impacts of utility HEs or associated costs are considered.

Besides reducing area and utility usage, a decision maker can have some different objectives. Therefore, this kind of attribute of our approach provides flexibility and alternatives for the decision maker.

Table 4.21: Second best solutions for instance HC-E2 from Huang and Chang (2012)

HC-E2	Best	1^{st} arc	2^{nd} or 3^{rd} arc
# of Process HEs	2	2	2
# of Utility HEs	2	3	2
Total Process HE Area (m^2)	76.6	80.4	91.6
Total Utility HE Area (m^2)	13.4	13.4	12.0
Total Area (m^2)	90.0	93.9	103.7
Total Utility (kW)	480.0	480.0	420.0
Total Capital Cost ($/yr)	47564.6	52591.9	50707.3
Utility Operating Cost ($/yr)	20400.0	20400.0	17400.0
Total Annual Cost ($/yr)	67964.6	72991.9	68107.3

4.3 Remarks

There are some points to be stressed out about our solution approach based on our computational experiments:

- In our approach, all the solutions for HEN in parallel with our assumptions are created. A decision maker can select one among these solutions according to his/her preferences.
- One can adjust the sensitivity of the problem solution by deciding the heat load difference parameter.
- Our approach is flexible. We do not restrict ourselves with a predefined network structure as it is done by Yee and Grossmann (1990).
- One can easily change and add features to the equipment design part without a need to change the entire HEN solution approach.
- Our approach performs better for the solution of HEN combined with detailed HE design.
- We take the physical and thermal properties of the streams at their environment temperature to provide a more realistic result. Unfortunately we could not have the chance to compare this feature with an example from the literature, but it is clear that a more realistic solution is always better.
- As the step size of heat load difference is decreased, thus the number of steps to reach the target temperatures increases, we obtain better results since we explore a greater

Table 4.22: Problem sizes for instances

Instance	Size	Current best solution setting			# of unique HEs	# of nodes
		Hot str. steps	Cold str. steps	ΔQ (kW)		
HC-E3	1H2C	22	18-4	90	1,155	6,601
HC-E2	1H2C	70	26-40	30	20,254	618,314
PO-E2	2H1C	50-47	75	16	30,360	1,520,742
4S1	2H2C	4-8	9-4	300	203	8,390
MG-E1	2H2C	4-10	24-5	100	1,235	66,400
HC-E1	2H2C	14-22	18-10	200	1,614	439,222
YG-E2	2H2C	12-16	18-15	150	3,134	831,766
YG-E1	2H2C	33-18	23-24	100	8,492	4,527,556
PO-E3	2H3C	9-14	12-6-6	1150	608	519,470
5SP	3H2C	10-2-7	5-15	19	211	98,684
MG-E2	3H3C	5-6-2	7-6-1	400	256	101,094
CH13-E2	3H3C	12-2-5	5-8-6	100	556	557,010
YG-E3	5H1C	9-3-5-3-6	55	120	292	260,720

portion of the solution space, except cases with very large heat load differences (see Table 4.8).

- The number of generated nodes for the best solution of instances are given in Table 4.22. The problem size rapidly increases as the number of streams and number of steps for streams increases.

- Although creating the nodes is time consuming, the algorithm consumes more time while connecting the nodes.

CHAPTER 5

CONCLUSION

In this study, we suggest a new solution approach to the heat exchanger network synthesis problem with detailed heat exchanger design. By its nature, it is a complex problem because combining detailed HE design with HEN synthesis results in more complicated problem nature. Various solution methods are suggested in the literature for the solution of the heat exchanger network synthesis, as a subproblem of our problem. Main methodologies are based on using a superstructure model and solving the problem with a nonlinear mathematical model or using the pinch analysis, both are heuristic methods. Usage of mixed integer nonlinear/nonlinear mathematical models dominates the HEN literature. These kinds of models are also used for the detailed design of heat exchangers. In the literature, however, there are limited number of works that consider HEN synthesis with detailed HE design.

How we handle a problem may actually decrease the complexity of the problem as we did in this study. We consider HENS and detailed HE design separately but integrated. This enables us to change detailed HE design part without any need of changing the HENS algorithm.

Our approach is flexible and successfully finds the required number of heat exchangers, their connections, and properties for each HE.

Future work directions are:

- A better way for generation of nodes and arcs of the alternative HEN network to handle the memory problems wisely for solving larger size problems.
- Creating a network by not creating copies of a HE and formulating a kind of network flow model for heat exchanger network synthesis.

- Including pressure drop, heat exchanger effectiveness, and phase change equations to the detailed heat exchanger design models.
- Considering topological aspects for placing heat exchangers.
- Implementing stream splitting and placing utility heat exchangers between process heat exchangers, which definitely increase the alternatives of solutions for decision makers.
- Developing a multiobjective approach for conflicting objectives of the problem like decreasing utility usage and process HE area at the same time.

Because of memory and solution time problems for increased size of instances, we are not able to decrease the step heat load for streams, ΔQ to smaller values. By making use of an initial solution, the solution space can be iteratively searched. For example, consider a solution which is obtained with ΔQ = 100 kW and there are four HEs placed in the HEN. Then, again by discretization new nodes (hence a new network) can be created for ΔQ = 10 kW based on the information obtained from the initial solution. The new solution can be worse or better. But by doing this, solution time can be reduced for a great amount and one can try for different values of ΔQ until a better and desired solution is reached.

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APPENDIX A

TERMINOLOGY

Turner et al. (1993) gives the following explanation while making the distinction between *analysis*, *design* and *synthesis*, which applies to our problem as well:

> "We distinguished between analysis and design ... [where] we learned that *analysis* is the investigation of the properties of a given (existing) system, while *design* involves the choice and arrangement of system components to perform a specific function. Furthermore, we described *synthesis* as the creation and structuring of components into a whole, so as to obtain optimal performance from the total system.
>
> This suggests that there are two basic approaches to system design:
>
> - Design via analysis
> - Design via synthesis
>
> Design by analysis is accomplished by modifying the characteristics of an existing or standard system configuration. Design by synthesis is performed by defining the form of the system directly from its specifications.
>
> Although we would like to always perform systems design generically (by synthesis), in reality, most system design work is related to ongoing systems that we "inherit." For these cases, considerable analysis is required before we are able to begin our design work. Most design work, therefore, involves both analysis and synthesis."

APPENDIX B

PINCH ANALYSIS METHOD

Pinch technology is one of the oldest methodologies used while solving the HENS problem. Here, we give excerpts from Turton et al. (2007) for the reader who is unfamiliar to this field.

> "Whenever the design of a system is considered, limits exist that constrain the design. These limits often manifest themselves as mechanical constraints. ... These mechanical limitations are often (but not always) a result of a constraint in the process design. ... When designing heat exchangers and other unit operations, limitations imposed by the first and second laws of thermodynamics constrain what can be done with such equipment. For example, in a heat exchanger, a close approach between hot and cold streams requires a large heat transfer area. ... Whenever the driving forces for heat or mass exchange are small, the equipment needed for transfer becomes large and we say that the design has a "pinch." When considering systems of many heat or mass exchange devices (called exchanger networks), there will exist somewhere in the system a point where the driving force for energy or mass exchange is a minimum. This represents a pinch or pinch point. The successful design of these networks involves defining where the pinch exists and using the information at the pinch point to design the whole network. We define this design process as pinch technology.
>
> The concepts of pinch technology can be applied to a wide variety of problems in heat and mass transfer. As with other problems encountered in this text, both design and performance cases can be considered. The focus of this chapter is on the implementation of pinch technology to new processes for both heat exchanger and mass exchanger networks. Retrofitting an existing process for heat or mass conservation is an important but more complicated problem. The opti-

mization of such a retrofit must consider the reuse of existing equipment, and this involves extensive research into the conditions that exist within the process, the suitability of materials of construction to new services, and a host of other issues. By considering the design of a heat (or mass) exchange network for existing systems, the solution that minimizes the use of utility streams can be identified and this can be used to guide the retrofit to this minimum utility usage goal.

The approach followed in the remainder of this chapter consists of establishing an algorithm for designing a heat (mass) exchanger network, HEN (MEN) that consumes the minimum amount of utilities and requires the minimum number of exchangers (MUMNE). Although this network may not be optimal in an economic sense, it does represent a feasible solution and will often be close to the optimum.

. . . As the Process Flow Diagram improves, the need to heat and cool process streams becomes apparent. For example, feed usually enters a process from a storage vessel that is maintained at ambient temperature. If the feed is to be reacted at an elevated temperature, then it must be heated. Likewise, after the reaction has taken place, the reactor effluent stream must be purified, which usually requires cooling the stream, and possibly condensing it, prior to separating it. Thus, energy must first be added and then removed from the process. The concept of heat integration, in its simplest form, is to find matches between heat additions and heat removals within the process. In this way, the total utilities that are used to perform these energy transfers can be minimized or rather optimized.

. . . We present the general algorithm to give the minimum number of exchangers requiring the minimum utility requirements for a given minimum approach temperature. The algorithm to solve the minimum utility, MUMNE problem consists of the following steps:

1. Choose a minimum approach temperature. This is part of a parametric optimization. . . . For every minimum approach temperature a different solution will be found.

2. Construct a temperature interval diagram.

3. Construct a cascade diagram and determine the minimum utility requirements and the pinch temperatures.

4. Calculate the minimum number of heat exchangers above and below the pinch.
5. Construct the heat exchanger network.

It is important to remember that the objective of this exercise is to obtain a heat exchanger network that exchanges the minimum amount of energy between the process streams and the utilities and uses the minimum number of heat exchangers to accomplish this. This network is almost never the optimum economic design. However, it does represent a good starting point for further study and optimization."

APPENDIX C

SOLUTION OF DME EXAMPLE

In this section, network generation steps of the illustrative example given in Section 4.1 is explained by doing the necessary calculations. Table 4.1 in 52 includes the data of the example.

Step 1: Discretization of stream inlet and outlet temperatures

Let us consider the hot stream H1 where $T_1^{system} = 364°C$ and $T_1^{target} = 100°C$ are its system inlet and target temperatures, respectively.

For discretization, heat capacity of the stream is needed at the average temperature. The equations for calculating the thermophysical properties of the streams are taken from Yaws (2004). The average temperature of H1 throughout the process is (364°C + 100°C)/2 = 232°C.

Mass flow rates of the components:

$$m_1^{h,DME} = \frac{130.5 \text{ kmol/h } \times 46.0684 \text{ kg/kmol}}{3600\text{s/h}} = 1.67 \text{ kg/s}$$
$$m_1^{h,water} = \frac{132.9 \text{ kmol/h } \times 18.0153 \text{ kg/kmol}}{3600\text{s/h}} = 0.66 \text{ kg/s}$$
$$m_1^{h,methanol} = \frac{64.9 \text{ kmol/h } \times 32.0419 \text{ kg/kmol}}{3600\text{s/h}} = 0.58 \text{ kg/s}$$
$$m_1^h = m_1^{h,DME} + m_1^{h,water} + m_1^{h,methanol} = 2.91 \text{ kg/s}$$

For DME at gas state from Yaws (2004):

$$Cp^{DME} = 34.668 + 7.0293 \times 10^{-2} T + 1.6530 \times 10^{-4} T^2 - 1.767 \times 10^{-7} T^3 + 4.9313 \times 10^{-11} T^4$$

where T is in K and Cp is in J/mol.K.

