Globally Optimal Heat Exchanger Networks. Part II- Stages/Substages Superstructure with Variable Cp

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ABSTRACT

We extend the formulation of the Stages/Substages model (see Part I) to account heat capacity variable with temperature, whose influence in designs of heat exchanger network design was not studied. Variable heat capacity (*Cp*) frequently arises when streams of high molecular weight are used, or when temperature ranges are large, like in petroleum fractionation, where the range of temperatures in streams spans more than 100 ºC. We solve our model globally using RYSIA, a recently developed method bound contraction procedure (Faria and Bagajewicz, 2011c; Faria et al., 2015). We also tried BARON and ANTIGONE, two commercial global solvers, but they failed to find a solution.

1. INTRODUCTION

Of all the articles devoted to the design of Heat exchanger networks (see Furman and Sahinidis , 2002; Morar and Agachi, 2010)), very few, if any, have dealt with streams that have variable heat capacity (Cp), perhaps because it was thought that using average *Cp* for streams is a sufficiently good approximation for design purposes. Figure 1, for example, shows the enthalpy of petroleum as a function of temperature (Wauquier, 1995). The slope, which is the heat capacity, increases with temperature. This is consistent with mixtures of high molecular weight.

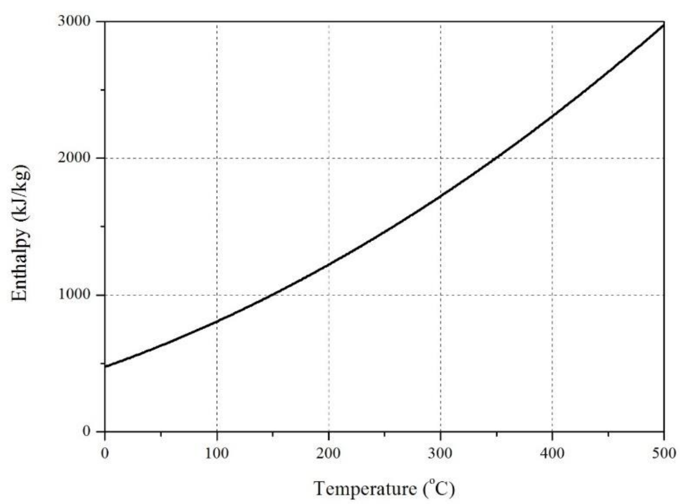


Figure 1. Enthalpy of Petroleum

This feature was pointed out and used in several petroleum fractionation design papers (Bagajewicz and Ji, 2001,2002; Ji and Bagajewicz, 2002a,b,c; Bagajewicz and Soto, 2001, Bagajewicz and Soto, 2003).

In addition, several methods, especially conceptual design methods like the Pinch Design method, have inherent inabilities to be extended to consider it.

On the other hand, as pointed out and shown in part I, the heat exchanger network design problem has been difficult to solve using local solvers, and even some global solvers have recently showed similar convergence difficulties. If one desire to approach in a mathematical programming purist form, one should use a generalized superstructure (Floudas et al., 1986), or its extension to multiple matches (Kim and Bagajewicz, 2016). While the purist approach guarantees, once solved a globally optimal solution can offer structures that are difficult to implement from the practical point of view. We solve this model using RYSIA, a global optimality method based on bound contraction without using branch and bound (Faria and Bagajewicz, 2011a, 2011b).

This paper is organized as follows: We present the revised stages/substages model first discussing critical aspects (reprodcuing all the equations in the appendix). We follow with the modications needed for variable Cp. We then discuss changes to the fixed Cp lower bound model (also shown in the appendix). We then discuss the bound contraction strategy next, including the use of lifting partitions. We then present results.

2. STAGES/SUB-STAGES SUPERSTRUCTURE MODEL

The original stage-wise superstructure proposed by Yee and Grossmann (1990), was extended to multiple substages (Jogunswat et al, 2013) and solved globally by Kim and Bagajewicz (2016) with non isothermal mixing. The model is based on the stages/substages shown in Figure 2.