DME $\longrightarrow$ @ T = 232°C $\longrightarrow$ gas state $\longrightarrow$ Cp^{DME} = 92.726 J/mol.K = 2.014 kJ/kg.K

Similarly:

Water $\longrightarrow$ @ T = 232°C $\longrightarrow$ gas state $\longrightarrow$ Cp^{water} = 1.951 kJ/kg.K

Methanol $\longrightarrow$ @ T = 232°C $\longrightarrow$ gas state $\longrightarrow$ $Cp^{methanol}$ = 1.849 kJ/kg.K

Average heat capacity of stream H1 is:

$$\begin{aligned}
&Cp_1^h = Cp^{DME} \times \frac{m_1^{h,DME}}{m_1^h} + Cp^{water} \times \frac{m_1^{h,water}}{m_1^h} + Cp^{methanol} \times \frac{m_1^{h,methanol}}{m_1^h} \\
&Cp_1^h = 2.014 \times \frac{1.67}{2.91} + 1.951 \times \frac{0.66}{2.91} + 1.849 \times \frac{0.58}{2.91} \\
&Cp_1^h = 1.967 \text{ kJ/kg.K}
\end{aligned}$$

Accordingly, $Fcp = m \cdot Cp$ for discreatization is Fcp = 2.91 · 1.967 = 5.729 kW/K.

Total temperature difference is 264°C = 264 K and total heat load difference is 5.729 kW/K × 264 K = 1512.535 kW.

Let β be 9 steps for stream H1, then ΔQ = 1512.535 kW / 9 = 168.06 kW.

Step temperature difference is $\alpha = \Delta Q / Fcp$ = 29.33 °C

Other streams are discretized by finding the best solutions to equate their system outlet temperatures.

Step 2: Construction of HE alternatives

Step 2.1: Selecting stream pairs and temperatures for each HE

Since, in this example, there is no phase change through the process, temperature steps should be equal to each other.

Pairs (i.e., HEs) consist of one hot and one cold streams. Thus, for example when H1 pairs with C1, their respective temperature levels are:

	Inlet	Outlet
H1:	8 (334.67°C) -	6 (276.01°C)
C1:	3 (154.00°C) -	1 (218.00°C)

Step 2.2: Elimination of HEs with infeasible stream inlet and outlet temperature pairings

Checking the feasibility of the previous example:

Since there is no phase change and temperature level differences (hence heat load differences) are equal, $\Delta Q_H = \Delta Q_C$.

Temperature feasibilities:

$T^{h(in)} > T^{h(out)} \longrightarrow 334.67°C > 276.01°C \rightarrow$ Feasible!

$T^{c(in)} < T^{c(out)} \longrightarrow 154.00°C < 218.00°C \rightarrow$ Feasible!

$T^{h(in)} > T^{c(out)} \longrightarrow 334.67°C > 218.00°C \rightarrow$ Feasible!

$T^{h(out)} > T^{c(in)} \longrightarrow 276.01°C > 154.00°C \rightarrow$ Feasible!

All conditions are satisfied, do not eliminate the HE alternative.

Step 2.3: Conducting detailed HE design for the remaining feasible HEs, using mathematical modeling

From HE design assumptions, cold fluid flows from tube side and hot fluid flows from shell side.

$$
\begin{aligned}
T^{bulk} &= T^{c(in)} + T^{c(out)}/2 = 1867°C \\
T^{wall} &= T^{h(in)} + T^{h(out)}/2 = 305.347°C \\
T^{film} &= T^{bulk} + T^{wall}/2 = 2457°C
\end{aligned}
$$

Tube side fluid properties @T^{bulk}: m^t=2.9 kg/s, ρ^t=12.3893 kg/m^3, μ^t=1×10^{-5} Pa.s, Cp^t = 1781.8196 J/kg.K, k^t=0.0386 W/m.K, k^{tube} = 43.19 W/m.K, y^{gas}=0, y^{liq}=1, y^{wat}=0, μ^{avg} = 0.8394

Shell side fluid properties @T^{film}: m^s=2.9 kg/s, ρ^s=13.3366 kg/m^3, μ^s=4×10^{-4} Pa.s, Cp^s = 1998.2885 J/kg.K, k^s=0.0442 W/m.K

Others: Tlm=87.22 K, Q^s=5.122e+005 W

Solving the CM model by using BARON solver: $Area$ = 11.3479 m^2 $\rightarrow$ Feasible solution, do not eliminate!

Step 3: Developing the alternative network

Step 3.1: Generation of nodes by HE copying, allowing to keep track of the inlet and outlet temperatures of all streams

Copying the HE for all temperatures of unprocessed stream H2:

Node 61: H1: 8-6 C1: 3-1 H2: 1-1

Node 62: H1: 8-6 C1: 3-1 H2: 2-2

Node 63: H1: 8-6 C1: 3-1 H2: 0-0

Step 3.2: Connecting nodes on the network (creating arcs)

Let us consider Node 60 where its temperatures are H1: 8-7 C1: 2-1 H2: 0-0.

All nodes should be connected to the Start and End dummy nodes. Therefore, arcs (Start, 60) and (60,End) are created.

For other nodes, the outlet temperatures of all streams of a node should be equal to the inlet temperatures of all streams of its subsequent node. Thus, Node 60 is connected to Node 36 in which the temperature levels are H1: 7-6 C1: 1-0 H2: 0-0, and arc (60,36) is generated.

Step 3.3: Placing utilities and calculating costs of arcs

In the outlet of Node 36, H2 and C1 are at their target temperatures. One utility HE should be placed for H1 for the connection (36,End).

Cold Utility inlet - outlet: 30°C - 40°C and H1 inlet - outlet: 305.34°C - 276.01°C

$$Q^{utility} = m^h Cp^h \Delta T = 2.9 \text{ kg/s } \times 1713.56 \text{ J/kg.K } \times (6 \times 29.33 \text{ K }) = 874.5 \text{ kW}$$

$$Area = Q^{utility} / U \cdot Tlm = 106.71 \text{ m}^2$$

Cost of arc (60,36) = $1000 + 60\,Area_{Node36}^{0.6} = 1000 + 60 \cdot 13.044^{0.6} = 1280.16$ \$/yr

Cost of arc (36,End) = $1000 + 60\,Area_{utility}^{0.6} + 6 \times Q^{utility} = 7425.72$ \$/yr

APPENDIX D

TEST PROBLEMS

Table D.1: Process data for instance YG-E1

	System Inlet (K)	Target (K)	$Fcp = m \cdot Cp$ (kW/K)	Cost ($/kW.yr)
H1	443	333	30	-
H2	423	303	15	-
C1	293	408	20	-
C2	353	413	40	-
HU*	450	450	-	20
CU**	293	313	-	80

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for HEs:
U = 800 W/m^2.K for all matches except ones involving steam,
U = 1200 W/m^2.K for matches involving steam.
Cost of heaters: $Cost(\$/\text{yr}) = 1000 \cdot A^{0.6}$ for all HEs except heaters, where A is heat exchange area in m^2.
Cost of coolers and process HEs: $Cost = 1200 \cdot A^{0.6}$ for heaters, where A is heat exchange area in m^2.

Table D.2: Process data for instance YG-E2

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/°C)	Cost ($/kW.yr)
H1	150	60	20	-
H2	90	60	80	-
C1	20	125	25	-
C2	25	100	30	-
HU*	180	180	-	80
CU**	10	15	-	20

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for HEs:
U = 50 W/m^2.K for all matches.
Cost of HEs: $Cost(\$/\text{yr}) = 8600 + 670 \cdot A^{0.83}$ for all HEs, where A is heat exchange area in m^2.

Table D.3: Process data for instance YG-E3

	System Inlet (K)	Target (K)	$Fcp = m \cdot Cp$ (kW/K)	Cost ($/kW.yr)
H1	500	320	6	-
H2	480	380	4	-
H3	460	360	6	-
H4	380	360	20	-
H5	380	320	12	-
C1	290	660	18	-
HU*	700	700	-	140
CU**	300	320	-	10

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for HEs:
U = 1000 W/m^2.K for all matches.
Cost of heaters: $Cost(\$/yr) = 1200 \cdot A^{0.60}$ for all HEs, where A is heat exchange area in m^2.

Table D.4: Process data for instance MG-E1

	System Inlet (K)	Target (K)	m (kg/s)	Cost ($/kW.yr)
H1	368	348	8.15	-
H2	353	348	81.5	-
C1	303	363	16.3	-
C2	333	343	20.4	-
HU*	500	500	-	60
CU**	300	320	-	6

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for utility HEs:
U = 444 W/m^2.K
Cost of HEs: $Cost(\$/yr) = 1000 + 60 \cdot A^{0.6}$ where A is heat exchange area in m^2.
For all streams the physical properties are:
viscosity: $\mu = 0.00024$ Pa.s
density: $\rho = 634$ kg/m^3
thermal(heat) capacity: $Cp = 2454$ J/kg.K
thermal conductivity: $k = 0.114$ W/m.K

Table D.5: Process data for instance MG-E2

	System Inlet (K)	Target (K)	m (kg/s)	Cost ($/kW.yr)
H1	426	333	16.3	-
H2	363	333	65.2	-
H3	454	433	32.6	-
C1	293	398	20.4	-
C2	293	373	24.4	-
C3	283	288	65.2	-
HU*	700	700	-	60
CU**	300	320	-	6

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient for utility HEs:
U = 444 W/m^2.K
Cost of HEs: $Cost(\$/\text{yr}) = 1000 + 60 \cdot A^{0.6}$ where A is heat exchange area in m^2.
For all streams the physical properties are:
viscosity: $\mu = 0.00024$ Pa.s
density: $\rho = 634$ kg/m^3
thermal(heat) capacity: $Cp = 2454$ J/kg.K
thermal conductivity: $k = 0.114$ W/m.K

Table D.6: Process data for instance PO-E2

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	105	25	10	0.5	-
H2	185	35	5	0.5	-
C1	25	185	7.5	0.5	-
HPS[a]	210	209	-	5.00	160
MPS[b]	160	159	-	5.00	110
LPS[c]	130	129	-	5.000	50
CW[d]	5	6	-	2.6	10

[a]High pressure steam [b]Medium pressure steam [c] Low pressure steam [d]Cooling water
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/\text{yr}) = \eta \cdot 800 \cdot A$ where A is heat exchange area in m^2 and η is the annualization factor of 0.298/yr.

Table D.7: Process data for instance PO-E3

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	155	85	150	0.5	-
H2	230	40	85	0.5	-
C1	115	210	140	0.5	-
C2	50	180	55	0.5	-
C3	60	175	60	0.5	-
HPS[a]	255	254	-	0.5	70
MPS[b]	205	204	-	0.5	50
LPS[c]	150	149	-	0.5	20
CW[d]	30	40	-	0.5	10
AC[e]	40	65	-	0.5	5

[a]High pressure steam [b]Medium pressure steam [c] Low pressure steam [d]Cooling water [e]Air cooling
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/\text{yr}) = \eta\left(13000 + 1000 \cdot A^{0.83}\right)$ where A is heat exchange area in m^2 and η is the annualization factor of 0.322.

Table D.8: Process data for instance 5SP

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	159	77	2.285	0.10	-
H2	267	80	0.204	0.04	-
H3	343	90	0.538	0.50	-
C1	26	127	0.933	0.01	-
C2	118	265	1.961	0.50	-
HU*	300	300	-	0.05	110
CU**	20	60	-	0.20	10

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/\text{yr}) = 7400 + 80 \cdot A$ where A is heat exchange area in m^2.

Table D.9: Process data for instance HC-E1

	System Inlet (K)	Target (K)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	650	370	10	1	-
H2	590	370	20	1	-
C1	410	650	15	1	-
C2	350	500	13	1	-
HU*	680	680	-	5	80
CU**	300	320	-	1	15

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/yr) = 5500 + 150 \cdot A$ where A is heat exchange area in m^2.

Table D.10: Process data for instance HC-E2

	System Inlet (K)	Target (K)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	423.15	318.15	20	2	-
C1	333.15	393.15	13	2	-
C2	293.15	393.15	12	2	-
HU*	483.15	483.15	-	1	80
CU**	278.15	288.15	-	1	20

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/yr) = 4000 + 700 \cdot A^{0.8}$ where A is heat exchange area in m^2.

Table D.11: Process data for instance HC-E3

	System Inlet (K)	Target (K)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	440	350	22	2	-
C1	349	430	20	2	-
C2	320	368	7.5	0.67	-
HU*	500	500	-	1	120
CU**	300	320	-	1	20

*Hot utility (Superheated steam) **Cold utility (Cooling water)
Overall heat transfer coefficient calculation:
$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$
Cost of HEs: $Cost(\$/yr) = 6600 + 670 \cdot A^{0.83}$ where A is heat exchange area in m^2.

Table D.12: Process data for instance 4S1

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/m^2.K)	Cost ($/kW.yr)	Cp (J/kg.K)	ρ (kg/m^3)	μ (Pa.s)	k (W/m.K)
H1	175	45	10	-	1658	716	0.24×10^{-3}	1.100
H2	125	65	40	-	2684	777	0.23×10^{-3}	0.240
C1	20	155	20	-	2456	700	0.23×10^{-3}	0.120
C2	40	112	15	-	2270	680	0.23×10^{-3}	0.011
HU*	180	179	-	110	-	-	-	-
CU**	15	25	-	10	-	-	-	-

*Hot utility (Superheated steam) **Cold utility (Cooling water)

Overall heat transfer coefficient calculation:

$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$

Cost of HEs: $Cost(\$/\mathrm{yr}) = \eta \cdot n^s \left(30800 + 890 \cdot A^{0.8}\right)$ where A is heat exchange area in m^2, n^s is the number of shell passes in the HE, and η is the annualization factor of 0.2309748.

Table D.13: Process data for instance CH13-E2

	System Inlet (°C)	Target (°C)	$Fcp = m \cdot Cp$ (kW/K)	h (kW/m^2.K)	Cost ($/kW.yr)
H1	300	150	8	0.4	-
H2	150	50	2	0.27	-
H3	200	50	3	0.53	-
C1	190	290	5	0.10	-
C2	90	190	8	0.25	-
C3	40	190	4	0.08	-
HU*	255	255	-	2.00	6
CU**	30	40	-	1.00	60

*Hot utility (Superheated steam) **Cold utility (Cooling water)

Overall heat transfer coefficient calculation:

$U = \frac{1}{(1/h^{hot})+(1/h^{cold})}$

Cost of HEs: $Cost(\$/\text{yr}) = 1000 + 60 \cdot A^{0.6}$ where A is heat exchange area in m^2.

Table D.14: Problem setups for instance YG-E1 from Yee and Grossmann (1990)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	170	60	30	110	3300	150	5.00	22
H2	150	30	15	120	1800	150	10.00	12
C1	20	135	20	115	2300	153.33	7.67	15
C2	80	140	40	60	2400	150	3.75	16
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	170	60	30	110	3300	100	3.33	33
H2	150	30	15	120	1800	100	6.67	18
C1	20	135	20	115	2300	100	5.00	23
C2	80	140	40	60	2400	100	2.50	24

Table D.15: Problem setups for instance YG-E2 from Yee and Grossmann (1990)

EXP. 1	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	150	60	20	90	1800	300	15	6
H2	90	60	80	30	2400	300	3.75	8
C1	20	125	25	105	2625	291.67	11.66667	9
C2	25	100	30	75	2250	281.25	9.375	8
EXP. 2	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	150	60	20	90	1800	150	7.50	12
H2	90	60	80	30	2400	150	1.88	16
C1	20	125	25	105	2625	145.83	5.83	18
C2	25	100	30	75	2250	150	5.00	15

Table D.16: Problem setups for instance YG-E3 from Yee and Grossmann (1990)

EXP. 1	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	227	47	6	180	1080	120	20	9
H2	207	107	4	100	400	133.33	33.33	3
H3	187	87	6	100	600	120	20	5
H4	107	87	20	20	400	133.33	6.67	3
H5	107	47	12	60	720	120	10	6
C1	17	387	18	370	6660	121.09	6.73	55
EXP. 2	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	227	47	6	180	1080	98.18	16.36	11
H2	207	107	4	100	400	100	25	4
H3	187	87	6	100	600	100	16.67	6
H4	107	87	20	20	400	100	5	4
H5	107	47	12	60	720	102.86	8.57	7
C1	17	387	18	370	6660	100.91	5.61	66

Table D.17: Problem setup for instance MG-E1 from Mizutani et al. (2003b)

EXP. 1	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	95	75	20	20	400	100	5	4
H2	80	75	200	5	1000	100	0.5	10
C1	30	90	40	60	2400	100	2.5	24
C2	60	70	50	10	500	100	2	5

Table D.18: Problem setup for instance MG-E2 from Mizutani et al. (2003b)

EXP. 1	**System in** (°C)	**Target** (°C)	**Fcp** (kW/°C)	**Total T diff.** (°C)	**Total Q diff.** (kW)	ΔQ (kW)	α (°C)	β (steps)
H1	153	60	40	93	3720	744	18.6	5
H2	90	60	160	30	4800	800	5	6
H3	181	160	80	21	1680	840	10.5	2
C1	20	125	50	105	5250	750	15	7
C2	20	100	60	80	4800	800	13.3	6
C3	10	15	160	5	800	800	5	1

Table D.19: Problem setups for instance PO-E2 from Ponce-Ortega et al. (2010)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	105	25	10	80	800	72.73	7.3	11
H2	185	35	5	150	750	75	15	10
C1	25	185	7.5	160	1200	75	10	16
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	105	25	10	80	800	36.36	3.6	22
H2	185	35	5	150	750	37.50	7.5	20
C1	25	185	7.5	160	1200	37.50	5.0	32
Exp. 3	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	105	25	10	80	800	16	1.6	50
H2	185	35	5	150	750	15.96	3.2	47
C1	25	185	7.5	160	1200	16	2.1	75

Table D.20: Problem setups for instance PO-E3 from Ponce-Ortega et al. (2010)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	155	85	150	70	10500	1500	10	7
H2	230	40	85	190	16150	1468.18	17.27	11
C1	115	210	140	95	13300	1477.78	10.56	9
C2	50	180	55	130	7150	1430	26	5
C3	60	175	60	115	6900	1380	23	5
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	155	85	150	70	10500	1166.67	7.78	9
H2	230	40	85	190	16150	1153.57	13.57	14
C1	115	210	140	95	13300	1108.33	7.92	12
C2	50	180	55	130	7150	1191.67	21.67	6
C3	60	175	60	115	6900	1150	19.17	6

Table D.21: Problem setup for instance HC-E1 from Huang and Chang (2012)

EXP. 1	**System in (°C)**	**Target (°C)**	**Fcp (kW/°C)**	**Total T diff. (°C)**	**Total Q diff. (kW)**	ΔQ **(kW)**	α **(°C)**	β **(steps)**
H1	377	97	10	280	2800	200	20	14
H2	317	97	20	220	4400	200	10	22
C1	137	377	15	240	3600	200	13.33	18
C2	77	227	13	150	1950	195	15	10

Table D.22: Problem setups for instance HC-E2 from Huang and Chang (2012)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	150	45	20	105	2100	60	3	35
C1	60	120	13	60	780	60	4.62	13
C2	20	120	12	100	1200	60	5	20
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	150	45	20	105	2100	30	1.5	70
C1	60	120	13	60	780	30	2.31	26
C2	20	120	12	100	1200	30	2.5	40

Table D.23: Problem setups for instance HC-E3 from Huang and Chang (2012)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	167	77	22	90	1980	180	8.18	11
C1	76	157	20	81	1620	180	9	9
C2	47	95	7.5	48	360	180	24	2
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	167	77	22	90	1980	90	4.09	22
C1	76	157	20	81	1620	90	4.50	18
C2	47	95	7.5	48	360	90	12	4

Table D.24: Problem setup for instance 4S1 from Ponce-Ortega et al. (2007)

EXP. 1	System in (°C)	Target (°C)	Fcp (kW/°C)	Total T diff. (°C)	Total Q diff. (kW)	ΔQ (kW)	α (°C)	β (steps)
H1	175	45	10	130	1300	325	32.5	4
H2	125	65	40	60	2400	300	7.5	8
C1	20	155	20	135	2700	300	15	9
C2	40	112	15	72	1080	270	18	4

Table D.25: Problem setup for instance CH13-E2 from Turton et al. (2007)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	300	150	8	150	1200	100	12.5	12
H2	150	50	2	100	200	100	50	2
H3	200	50	3	150	450	90	30	5
C1	190	290	5	100	500	100	20	5
C2	90	190	8	100	800	100	12.5	8
C3	40	190	4	150	600	100	25	6

Table D.26: Problem setups for instance 5SP from Gupta and Ghosh (2010)

EXP. 1	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	159	77	2.285	82	187.37	18.737	8.2	10
H2	267	80	0.204	187	38.148	19.074	93.5	2
H3	343	90	0.538	253	136.114	19.44486	36.14286	7
C1	26	127	0.933	101	94.233	18.8466	20.2	5
C2	118	265	1.961	147	288.267	19.2178	9.8	15
EXP. 2	**System in**	**Target**	**Fcp**	**Total T diff.**	**Total Q diff.**	ΔQ	α	β
	(°C)	**(°C)**	**(kW/°C)**	**(°C)**	**(kW)**	**(kW)**	**(°C)**	**(steps)**
H1	159	77	2.285	82	187.37	11.71063	5.125	16
H2	267	80	0.204	187	38.148	12.716	62.33333	3
H3	343	90	0.538	253	136.114	12.374	23	11
C1	26	127	0.933	101	94.233	11.77913	12.625	8
C2	118	265	1.961	147	288.267	12.01113	6.125	24

In Tables D.27–D.49, the following abbreviations are used:

HL	:	Heat Load (in kW)
L	:	Level
T	:	Temperature (in °C)
A	:	Area (in m^2)
CC	:	Capital Cost (in \$/yr)
OC	:	Operating Cost (in \$/yr)

Table D.27: Result of Experiment 1 of Instance YG-E1 from Yee and Grossmann (1990)

		Heat Exchangers						**Utilities**	
		1		**2**		**3**			
		In	Out	In	Out	In	Out	A	HL
H1	L	22	6	6	0	0	0	0.0	0.0
	T	170.0	90.0	90.0	60.0	60.0	60.0		
H2	L	12	12	12	12	12	4	41.2	600.0
	T	150.0	150.0	150.0	150.0	150.0	70.0		
C1	L	15	15	15	9	9	1	2.8	153.3
	T	20.0	20.0	20.0	66.0	66.0	127.3		
C2	L	16	0	0	0	0	0	0.0	0.0
	T	80.0	140.0	140.0	140.0	140.0	140.0		
HL (kW)		2400.0		920.0		1226.7		753.3	
A (m^2)		164.8		36.2		170.4		44.0	
γ (%)		0.0%		2.2%		2.2%		-	
CC (\$/yr)		21387.6		8621.0		21820.8		11532.6	
OC (\$/yr)		-		-		-		24266.7	
Total Cost		**87628.5**							