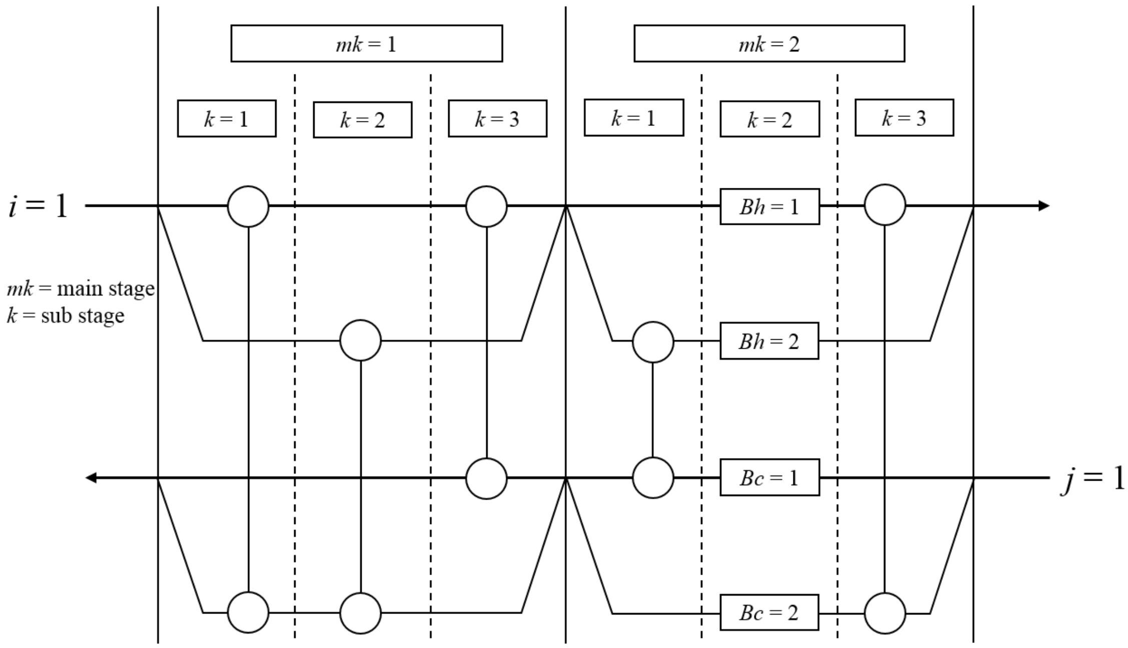


Figure 2. Stage/Sub-stages network superstructure.

Basically, the proposed stage/substage-wise superstructure allows stream branching and the split stream to contain more than one heat exchanger. The original equations for fixed Cp are shown in the Appendix without discussion. We also include the equation for the Lower bound.

3. MODIFICATIONS TO THE STAGES/SUBSTAGES MODEL

We now add the following parameters to the model (see Part I):

$$Cph_i^{IN} = a_i^h + b_i^h Th_i^{IN} + c_i^h \left(Th_i^{IN}\right)^2 \qquad \forall \boldsymbol{i} \qquad (1)$$

$$Cph_i^{OUT} = a_i^h + b_i^h Th_i^{OUT} + c_i^h \left(Th_i^{IN}\right)^2 \qquad \forall \boldsymbol{i} \qquad (2)$$

$$Cpc_j^{IN} = a_j^c + b_j^c Tc_j^{IN} + c_j^c \left(Tc_j^{IN}\right)^2 \qquad \forall \boldsymbol{j} \qquad (3)$$

$$Cpc_j^{OUT} = a_j^c + b_j^c Tc_j^{OUT} + c_j^c \left(T_j^{OUT}\right)^2 \qquad \forall \boldsymbol{j} \qquad (4)$$

We also add the following equations:

$$Cph_{i,mk} = a_i^h + b_i^h Th_{i,mk} + c_i^h \left(Th_{i,mk}\right)^2 \qquad \forall i, mk \qquad (5)$$

$$Cpc_{j,mk} = a_j^c + b_j^c Tc_{j,mk} + c_j^c \left(Tc_{j,mk}\right)^2 \qquad \forall j, mk \qquad (6)$$

$$Cphb_{i,mk,bh,k} = a_i^h + b_i^h Tbh_{i,mk,bh,k} + c_i^h \left(Tbh_{i,mk}\right)^2 \qquad \forall i, mk, bh, k \qquad (7)$$

$$Cpcb_{j,mk,bh,k} = a_j^c + b_j^c Tbc_{j,mk,bh,k} + c_j^c \left(Tbc_{j,mk,bh,k}\right)^2 \qquad \forall j, mk, bh, k \qquad (8)$$

Clearly, these equations can be extended to include cubic terms, logarithm terms and inverse terms.

LOWER BOUND MODEL MODIFICATIONS

The lower bound for constant *Cp* is based on the partition of flowrates and differences of temperature. In turn the *LMTD* function image is partitioned using the partitioned temperature differences. Here we simply add the partition of temperatures as follows:

$$ThD_{i,mk,ph} = T_i^{OUT} + \frac{(ph-1)}{phD}(T_i^{IN} - T_i^{OUT}) \qquad \forall i, mk, bh, k \qquad (9)$$

$$TbhD_{i,mk,bh,k,obh} = T_i^{OUT} + \frac{(obh-1)}{obhD}(T_i^{IN} - T_i^{OUT}) \qquad \forall i, mk, bh, k \qquad (10)$$

$$TbcD_{j,mk,pc} = T_j^{IN} + \frac{(pc-1)}{pcD}(T_j^{OUT} - T_i^{IN}) \qquad \forall i, mk, bh, k \qquad (11)$$

$$TbcD_{j,mk,bh,k,obc} = T_j^{IN} + \frac{(obc-1)}{obcD}(T_j^{OUT} - T_j^{IN}) \qquad \forall i, mk, bh, k \qquad (12)$$

Thus

$$\sum_{ph} ThD_{i,mk,ph} \cdot vTh_{i,mk,ph} \le Th_{i,mk} \le \sum_{ph} ThD_{i,mk,ph+1} \cdot vTh_{i,mk,ph} \qquad \forall i, mk \tag{13}$$

$$\sum_{ph} vTh_{i,mk,ph} = 1 \qquad \forall i, mk \tag{14}$$

$$\sum_{pc} TcD_{j,mk,pc} \cdot vTc_{j,mk,pc} \le Tc_{j,mk} \le \sum_{pc} TcD_{j,mk,pc+1} \cdot vTc_{j,mk,pc} \qquad \forall j, mk \tag{15}$$

$$\sum_{pc} vTc_{j,mk,pc} = 1 \qquad \forall j, mk \tag{16}$$

$$\sum_{obh} TbhD_{i,mk,bh,k,obh} \cdot vTbh_{i,mk,bh,k,obh} \le Tbh_{i,mk,bh,k} \le \sum_{obh} TbhD_{i,mk,bh,k,obh+1} \cdot vTbh_{i,mk,bh,k,obh} \quad \forall i, mk, bh, k \tag{17}$$

$$\sum_{obh} vTbh_{i,mk,bh,k,obh} = 1 \qquad \forall i, mk, bh, k \tag{18}$$

$$\sum_{obc} TbcD_{j,mk,bc,k,obc} \cdot vTbc_{j,mk,bc,k,obc} \le Tbc_{j,mk,bc,k} \le \sum_{obc_{j,mk,bc,k}} TbcD_{j,mk,bc,k,obc+1} \cdot vTbc_{j,mk,bc,k,obc} \quad \forall j, mk, bc, k \tag{19}$$

$$\sum_{obc} vTbc_{j,mk,bc,k,obc} = 1 \qquad \forall j, mk, bc, k \tag{20}$$

We introduce new parameters $CphThD_{i,mk}, CphTbhD_{i,mk,bh,k}$ as the product of temperature and *Cp* as follows:

$$CphThD_{i,mk,ph} = a_i^h ThD_{i,mk,ph} + b_i^h \left(ThD_{i,mk,ph}\right)^2 + c_i^h \left(ThD_{i,mk,ph}\right)^3 \qquad \forall i, mk \tag{21}$$

$$CphTbhD_{i,mk,bh,k,obh} = a_i^h TbhD_{i,mk,bh,k,obh} + b_i^h \left(TbhD_{i,mk,bh,k,obh}\right)^2 + c_i^h \left(TbhD_{i,mk,bh,k,obh}\right)^3 \quad \forall i, mk, bh, k \tag{22}$$

$$CpcTcD_{j,mk,pc} = a_j^c TcD_{j,mk,pc} + b_j^c \left(TcD_{j,mk,pc}\right)^2 + c_j^c \left(TcD_{j,mk,pc}\right)^3 \qquad \forall j, mk \tag{23}$$

$$CpcTbcD_{j,mk,bc,k,obc} = a_j^c TbcD_{j,mk,bc,k,obc} + b_j^c \left(TbcD_{j,mk,bc,k,obc}\right)^2 + c_j^c \left(TbcD_{j,mk,bc,k,obc}\right)^3 \quad \forall i, mk, bh, k \tag{24}$$

Then we rewrite the heat balance equation for the hot streams in each stage as follows:

$$QHM_{i,mk} = Fh_i \cdot CphTh_{i,mk} - Fh_i \cdot CphTh_{i,mk+1} \qquad \forall i, mk \qquad (25)$$

and relax $CphTh_{i,mk}$ as follows:

$$\sum_{ph} CphThD_{i,mk,ph} vTh_{i,mk,ph} \le CphTh_{i,mk} \le \sum_{ph} CphThD_{i,mk,ph+1} vTh_{i,mk,ph} \quad \forall i, mk \qquad (26)$$

In turn we rewrite the heat balance equation for the cold streams in each stage as follows:

$$QCM_{j,mk} = Fc_j CpcTc_{j,mk} - Fc_j CpcTc_{j,mk+1} \qquad \forall j, mk \qquad (27)$$

and relax $CpcTc_{j,mk}$ as follows:

$$\sum_{pc} CpcTcD_{j,mk,pc} vTc_{j,mk,pc} \le CpcTc_{j,mk} \le \sum_{pc} CpcTcD_{j,mk,pc+1} vTc_{j,mk,pc} \quad \forall j, mk \qquad (28)$$

We relax the equation defining $AH_{i,mk,bh,k}$ ($AH_{i,mk,bh,k} = Tbh_{i,mk,bh,k} Fbh_{i,mk,bh} Cphb_{i,mk,bh,k}$) as follows:

$$\begin{aligned} &\sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh} \cdot FbhD_{i,mk,bh,ofh} vTbh_{i,mk,bh,k,obh} vFbh_{i,mk,bh,ofh} \le AH_{i,mk,bh,k} \le \\ &\le \sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh+1} \cdot FbhD_{i,mk,bh,ofh+1} vTbh_{i,mk,bh,k,obh} vFbh_{i,mk,bh,ofh} \end{aligned} \qquad \forall i, mk, bh, k \qquad (29)$$

$$\sum_{obh} CphTbhD_{i,mk,bh,k,obh} vTbh_{i,mk,bh,k,obh} \le CphTbh_{i,mk,bh,k} \le \sum_{obh} CphTbhD_{i,mk,bh,k,obh+1} vTbh_{i,mk,bh,k,obh}$$
$$\forall i, mk, bh, k \qquad (30)$$

We now replace the product of binaries by a continuous variable $WTbhFbh_{i,mk,bh,k,obh,ofh} = vTbh_{i,mk,bh,k,obh} vFbh_{i,mk,bh,ofh}$ so we write the relaxed equation as follows:

$$\begin{aligned}&\sum_{obh}\sum_{ofh} CphTbhD_{i,mk,bh,k,obh}\cdot FbhD_{i,mk,bh,ofh} WTbhFbh_{i,mk,bh,k,obh,ofh} \le AH_{i,mk,bh,k} \le \\ &\le \sum_{obh}\sum_{ofh} CphTbhD_{i,mk,bh,k,obh+1}\cdot FbhD_{i,mk,bh,ofh+1} WTbhFbh_{i,mk,bh,k,obh,ofh}\end{aligned} \qquad \forall i,mk,bh,k \quad (31)$$

$$WTbhFbh_{i,mk,bh,k,obh,ofh} \le vTbh_{i,mk,bh,k,obh} \qquad \forall i,mk,bh,k,obh,ofh \quad (32)$$

$$WTbhFbh_{i,mk,bh,k,obh,ofh} \le vFbh_{i,mk,bh,ofh} \qquad \forall i,mk,bh,k,obh,ofh \quad (33)$$

$$WTbhFbh_{i,mk,bh,k,obh,ofh} \ge vTbh_{i,mk,bh,k,obh} + vFbh_{i,mk,bh,ofh} - 1 \qquad \forall i,mk,bh,k,obh,ofh \quad (34)$$