Table D.28: Result of Experiment 2 of Instance YG-E1 from Yee and Grossmann (1990)

		Heat Exchangers						**Utilities**	
		1		**2**		**3**			
		In	Out	In	Out	In	Out	A	HL
H1	L	33	9	9	0	0	0	0.0	0.0
	T	170.0	90.0	90.0	60.0	60.0	60.0		
H2	L	18	18	18	18	18	6	41.2	600.0
	T	150.0	150.0	150.0	150.0	150.0	70.0		
C1	L	23	23	23	14	14	2	3.6	200.0
	T	20.0	20.0	20.0	65.0	65.0	125.0		
C2	L	24	0	0	0	0	0	0.0	0.0
	T	80.0	140.0	140.0	140.0	140.0	140.0		
HL (kW)		2400.0		900.0		1200.0		800.0	
Area (m^2)		164.8		35.3		120.7		44.8	
γ (%)		0.0%		0.0%		0.0%		-	
CC ($/yr)		21387.6		8478.1		17743.6		11880.0	
OC ($/yr)		-		-		-		28000.0	
Total Cost		**87489.2**							

Table D.29: Result of Experiment 1 of Instance YG-E2 from Yee and Grossmann (1990)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	6	0	0	0	0.0	0.0
	T	150.0	60.0	60.0	60.0		
H2	L	8	8	8	4	437.6	1200.0
	T	90.0	90.0	90.0	75.0		
C1	L	9	3	3	3	246.2	875.0
	T	20.0	90.0	90.0	90.0		
C2	L	8	8	8	4	230.6	1125.0
	T	25.0	25.0	25.0	62.5		
HL (kW)		1800.0		1200.0		3200.0	
A (m^2)		743.1		665.2		914.5	
γ (%)		2.9%		6.7%		-	
CC ($/yr)		170429.3		156253.9		256046.2	
OC ($/yr)		-		-		184000.0	
Total Cost		**766729.7**					

Table D.30: Result of Experiment 2 of Instance YG-E2 from Yee and Grossmann (1990)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	12	12	12	0	0.0	0.0
	T	150.0	150.0	150.0	60.0		
H2	L	16	8	8	8	437.6	1200.0
	T	90.0	75.0	75.0	75.0		
C1	L	18	10	10	10	361.5	1458.3
	T	20.0	66.7	66.7	66.7		
C2	L	15	15	15	3	103.1	450.0
	T	25.0	25.0	25.0	85.0		
HL (kW)		1200.0		1800.0		3108.3	
A (m^2)		666.4		742.8		902.2	
γ (%)		2.9%		0.0%		-	
CC ($/yr)		156432.9		170378.7		250462.7	
OC ($/yr)		-		-		176666.7	
Total Cost		**753940.9**					

Table D.31: Result of Experiment 3 of Instance PO-E2 from Ponce-Ortega et al. (2010)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	50	24	24	24	25.8	384.0
	T	105.0	63.4	63.4	63.4		
H2	L	47	47	47	18	12.8	287.2
	T	185.0	185.0	185.0	92.4		
C1	L	75	49	49	20	16.6	320.0
	T	25.0	80.5	80.5	142.3		
HL (kW)		416.0		464.0		991.2	
A (m^2)		53.8		77.3		55.2	
γ (%)		0.0%		0.3%		-	
CC ($/yr)		12301.0		17675.5		12636.1	
OC ($/yr)		-		-		57912.3	
Total Cost		**100524.9**					

Table D.32: Result of Experiment 1 of Instance YG-E3 from Yee and Grossmann (1990)

		Utilities		**Heat Exchangers**										**Utilities**	
				1		**2**		**3**		**4**		**5**			
		A	HL	In	Out	In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	0.0	0.0	9	9	9	9	9	9	9	9	9	4	11.1	480.0
	T			227.0	227.0	227.0	227.0	227.0	227.0	227.0	227.0	227.0	127.0		
H2	L	0.0	0.0	3	3	3	3	3	3	3	0	0	0	0.0	0.0
	T			207.0	207.0	207.0	207.0	207.0	207.0	207.0	107.0	107.0	107.0		
H3	L	0.0	0.0	5	5	5	5	5	0	0	0	0	0	0.0	0.0
	T			187.0	187.0	187.0	187.0	187.0	87.0	87.0	87.0	87.0	87.0		
H4	L	0.0	0.0	3	3	3	0	0	0	0	0	0	0	0.0	0.0
	T			107.0	107.0	107.0	87.0	87.0	87.0	87.0	87.0	87.0	87.0		
H5	L	1.8	120.0	5	0	0	0	0	0	0	0	0	0	0.0	0.0
	T			97.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0		
C1	L	0.0	0.0	55	50	50	47	47	42	42	39	39	34	34.3	4117.1
	T			17.0	50.6	50.6	70.8	70.8	104.5	104.5	124.6	124.6	158.3		
HL (kW)		120.0		403.6		400.0		600.0		400.0		600.0		4597.1	
A (m^2)		1.8		16.1		11.2		15.0		17.8		34.2		45.2	
γ (%)		-		0.9%		10.1%		0.9%		10.1%		0.9%		-	
CC ($/yr)		1735.6		6351.2		5154.5		6104.9		6741.0		10023.2		15089.2	
OC ($/yr)		1200.0		-		-		-		-		-		581192.7	
Total Cost		**633592.9**													

Table D.33: Result of Experiment 2 of Instance YG-E3 from Yee and Grossmann (1990)

		Utilities		**Heat Exchangers**										**Utilities**	
				1		**2**		**3**		**4**		**5**			
		A	HL	In	Out	In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	0.0	0.0	11	11	11	11	11	11	11	11	11	5	11.2	490.9
	T			227.0	227.0	227.0	227.0	227.0	227.0	227.0	227.0	227.0	128.8		
H2	L	0.0	0.0	4	4	4	4	4	4	4	0	0	0	0.0	0.0
	T			207.0	207.0	207.0	207.0	207.0	207.0	207.0	107.0	107.0	107.0		
H3	L	0.7	100.0	5	5	5	5	5	0	0	0	0	0	0.0	0.0
	T			170.3	170.3	170.3	170.3	170.3	87.0	87.0	87.0	87.0	87.0		
H4	L	0.0	0.0	4	4	4	0	0	0	0	0	0	0	0.0	0.0
	T			107.0	107.0	107.0	87.0	87.0	87.0	87.0	87.0	87.0	87.0		
H5	L	1.6	102.9	6	0	0	0	0	0	0	0	0	0	0.0	0.0
	T			98.4	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0		
C1	L	0.0	0.0	66	60	60	56	56	51	51	47	47	41	34.4	4137.3
	T			17.0	50.6	50.6	73.1	73.1	101.1	101.1	123.5	123.5	157.2		
HL (kW)		202.9		403.6		400.0		500.0		400.0		589.1		4628.2	
A (m^2)		2.3		16.3		11.4		14.8		14.3		28.9		45.5	
γ (%)		-		0.9%		10.1%		0.9%		10.1%		0.9%		-	
CC ($/yr)		2546.2		6397.9		5171.5		6042.8		5932.7		9030.5		15129.0	
OC ($/yr)		2028.6		-		-		-		-		-		584127.3	
Total Cost		**636406.4**													

Table D.34: Result of Experiment 1 of Instance MG-E1 from Mizutani et al. (2003b)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	4	4	4	0	0.0	0.0
	T	95.0	95.0	95.0	75.0		
H2	L	10	0	0	0	0.0	0.0
	T	80.0	75.0	75.0	75.0		
C1	L	24	14	14	14	20.5	1400.0
	T	30.0	55.0	55.0	55.0		
C2	L	5	5	5	1	1.4	100.0
	T	60.0	60.0	60.0	68.0		
HL (kW)		1000.0		400.0		1500.0	
A (m^2)		12.0		17.4		21.9	
γ (%)		0.0%		0.0%		-	
CC ($/yr)		1266.1		1332.5		2441.6	
OC ($/yr)		-		-		90000.0	
Total Cost		**95040.2**					

Table D.35: Detailed Design Parameters for Experiment 1 of 4S1

Specifications	**Heat Exchangers**	
	1	**2**
Inner diameter of tubes (m)	0.0229	0.0173
Outer diameter of tubes (m)	0.0254	0.0191
Tube arrangement (m)	square	square
Pitch length (m)	0.0318	0.0254
TEMA type	U	P/S
Number of tubes	6	12
Number of tube passes	6	6
Number of shell passes	3	3
Shell diameter (m)	0.2032	0.2032
Length of HE (m)	16.9340	9.067861
Area (m^2)	48.6459	39.0735

Table D.36: Result of Experiment 1 of Instance MG-E2 from Mizutani et al. (2003b)

		Heat Exchangers										Utilities	
		1		2		3		4		5			
		In	Out	In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	5	5	5	5	5	5	5	5	5	0	0.0	0.0
	T	153.0	153.0	153.0	153.0	153.0	153.0	153.0	153.0	153.0	60.0		
H2	L	6	2	2	2	2	1	1	0	0	0	0.0	0.0
	T	90.0	70.0	70.0	70.0	70.0	65.0	65.0	60.0	60.0	60.0		
H3	L	2	2	2	0	0	0	0	0	0	0	0.0	0.0
	T	181.0	181.0	181.0	160.0	160.0	160.0	160.0	160.0	160.0	160.0		
C1	L	7	7	7	7	7	7	7	6	6	1	5.5	750.0
	T	20.0	20.0	20.0	20.0	20.0	20.0	20.0	35.0	35.0	110.0		
C2	L	6	2	2	0	0	0	0	0	0	0	0.0	0.0
	T	20.0	73.3	73.3	100.0	100.0	100.0	100.0	100.0	100.0	100.0		
C3	L	1	1	1	1	1	0	0	0	0	0	0.0	0.0
	T	10.0	10.0	10.0	10.0	10.0	15.0	15.0	15.0	15.0	15.0		
HL (kW)		4266.7		2133.3		250.0		2400.0		12000.0		750.0	
A (m^2)		39.2		10.9		12.9		11.6		73.4		5.5	
γ (%)		0.0%		5.0%		0.0%		6.7%		0.8%		-	
CC ($/yr)		1541.9		1251.0		1278.7		1260.7		1789.8		1166.1	
OC ($/yr)		-		-		-		-		-		45000.0	
Total Cost		**53288.2**											

Table D.37: Result of Experiment 1 of Instance PO-E2 from Ponce-Ortega et al. (2010)

		Heat Exchangers				Utilities	
		1		2			
		In	Out	In	Out	A	HL
H1	L	11	5	5	5	25.0	363.6
	T	105.0	61.4	61.4	61.4		
H2	L	10	10	10	4	13.2	300.0
	T	185.0	185.0	185.0	95.0		
C1	L	16	10	10	4	15.9	300.0
	T	25.0	85.0	85.0	145.0		
HL (kW)		450.0		450.0		963.6	
A (m^2)		65.1		83.2		54.1	
γ (%)		3.1%		0.0%		-	
CC ($/yr)		14899.2		19031.0		12368.9	
OC ($/yr)		-		-		54636.4	
Total Cost		**100935.5**					

Table D.38: Result of Experiment 2 of Instance PO-E2 from Ponce-Ortega et al. (2010)

		Heat Exchangers				Utilities	
		1		2			
		In	Out	In	Out	A	HL
H1	L	22	11	11	11	26.5	400.0
	T	105.0	65.0	65.0	65.0		
H2	L	20	20	20	8	13.2	300.0
	T	185.0	185.0	185.0	95.0		
C1	L	32	21	21	9	17.1	337.5
	T	25.0	80.0	80.0	140.0		
HL (kW)		412.5		450.0		1037.5	
A (m^2)		51.0		65.9		56.8	
γ (%)		3.1%		0.0%		-	
CC ($/yr)		11668.1		15081.7		12990.3	
OC ($/yr)		-		-		61000.0	
Total Cost		**100740.1**					