We do the same to (A13). We relaxed it as follows:

$$\begin{aligned}&\sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc}\cdot FbcD_{j,mk,bc,ofc} vTbc_{j,mk,bc,k,obc_{j,mk,bc,k}} vFbc_{j,mk,bc,ofc} \le AC_{j,mk,bc,k} \le \\ &\le \sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc+1}\cdot FbcD_{j,mk,bc,ofc+1} vTbc_{j,mk,bc,k,obc} vFbc_{j,mk,bc,ofc}\end{aligned} \qquad \forall j,mk,bc,k \quad (35)$$

$$\sum_{obc} CpcTbcD_{j,mk,bc,k,obc} vTbc_{j,mk,bc,k,obc} \le CpcTbc_{j,mk,bc,k} \le \sum_{obc_{j,mk,bc,k}} CpcTbcD_{j,mk,bc,k,obc+1} vTbc_{j,mk,bc,k,obc}$$

$$\forall j,mk,bc,k \qquad (36)$$

We introduce a new variable $WTbcFbc_{j,mk,bc,k,obc,ofc} = vTbc_{j,mk,bc,k,obc} vFbc_{j,mk,bc,ofc}$ so we write the relaxed equation as follows:

$$\begin{aligned}&\sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc}\cdot FbcD_{j,mk,bc,ofc_{j,mk,bc}} WTbcFbc_{j,mk,bc,k,obc,ofc} \le AC_{j,mk,bc,k} \le \\ &\le \sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc+1}\cdot FbcD_{j,mk,bc,ofc+1} WTbcFbc_{j,mk,bc,k,obc,ofc}\end{aligned} \qquad \forall j,mk,bc,k \quad (37)$$

$$WTbhFbh_{i,mk,bh,k,obh,ofh} \le vTbh_{i,mk,bh,k,obh} \qquad \forall i,mk,bh,k,obh,ofh \quad (38)$$

$$WTbhFbh_{i,mk,bh,k,obh_{i,mk,bh,k},ofh_{i,mk,bh}} \leq vFbh_{i,mk,bh,ofh_{i,mk,bh}} \qquad \forall i,mk,bh,k,obh,ofh \qquad (39)$$

$$WTbhFbh_{i,mk,bh,k,obh,ofh} \geq vTbh_{i,mk,bh,k,obh} + vFbh_{i,mk,bh,ofh} - 1 \qquad \forall i,mk,bh,k,obh,ofh \qquad (40)$$

We rewrite the equations linking $AC_{i,mk,bc,1}$ with the products of temperature, Cp and flow as follows :

$$\sum_{bh} AH_{i,mk,bh,1} = Fh_i CphTh_{i,mk} \qquad \forall i,mk \qquad (41)$$

$$\sum_{bh} AH_{i,mk,bh,SBNOK+1} = Fh_i CphTh_{i,mk+1} \qquad \forall i,mk \qquad (42)$$

$$\sum_{bc} AC_{i,mk,bc,1} = Fc_j CpcTc_{j,mk} \qquad \forall j,mk \qquad (43)$$

$$\sum_{bc} AC_{j,mk,bc,SBNOK+1} = Fc_j CpcTc_{j,mk+1} \qquad \forall j,mk \qquad (44)$$

$CphTh_{i,mk}$ and $CpcTc_{j,mk}$ are already relaxed in equations (26) and (28)

5. SOLUTION STRATEGY USED BY RYSIA

After partitioning each one of the variables in the bilinear terms and the nonconvex terms, our method consists of a bound contraction step that uses a procedure for eliminating partitions. In the heat exchanger network problems the bilinear terms are composed of the product of heat capacity flow rates and stream temperatures, and the nonconvex terms are the logarithmic mean temperature differences of the area calculation. Details of this strategy were discussed in Part I.

6. EXAMPLES

Our examples were implemented in GAMS (version 23.7) (Brooke et al., 2007) and solved using CPLEX (version 12.3) as the MIP solver and DICOPT (Viswanathan and Grossmann, 1990) as the MINLP solver on a PC machine (i7 3.6GHz, 8GB RAM).

6.1. Example 1: The first example is an example to find the optimum HEN design consist of three hot streams, two cold streams. We illustrate the proposed approach in detail and make a comparison between the fixed Cp and the variable Cp models using this example, which is adapted from Nguyen et al. (2010). The data are presented in Table 1 and 2. We used a minimum temperature approach of 10° C, a fixed cost of units is 250,000$, and the area cost coefficient is 550$/m^2. We solved using two main stages and two sub-stages model. We assumed that the limit of number of branched stream for hot and cold stream was 2.

Table 1. Data for example 1

Stream	F [kg/s]	T_{in} [C]	T_{out} [°C]	h [KW/m^2·°C]
H1	210	159	77	0.4
H2	18	267	88	0.3
H3	50	343	90	0.25
C1	90	26	127	0.15
C2	180	118	265	0.5
HU		500	499	0.53
CU		20	40	0.53

Table 2. Cost data for example 1.

Heating utility cost	100 [$/KJ]
Cooling utility cost	10 [$/KJ]
Fixed cost for heat exchangers	250,000 [$/unit]
Variable cost for heat exchanger area	550 [$/m^2]

The globally optimal solution for the fixed Cp model has an annualized cost of $1,783,257 and was obtained in the root node of 7th iteration satisfying 1% gap between UB and LB. The optimal solution network is presented in Figure 3. We showed alternative solutions with a different number of sub-stages in Part I of the paper using the fixed Cp model. One of these solutions was also obtained by Kim and Bagajewicz (2016) using a new generalized superstructure solved using RYSIA.

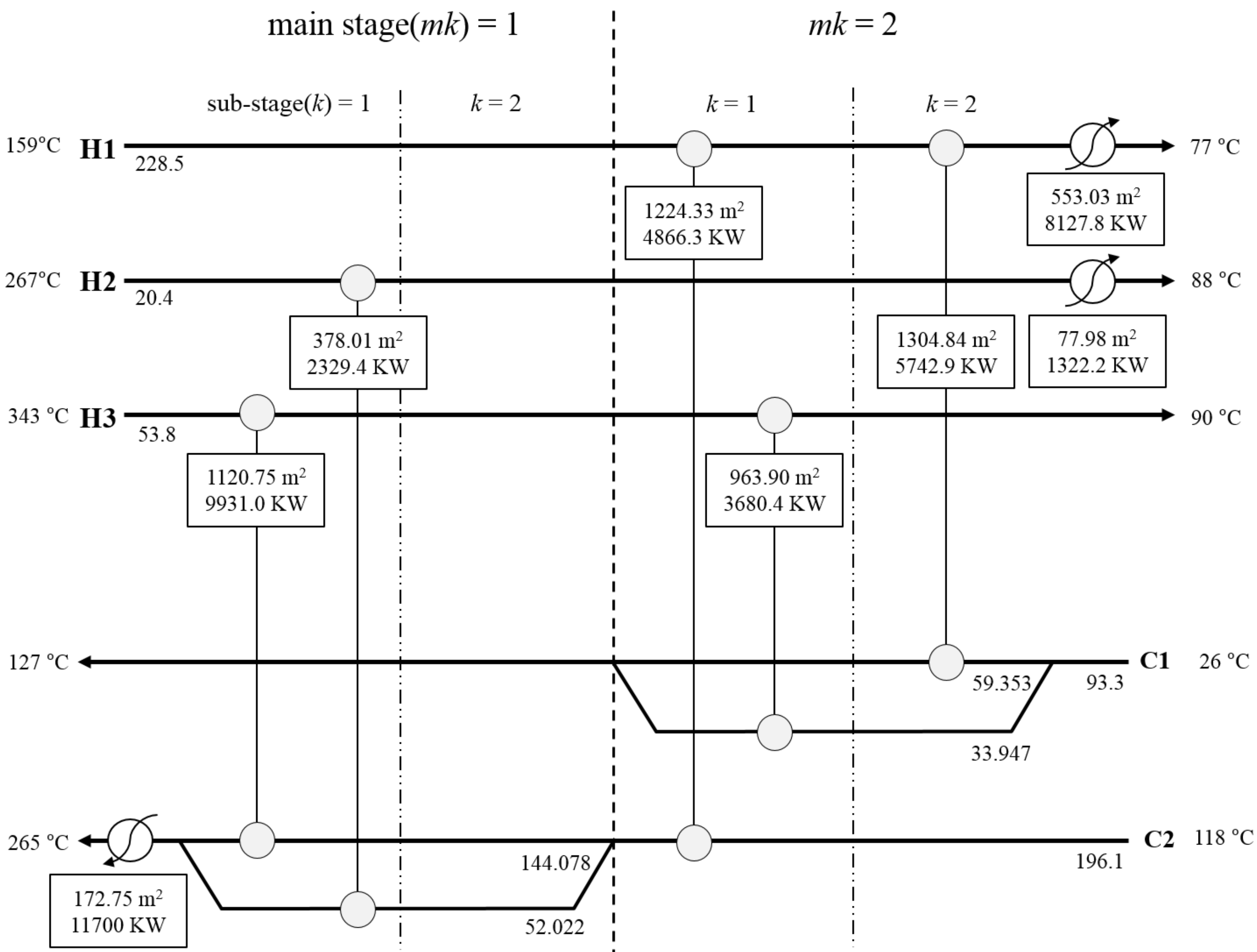


Figure 3. The solution network for example 1 with 2 main stages and 2 sub-stages.

We now introduce variable Cp. The values of parameters *a*, *b* and *c* are presented in Table 3. These parameters are produced by varying with temperature so that the amount of heat is the same for each stream.

Table 3. Parameters of variable Cp for example 1.

	a	*b*	*c*
H1	0.16135	0.01083	-2.49681×10^{-5}
H2	0.70678	0.00334	-5.05484×10^{-6}
H3	0.77039	0.00198	-2.46313×10^{-6}
C1	0.25693	0.01445	-5.13029×10^{-5}
C2	0.57327	0.00372	-5.25405×10^{-6}

We partitioned flows and temperatures in the bilinear terms of the energy balances and ΔT in the area calculations using 2 partitions. Extended partition forbidding (applied only when the number of partitions increases above 2) is used in bound contraction. The lower limits of total area and total heat of heating utilities in the lifting partitioning are used for 5590 m^2 and 11700 kW calculated using pinch analysis. The globally optimal solution for variable Cp has an annualized cost of $1,783,727 using 9 iterations and 29 min 22 sec cpu time with 0% gap between UB and LB. The results are summarized in Table 4 and the optimal solution network is presented in Figure 4.

Table 4. Global optimal solution of example 1 for variable Cp.