Table D.39: Result of Experiment 1 of Instance PO-E3 from Ponce-Ortega et al. (2010)

		Heat Exchangers								Utilities	
		1		2		3		4			
		In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	7	5	5	2	2	2	2	2	282.7	3000.0
	T	155.0	135.0	135.0	105.0	105.0	105.0	105.0	105.0		
H2	L	11	11	11	11	11	6	6	3	693.1	4404.5
	T	230.0	230.0	230.0	230.0	230.0	143.6	143.6	91.8		
C1	L	9	7	7	7	7	2	2	2	217.2	2955.6
	T	115.0	136.1	136.1	136.1	136.1	188.9	188.9	188.9		
C2	L	5	5	5	2	2	2	2	2	116.4	2860.0
	T	50.0	50.0	50.0	128.0	128.0	128.0	128.0	128.0		
C3	L	5	5	5	5	5	5	5	2	109.5	2760.0
	T	60.0	60.0	60.0	60.0	60.0	60.0	60.0	129.0		
HL (kW)		3000.0		4500.0		7388.9		4404.5		15980.1	
A (m^2)		622.5		990.0		1527.1		926.1		1418.8	
γ (%)		1.5%		4.9%		0.7%		6.4%		-	
CC ($/yr)		71328.2		102863.5		145587.9		97554.2		189778.7	
OC ($/yr)		-		-		-		-		674334.3	
Total Cost		**1281446.8**									

Table D.40: Result of Experiment 2 of Instance PO-E3 from Ponce-Ortega et al. (2010)

		Heat Exchangers										Utilities	
		1		2		3		4		5			
		In	Out	In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	9	7	7	3	3	3	3	3	3	3	317.0	3500.0
	T	155.0	139.4	139.4	108.3	108.3	108.3	108.3	108.3	108.3	108.3		
H2	L	14	14	14	14	14	12	12	8	8	4	705.0	4614.3
	T	230.0	230.0	230.0	230.0	230.0	202.9	202.9	148.6	148.6	94.3		
C1	L	12	10	10	10	10	10	10	6	6	6	406.0	6650.0
	T	115.0	130.8	130.8	130.8	130.8	130.8	130.8	162.5	162.5	162.5		
C2	L	6	6	6	2	2	0	0	0	0	0	0.0	0.0
	T	50.0	50.0	50.0	136.7	136.7	180.0	180.0	180.0	180.0	180.0		
C3	L	6	6	6	6	6	6	6	6	6	2	94.4	2300.0
	T	60.0	60.0	60.0	60.0	60.0	60.0	60.0	60.0	60.0	136.7		
HL (kW)		2333.3		4766.7		2383.3		4614.3		4614.3		17064.3	
A (m^2)		390.8		1031.5		161.0		683.3		879.6		1522.4	
γ (%)		5.3%		2.1%		3.3%		4.1%		0.3%		-	
CC ($/yr)		49805.3		106286.2		26043.6		76725.1		93646.2		190660.7	
OC ($/yr)		-		-		-		-		-		707642.9	
Total Cost		**1250810.1**											

Table D.41: Result of Experiment 1 of Instance HC-E1 from Huang and Chang (2012)

		Heat Exchangers						Utilities	
		1		2		3			
		In	Out	In	Out	In	Out	A	HL
H1	L	14	14	14	10	10	0	0.0	0.0
	T	377.0	377.0	377.0	297.0	297.0	97.0		
H2	L	22	11	11	11	11	11	40.4	2200.0
	T	317.0	207.0	207.0	207.0	207.0	207.0		
C1	L	18	7	7	3	3	3	15.3	600.0
	T	137.0	283.7	283.7	337.0	337.0	337.0		
C2	L	10	10	10	10	10	0	0.0	0.0
	T	77.0	77.0	77.0	77.0	77.0	227.0		
HL (kW)		2200.0		800.0		2000.0		2800.0	
A (m^2)		89.0		65.9		103.7		55.7	
γ (%)		0.0%		0.0%		2.6%		-	
CC ($/yr)		18854.9		15387.5		21051.3		19350.0	
OC ($/yr)		-		-		-		81000.0	
Total Cost		**155643.7**							

Table D.42: Result of Experiment 1 of Instance HC-E2 from Huang and Chang (2012)

		Heat Exchangers				Utilities	
		1		2			
		In	Out	In	Out	A	HL
H1	L	35	22	22	5	10.6	300.0
	T	150.0	111.0	111.0	60.0		
C1	L	13	0	0	0	0.0	0.0
	T	60.0	120.0	120.0	120.0		
C2	L	20	20	20	3	2.8	180.0
	T	20.0	20.0	20.0	105.0		
HL (kW)		780.0		1020.0		480.0	
A (m^2)		19.7		56.9		13.4	
γ (%)		0.0%		0.0%		-	
CC ($/yr)		11600.3		21753.0		14211.3	
OC ($/yr)		-		-		20400.0	
Total Cost		**67964.6**					

Table D.43: Result of Experiment 2 of Instance HC-E2 from Huang and Chang (2012)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	70	44	44	10	10.6	300.0
	T	150.0	111.0	111.0	60.0		
C1	L	26	0	0	0	0.0	0.0
	T	60.0	120.0	120.0	120.0		
C2	L	40	40	40	6	2.8	180.0
	T	20.0	20.0	20.0	105.0		
HL (kW)		780.0		1020.0		480.0	
A (m^2)		19.7		56.9		13.4	
γ (%)		0.0%		0.0%		-	
CC ($/yr)		11600.3		21753.0		14211.3	
OC ($/yr)		-		-		20400.0	
Total Cost		**67964.6**					

Table D.44: Result of Experiment 1 of Instance HC-E3 from Huang and Chang (2012)

		Heat Exchangers				**Utilities**	
		1		**2**			
		In	Out	In	Out	A	HL
H1	L	44	8	8	1	1.7	45.0
	T	167.0	93.4	93.4	79.0		
C1	L	36	0	0	0	0.0	0.0
	T	76.0	157.0	157.0	157.0		
C2	L	8	8	8	1	0.8	45.0
	T	47.0	47.0	47.0	89.0		
HL (kW)		1620.0		315.0		90.0	
A (m^2)		121.4		45.2		2.5	
γ (%)		0.0%		0.0%		-	
CC ($/yr)		42571.6		22445.4		14801.3	
OC ($/yr)		-		-		6300.0	
Total Cost		**86118.3**					

Table D.45: Result of Experiment 2 of Instance HC-E3 from Huang and Chang (2012)

		Heat Exchangers				Utilities	
		1		2			
		In	Out	In	Out	A	HL
H1	L	88	16	16	2	1.7	45.0
	T	167.0	93.4	93.4	79.0		
C1	L	72	0	0	0	0.0	0.0
	T	76.0	157.0	157.0	157.0		
C2	L	16	16	16	2	0.8	45.0
	T	47.0	47.0	47.0	89.0		
HL (kW)		1620.0		315.0		90.0	
A (m^2)		121.4		45.2		2.5	
γ (%)		0.0%		0.0%		-	
CC ($/yr)		42570.8		22442.5		14801.2	
OC ($/yr)		-		-		6300.0	
Total Cost		**86114.5**					

Table D.46: Result of Experiment 1 of Instance 4S1 from Ponce-Ortega et al. (2007)

		Heat Exchangers				Utilities	
		1		2			
		In	Out	In	Out	A	HL
H1	L	4	0	0	0	0.0	0.0
	T	175.0	45.0	45.0	45.0		
H2	L	8	8	8	2	4.6	600.0
	T	125.0	125.0	125.0	80.0		
C1	L	9	9	9	3	4.2	900.0
	T	20.0	20.0	20.0	110.0		
C2	L	4	0	0	0	0.0	0.0
	T	40.0	112.0	112.0	112.0		
HL (kW)		1300.0		1800.0		1500.0	
A (m^2)		48.6		39.1		8.7	
γ (%)		20.4%		0.0%		-	
CC ($/yr)		20908.8		18690.6		15564.1	
OC ($/yr)		-		-		105000.0	
Total Cost		**160163.5**					

Table D.47: Result of Experiment 1 of Instance CH13-E2 from Turton et al. (2007)

		Heat Exchangers										**Utilities**	
		1		**2**		**3**		**4**		**5**			
		In	Out	In	Out	In	Out	In	Out	In	Out	A	HL
H1	L	12	12	12	12	12	7	7	0	0	0	0.0	0.0
	T	300.0	300.0	300.0	300.0	300.0	237.5	237.5	150.0	150.0	150.0		
H2	L	2	1	1	0	0	0	0	0	0	0	0.0	0.0
	T	150.0	100.0	100.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0		
H3	L	5	5	5	5	5	5	5	5	5	1	9.0	90.0
	T	200.0	200.0	200.0	200.0	200.0	200.0	200.0	200.0	200.0	80.0		
C1	L	5	5	5	5	5	0	0	0	0	0	0.0	0.0
	T	190.0	190.0	190.0	190.0	190.0	290.0	290.0	290.0	290.0	290.0		
C2	L	8	7	7	7	7	7	7	0	0	0	0.0	0.0
	T	90.0	102.5	102.5	102.5	102.5	102.5	102.5	190.0	190.0	190.0		
C3	L	6	6	6	5	5	5	5	5	5	1	16.9	100.0
	T	40.0	40.0	40.0	65.0	65.0	65.0	65.0	65.0	65.0	165.0		
HL (kW)		100.0		200.0		500.0		700.0		800.0		190.0	
A (m^2)		32.0		81.2		259.7		95.8		473.0		25.9	
γ (%)		0.0%		0.0%		0.0%		0.0%		11.1%		-	
CC ($/yr)		1480.1		1839.2		2685.9		1926.7		3416.0		2551.8	
OC ($/yr)		-		-		-		-		-		6540.0	
Total Cost		**20439.7**											

Table D.48: Result of Experiment 1 of Instance 5SP from Gupta and Ghosh (2010)

		Utilities		Heat Exchangers 1		Utilities	
		A	HL	In	Out	A	HL
H1	L	36.9	187.4	0	0	0.0	0.0
	T			77.0	77.0		
H2	L	0.0	0.0	2	2	9.6	38.1
	T			267.0	267.0		
H3	L	0.0	0.0	7	2	3.2	38.9
	T			343.0	162.3		
C1	L	0.0	0.0	5	0	0.0	0.0
	T			26.0	127.0		
C2	L	0.0	0.0	15	15	71.1	288.3
	T			118.0	118.0		
HL (kW)		187.4		97.2		365.3	
A (m^2)		36.9		57.8		84.0	
γ (%)		-		3.2%		-	
CC ($/yr)		10355.5		12020.3		28917.2	
OC ($/yr)		1873.7		-		32479.7	
Total Cost		**85646.5**					

Table D.49: Result of Experiment 2 of Instance 5SP from Gupta and Ghosh (2010)

		Heat Exchangers 1		Utilities	
		In	Out	A	HL
H1	L	16	16	36.9	187.4
	T	159.0	159.0		
H2	L	3	3	9.6	38.1
	T	267.0	267.0		
H3	L	11	3	3.1	37.1
	T	343.0	159.0		
C1	L	8	0	0.0	0.0
	T	26.0	127.0		
C2	L	24	24	71.1	288.3
	T	118.0	118.0		
HL (kW)		99.0		550.9	
A (m^2)		59.8		120.8	
γ (%)		3.2%		-	
CC ($/yr)		12180.7		39265.3	
OC ($/yr)		-		34335.8	
Total Cost		**85781.8**			