# of starting partitions	Objective value ($) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	1,783,727	0%	9	2	29m 22s

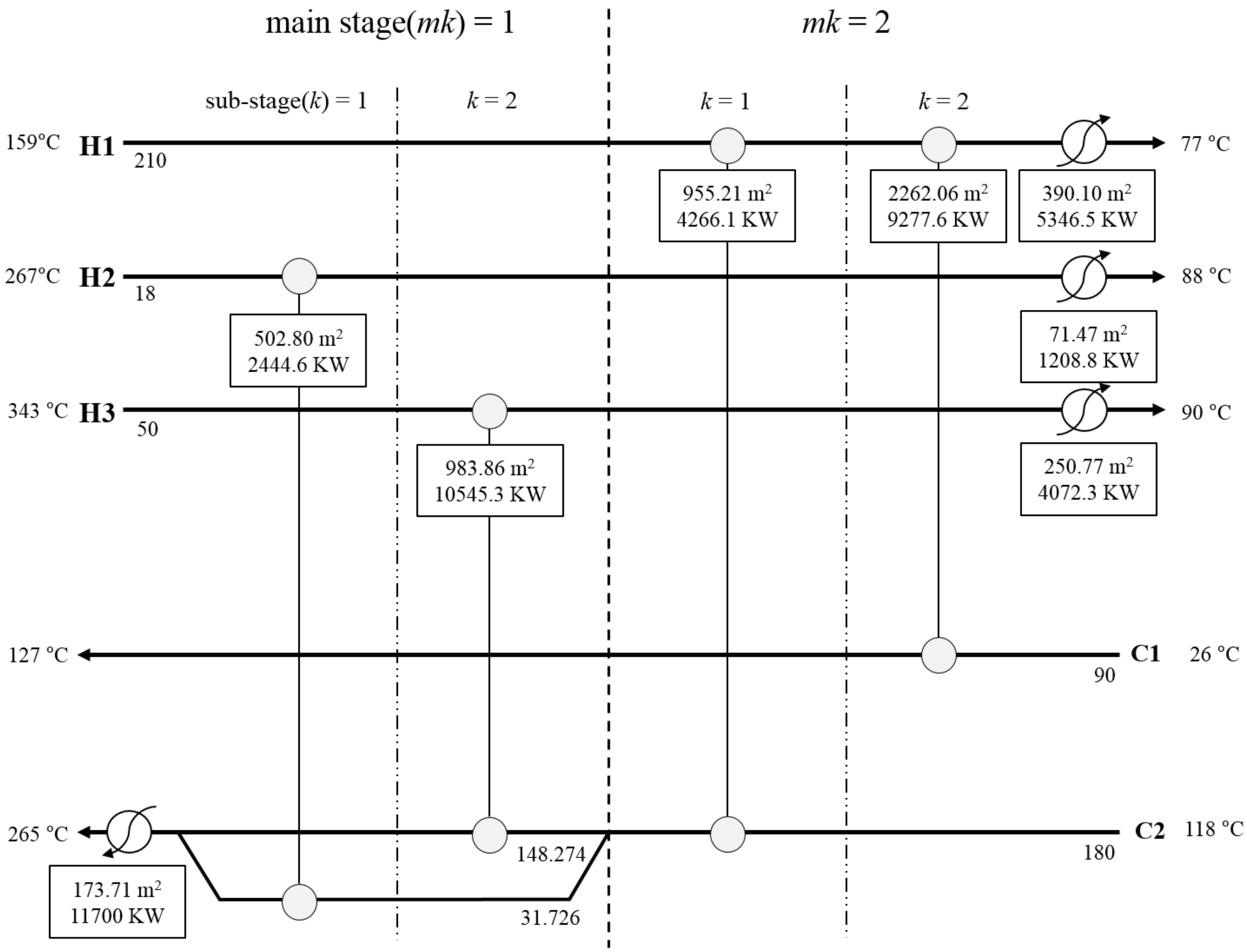


Figure 4. The solution network of example 1 for variable Cp.

If we use that the value of parameter *a* is one and the others are zero (i.e. Cp=1) for the same condition with the fixed Cp. We obtained a globally optimal solution of 1,786,076 with 0.79% gap using 4 iterations and 5 min 10 sec cpu time. A very similar solution network with the fixed Cp model (Figure 3) is obtained when using Cp=1 and this optimum solution network is presented in Figure 5.

We tried to solve this problem using BARON (version 14.4) (Sahinidis, 1996), and ANTIGONE (version 1.1) (Misener and Floudas, 2014). None of them rendered a feasible solution.