Table D.50: Detailed Design Parameters for Experiment 1 of MG-E2

Specifications	**Heat Exchangers**				
	1	**2**	**3**	**4**	**5**
Inner diameter of tubes (m)	0.0173	0.0236	0.0300	0.0135	0.0173
Outer diameter of tubes (m)	0.0191	0.0254	0.0318	0.0191	0.0191
Tube arrangement (m)	square	square	square	triangular	square
Pitch length (m)	0.0254	0.0318	0.0397	0.0238	0.0254
TEMA type	P/S	U	U	P/S	P/S
Number of tubes	12	8	32	18	12
Number of tube passes	6	4	6	6	6
Number of shell passes	3	2	3	3	3
Shell diameter (m)	0.2032	0.2032	0.3874	0.2032	0.2032
Length of HE (m)	9.0909	4.2541	0.6751	1.7896	17.0300
Area (m^2)	39.1729	10.8627	12.9299	11.5669	73.3826

Table D.51: Detailed Design Parameters for Experiment 1 of MG-E1

Specifications	**Heat Exchangers**	
	1	**2**
Inner diameter of tubes (m)	0.0173	0.0166
Outer diameter of tubes (m)	0.0191	0.0191
Tube arrangement (m)	square	square
Pitch length (m)	0.0254	0.0254
TEMA type	P/S	P/S
Number of tubes	12	12
Number of tube passes	6	6
Number of shell passes	3	3
Shell diameter (m)	0.2032	0.2032
Length of HE (m)	2.7777	4.0275
Area (m^2)	11.9693	17.3546

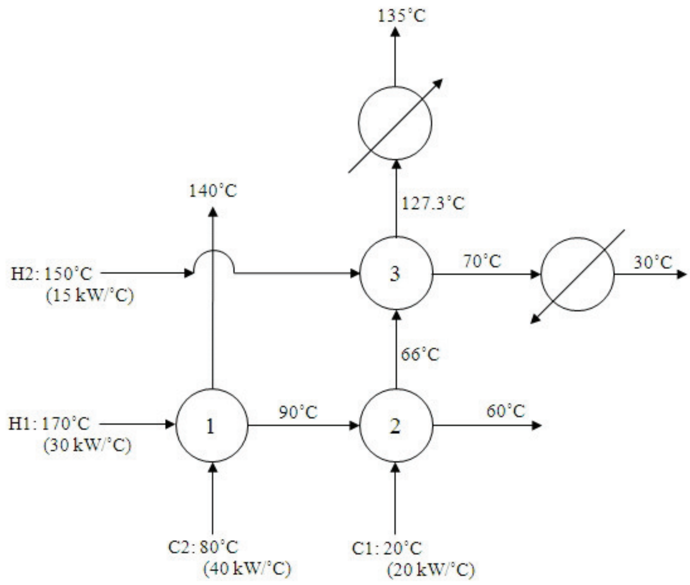

Figure D.1: The resulting HEN of Experiment 1 of instance YG-E1

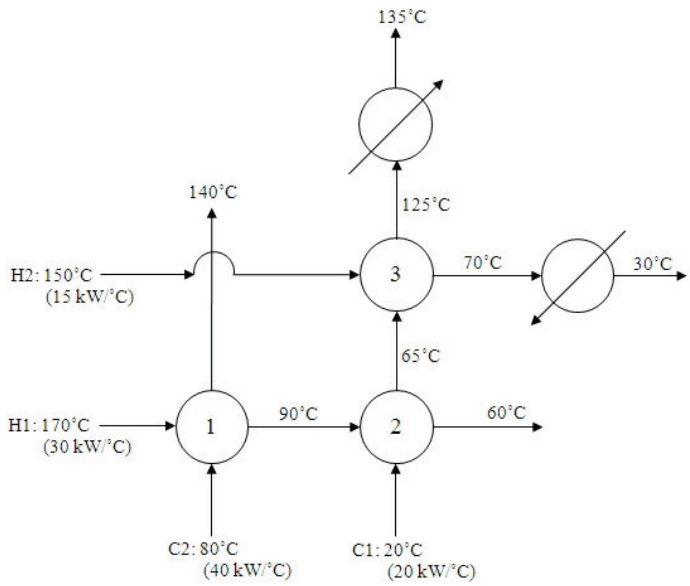

Figure D.2: The resulting HEN of Experiment 2 of instance YG-E1

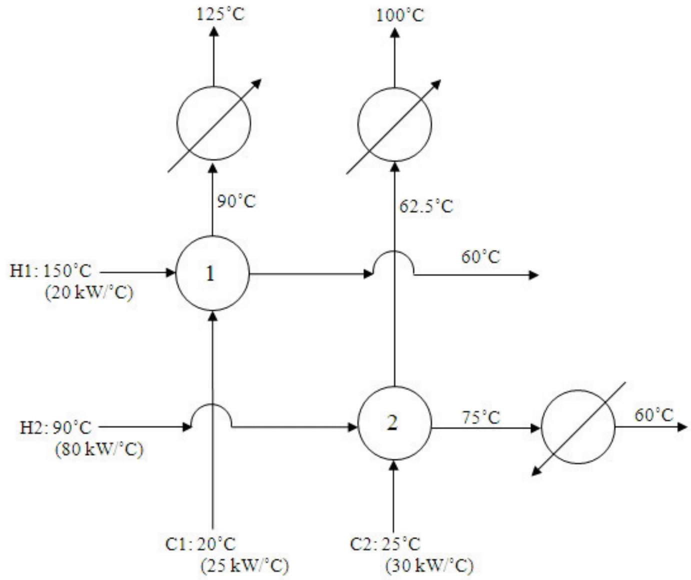

Figure D.3: The resulting HEN of Experiment 1 of instance YG-E2

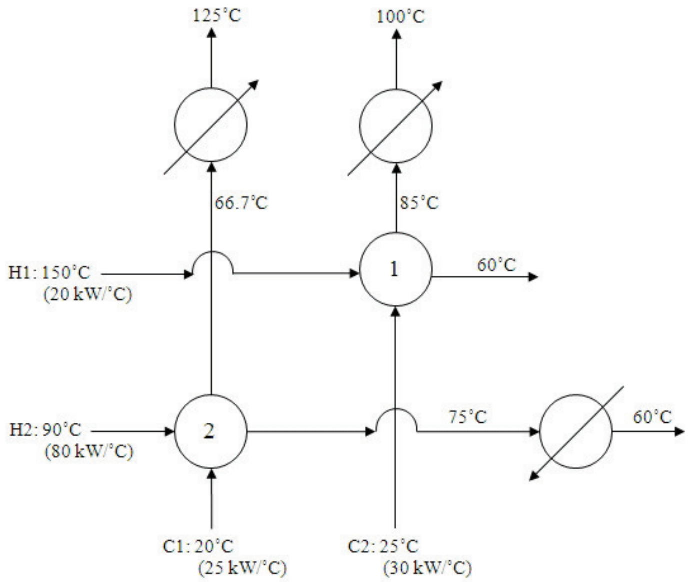

Figure D.4: The resulting HEN of Experiment 2 of instance YG-E2

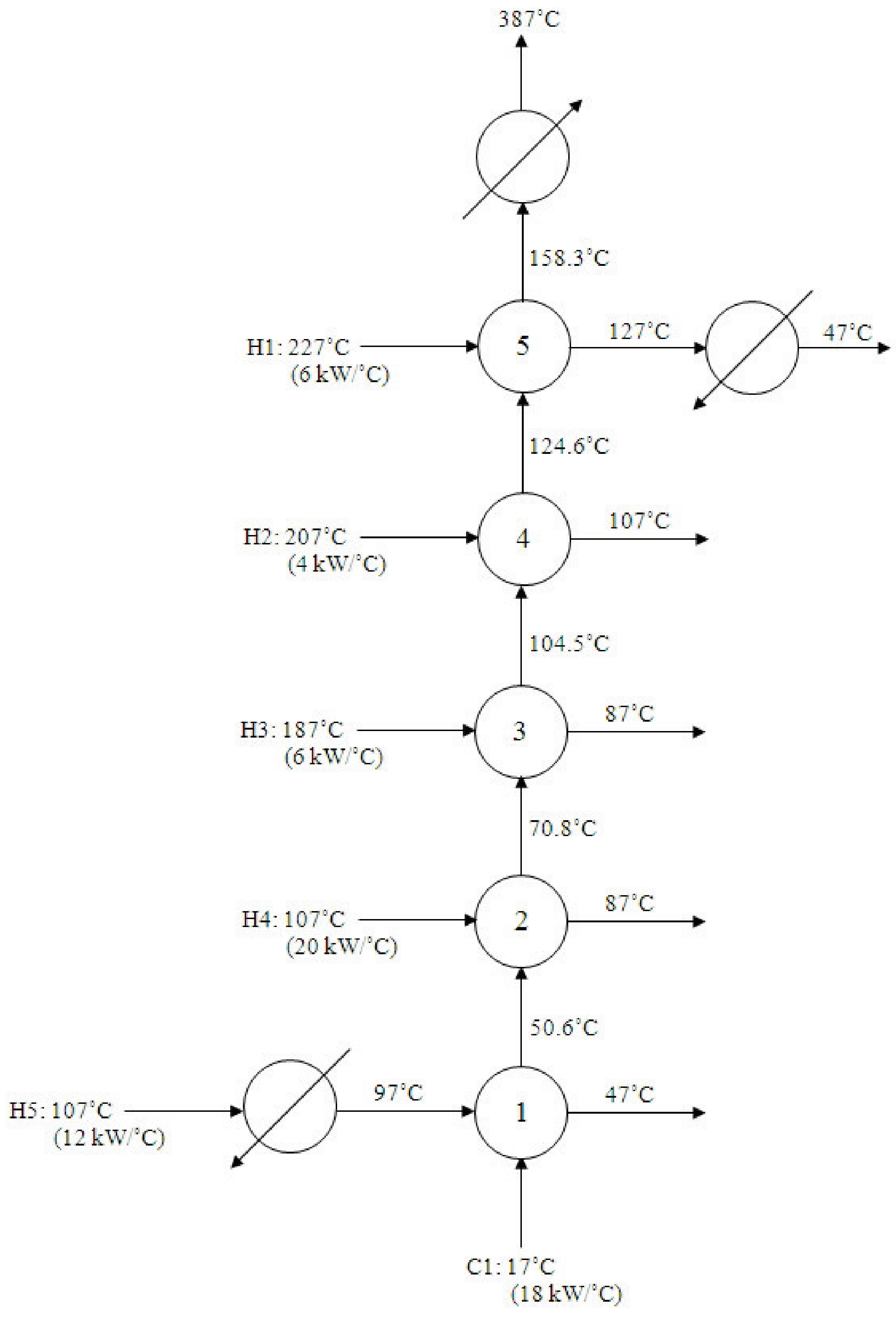

Figure D.5: The resulting HEN of Experiment 1 of instance YG-E3

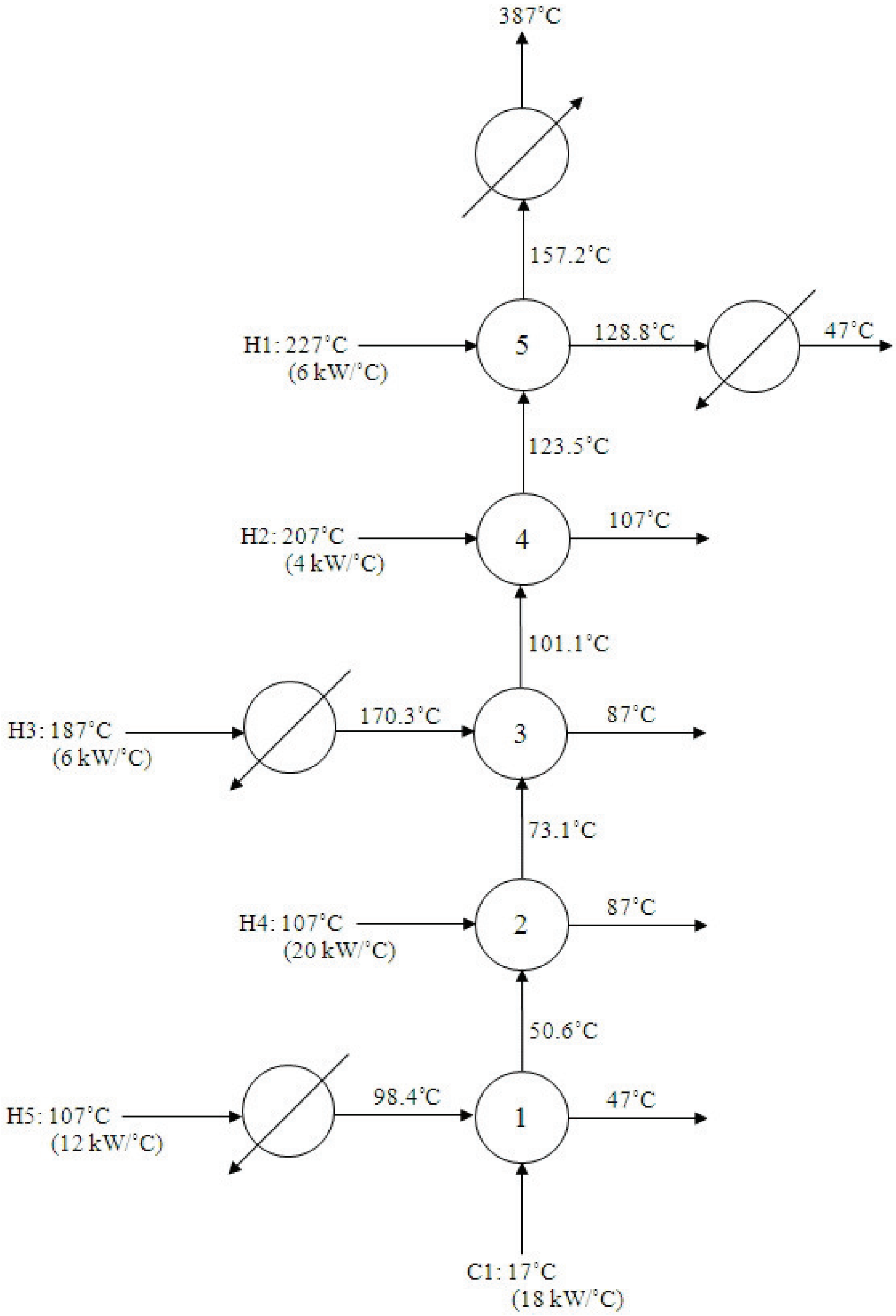

Figure D.6: The resulting HEN of Experiment 2 of instance YG-E3

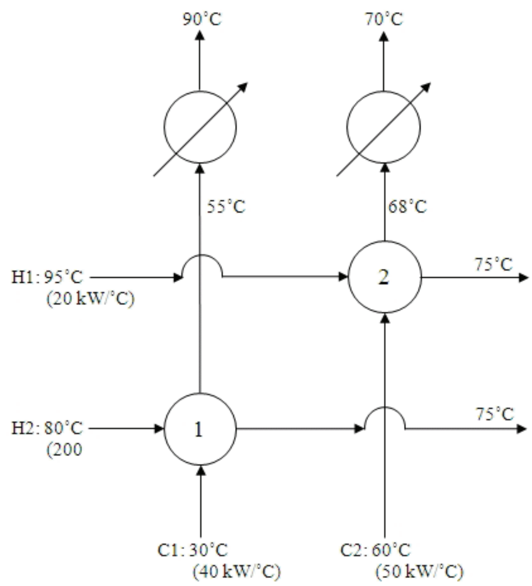

Figure D.7: The resulting HEN of Experiment 1 of instance MG-E1

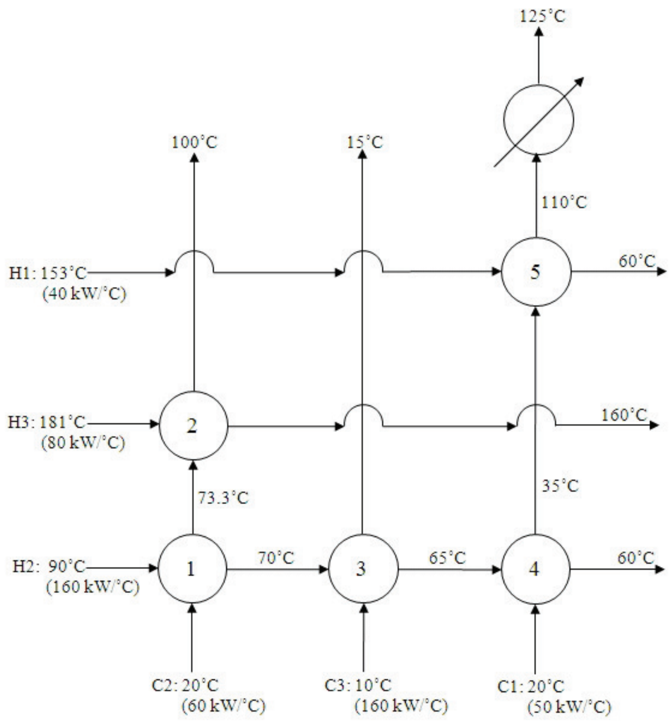

Figure D.8: The resulting HEN of Experiment 1 of instance MG-E2

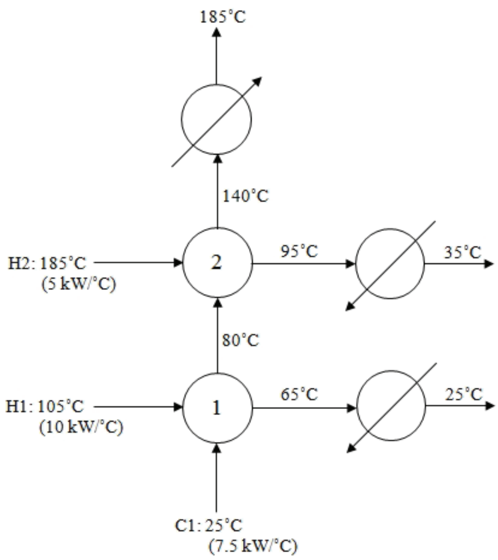

Figure D.9: The resulting HEN of Experiment 2 of instance PO-E2

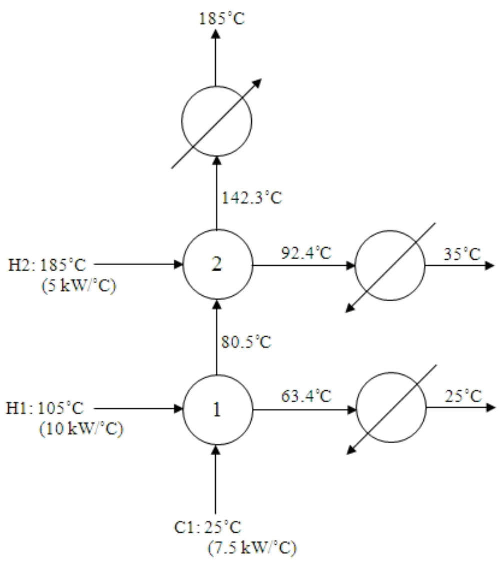

Figure D.10: The resulting HEN of Experiment 3 of instance PO-E2

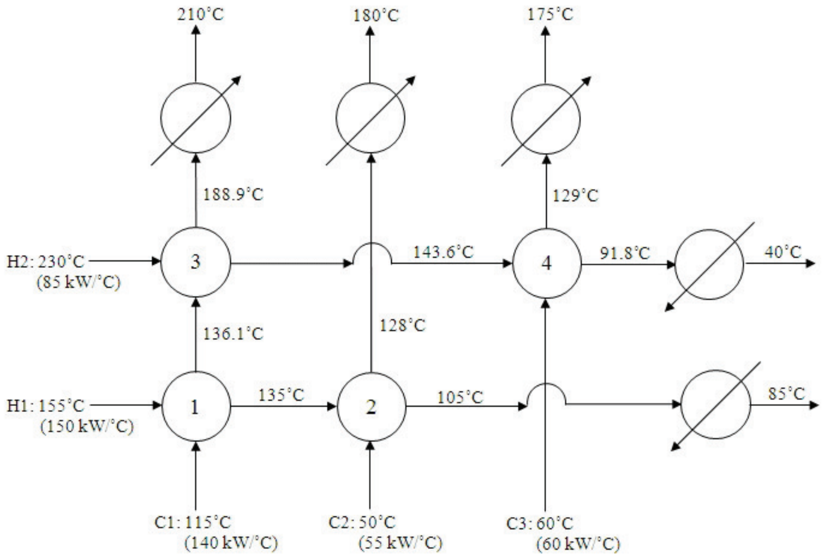

Figure D.11: The resulting HEN of Experiment 1 of instance PO-E3

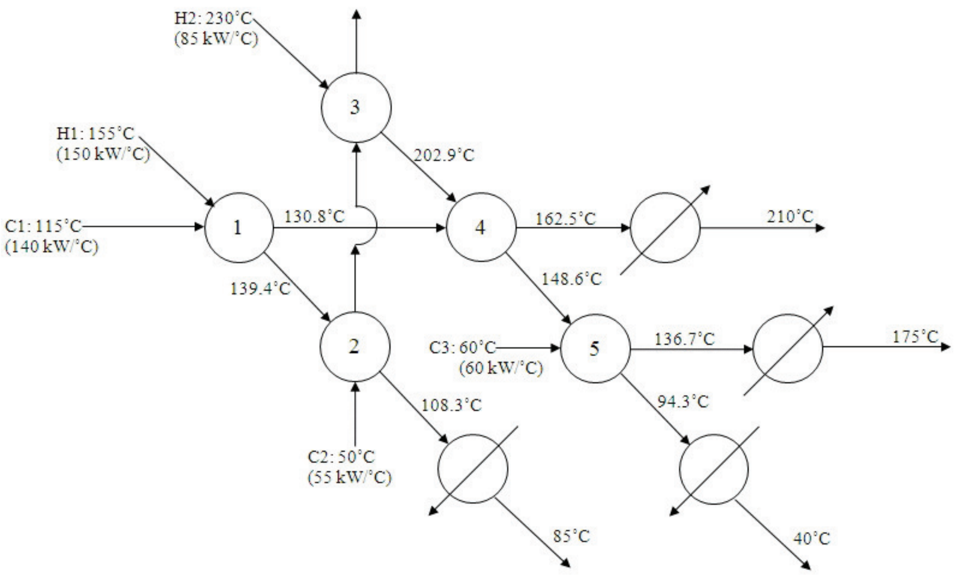

Figure D.12: The resulting HEN of Experiment 2 of instance PO-E3

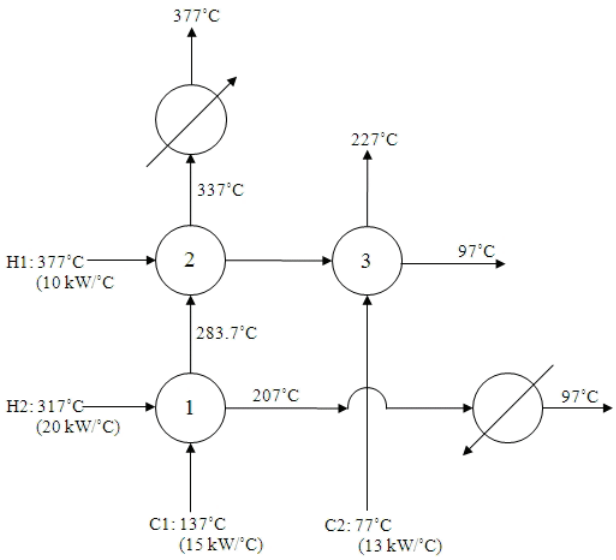

Figure D.13: The resulting HEN of Experiment 1 of instance HC-E1

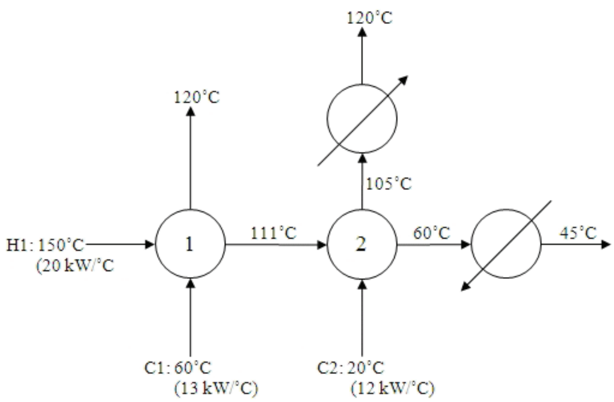

Figure D.14: The resulting HEN of Experiment 1 of instance HC-E2

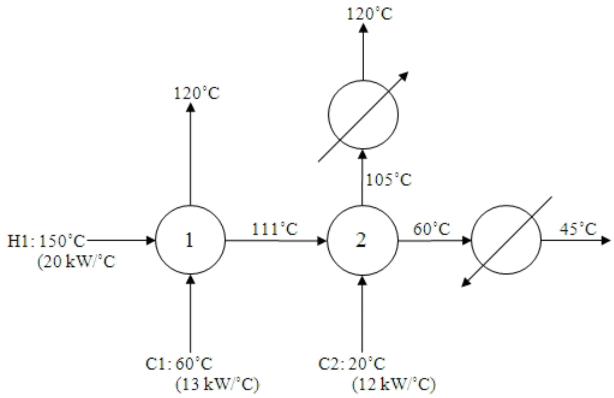

Figure D.15: The resulting HEN of Experiment 2 of instance HC-E2

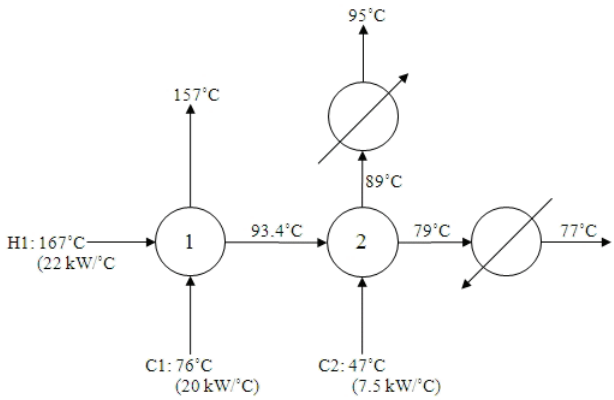