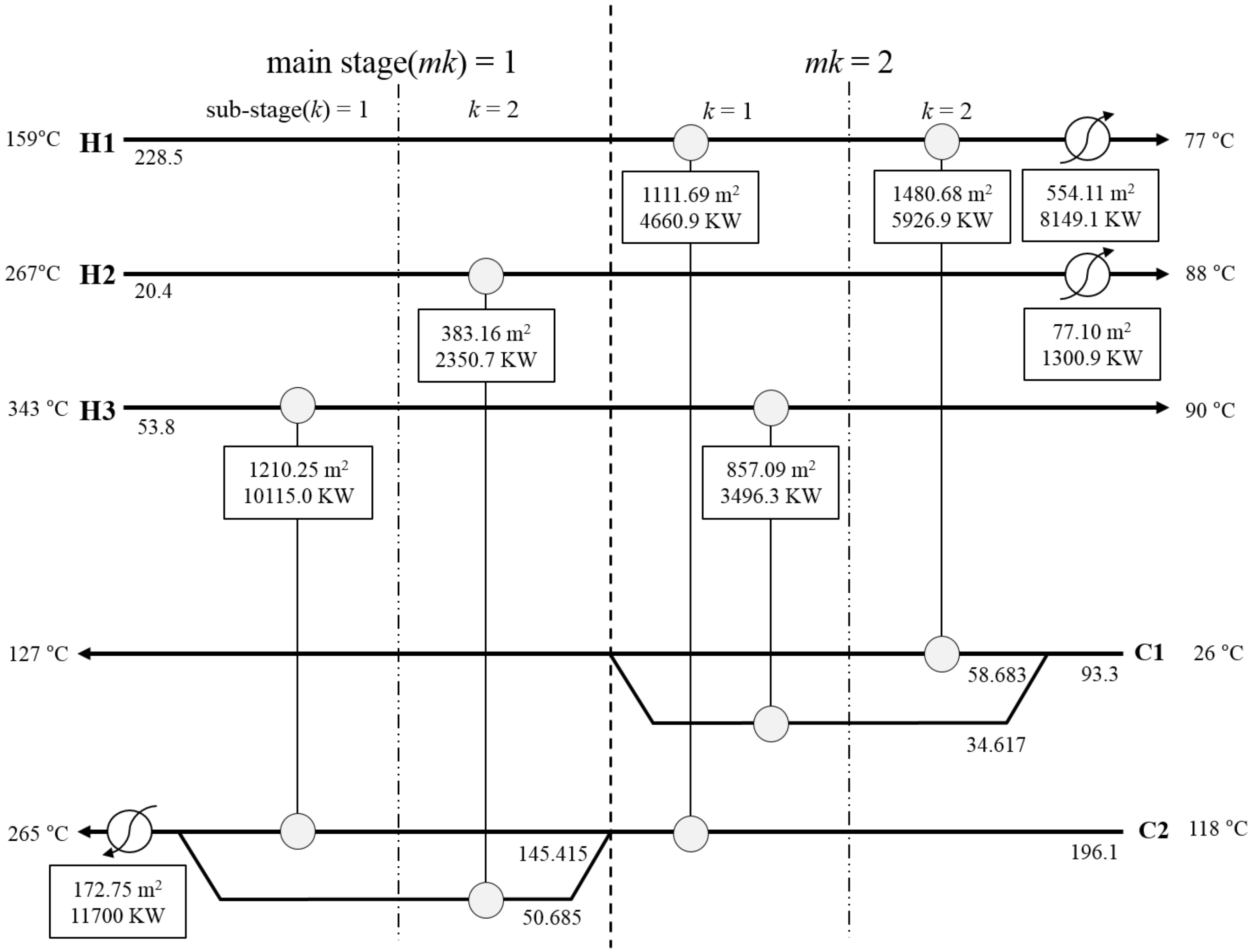


Figure 5. The solution network of example 1 for Cp=1.

6.2. Example 2: The second example is 10SP1 (Cerda, 1980). This example consists of four hot and five cold streams and the data is given in Table 5 and 6. We assumed a minimum temperature approach of 10º C. The fixed cost of units is 5,291.9$, and the area cost coefficient is 77.79$/m^2. We solved using two main stages and two sub-stages model. We assumed that the limit of number of branched stream for hot and cold stream was 2.

Table 5. Data for example 2

Stream	F [Kg/s]	T_{in} [ºC]	T_{out} [ºC]	h [kJ/s·m^2·ºC]
H1	2	160	93	0.06
H2	3	249	138	0.06
H3	4	227	66	0.06
H4	5	199	66	0.06
C1	2	60	160	0.06
C2	1	116	222	0.06
C3	2	38	221	0.06
C4	5	82	177	0.06
C5	4	93	205	0.06
HU		38	82	0.06
CU		271	149	0.06

Table 6. Cost data for example 2.

Heating utility cost	566,167 [$/(kJ/s)]
Cooling utility cost	53,349 [$/(kJ/s)]
Fixed cost for heat exchangers	5,291.9 [$/unit]
Variable cost for heat exchanger area	77.79 [$/m^2]

We partitioned flows, temperature and ΔT with 2 intervals and used the extended interval forbidding. Lower limits of total area and total heat of heating utilities in the lifting partitioning are used for 3000 m^2 and 150 KJ/s from (Faria et al., 2015). Upper limits are used 50% higher values than lower limits. We produced the value of parameters *a*, *b* and *c* in Table 7 for variable Cp by varying with temperature so that the amount of heat is the same for each stream.

Table 7. Parameters of variable Cp for example 2.

	a	b	c
H1	-0.49215	0.01250	$-2.800*10^{-5}$
H2	-0.03388	0.00492	$-7.200*10^{-6}$
H3	0.36506	0.00454	$-8.400*10^{-6}$
H4	0.16632	0.00600	-1.220×10^{-5}
C1	-0.05020	0.00952	-2.370×10^{-5}
C2	0.68902	0.00580	-9.700×10^{-6}
C3	0.60183	0.00480	-1.010×10^{-5}
C4	-0.22326	0.00850	-1.810×10^{-5}
C5	-0.02567	0.00625	-1.150×10^{-5}

The globally optimal solution features an annualized cost of $99,629,274 and was obtained in the root node of the 8^{th} iteration satisfying 1% gap between UB and LB able in Table 8. The optimal solution network is presented in Figure 6.

Table 8. Global optimal solution of example 1 for variable Cp.