Figure D.16: The resulting HEN of Experiment 1 of instance HC-E3

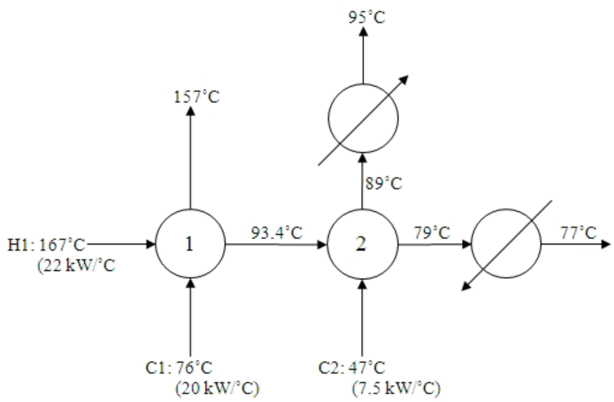

Figure D.17: The resulting HEN of Experiment 2 of instance HC-E3

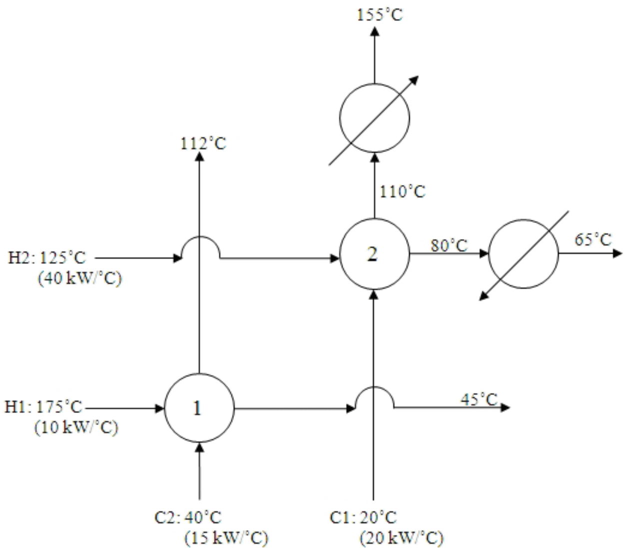

Figure D.18: The resulting HEN of Experiment 1 of instance 4S1

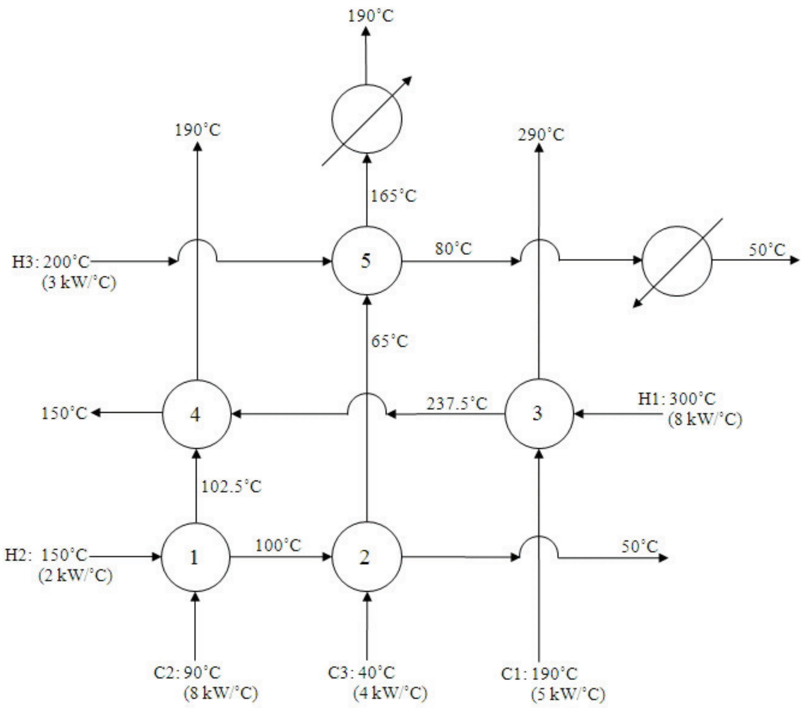

Figure D.19: The resulting HEN of Experiment 1 of instance CH13-E2

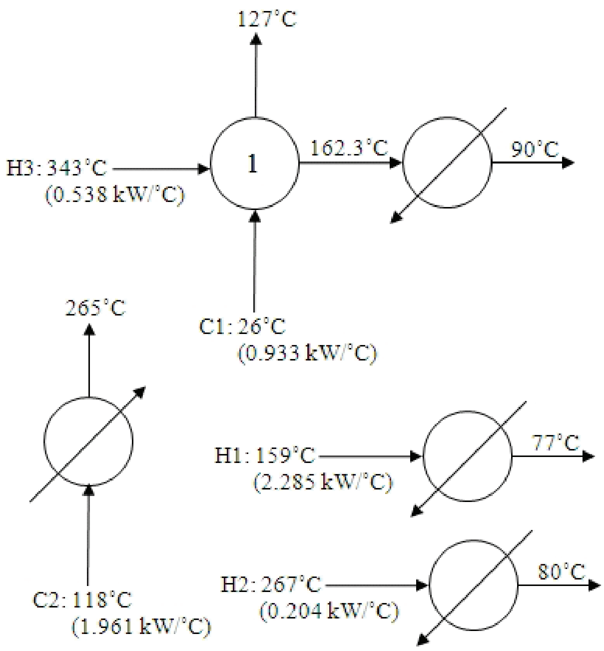

Figure D.20: The resulting HEN of Experiment 1 of instance 5SP

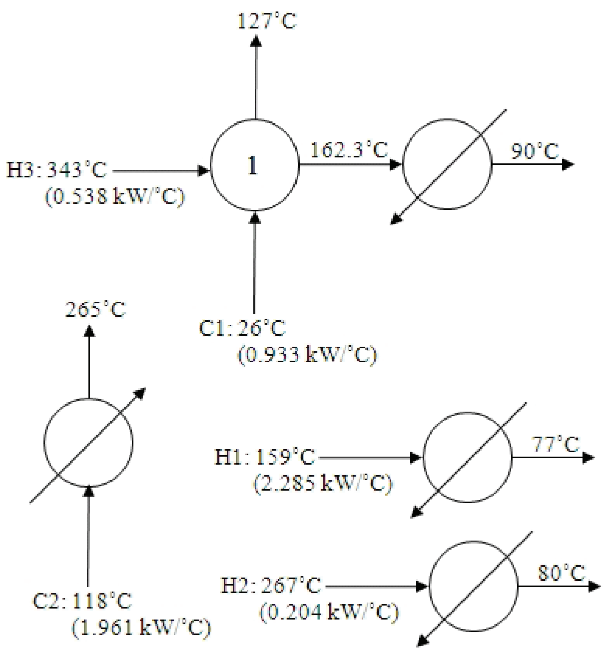

Figure D.21: The resulting HEN of Experiment 2 of instance 5SP

APPENDIX E

DESCRIPTION OF SOME TECHNICAL TERMS

Heat Exchanger (HE):	A device that is used to transfer thermal energy between two or more fluids, between a solid surface and a fluid, or between solid particulates and a fluid, at different temperatures and in thermal contact.
Heat Exchanger Network (HEN):	An overall system of HEs that combines the heat release and neediness points in a process for efficient utilization of energy.
Utility:	Cold water for cooling or superheated steam for heating the process streams.
Process Heat Exchanger:	Heat exchangers that two process streams interact.
Utility Heat Exchanger:	Heat exchangers that a process stream and a utility stream interacts.
Heat capacity:	The amount of heat required to raise the temperature of a substance by one degree
Thermal conductivity:	The ability of a material to allow heat to pass through
Viscosity:	A liquid's internal resistance to flowing
Density:	The quantity of mass per unit of volume
Stream splitting:	Partitioning a process in a heat exchanger network and processing each portion in different HEs.