# of starting partitions	Objective value ($) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	99,629,274	0.01%	8	2	17m 34s

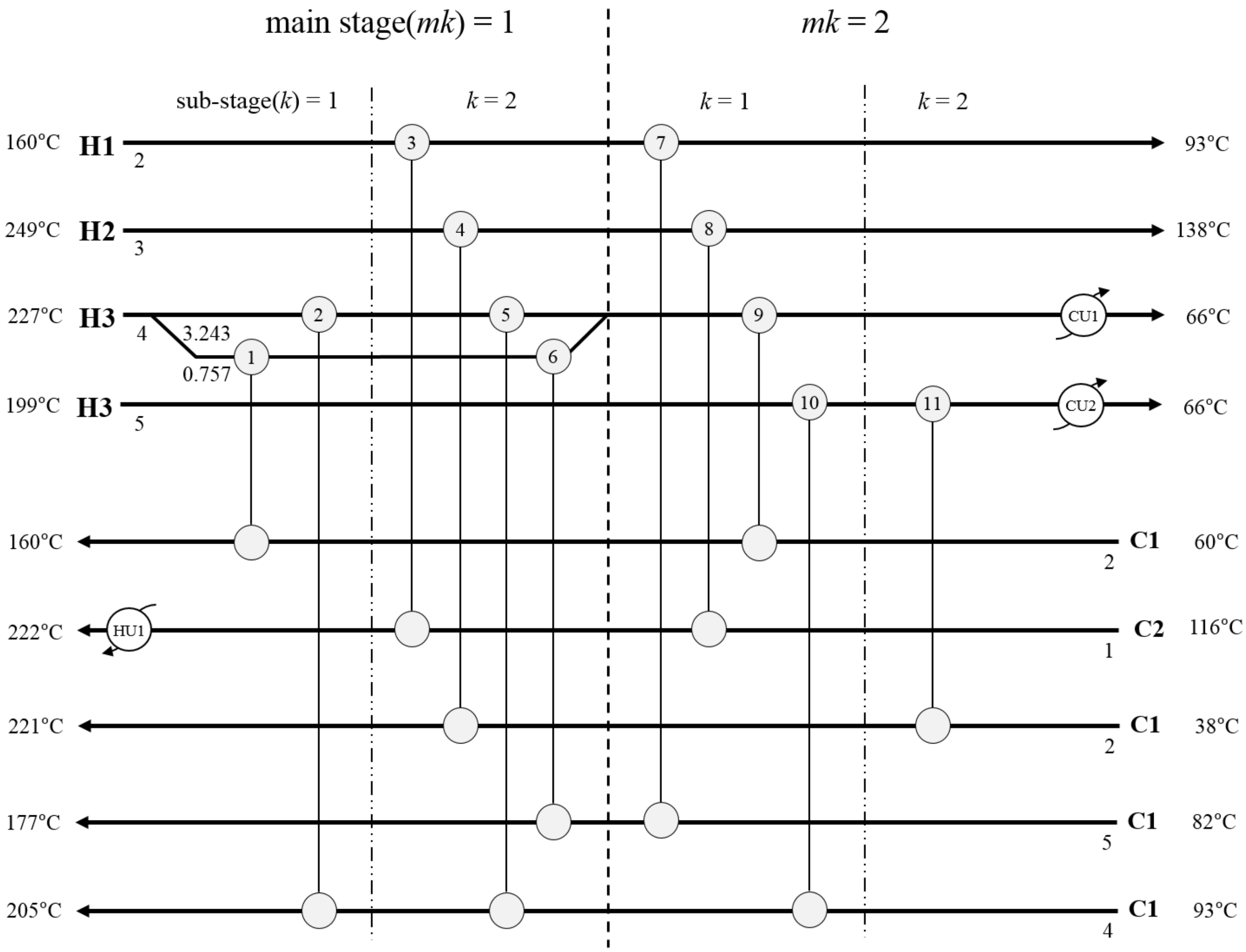


Figure 6. The solution network of example 2 for variable Cp.

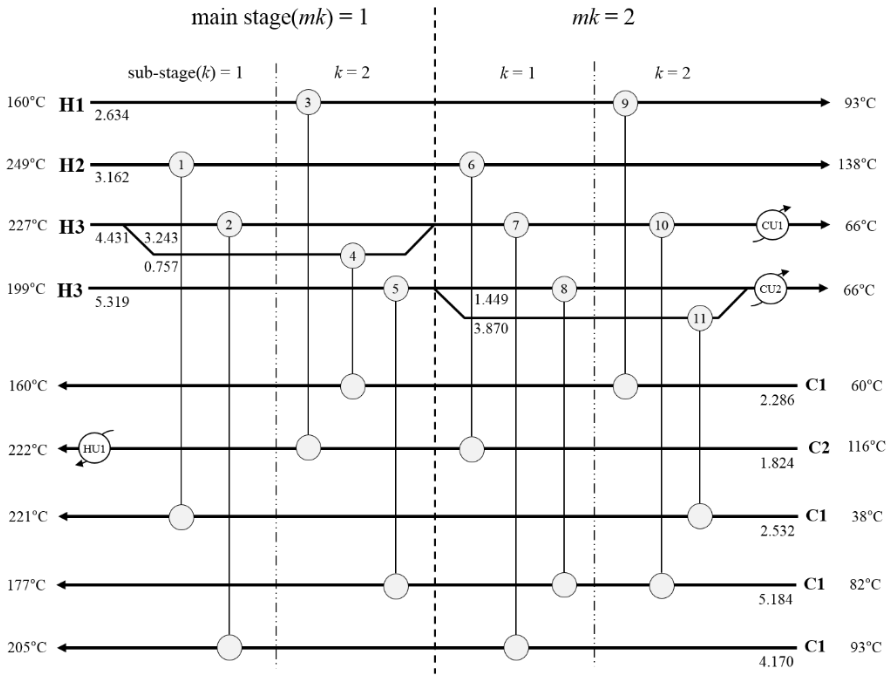
We also tested with Cp=1 and we obtained a globally optimal solution of $99,369,753 with 0.2% gap using 15 min 24 sec cpu time (Table 9). We compared this optimal solution with the fixed Cp solution from the generalized superstructure model in Table 10 and figure 7. Finally, we tried to solve this problem using BARON (version 14.4) (Sahinidis, 1996), and ANTIGONE (version 1.1) (Misener and Floudas, 2014). None of them rendered a feasible solution.

Table 9. Heat exchanger results for example 2.

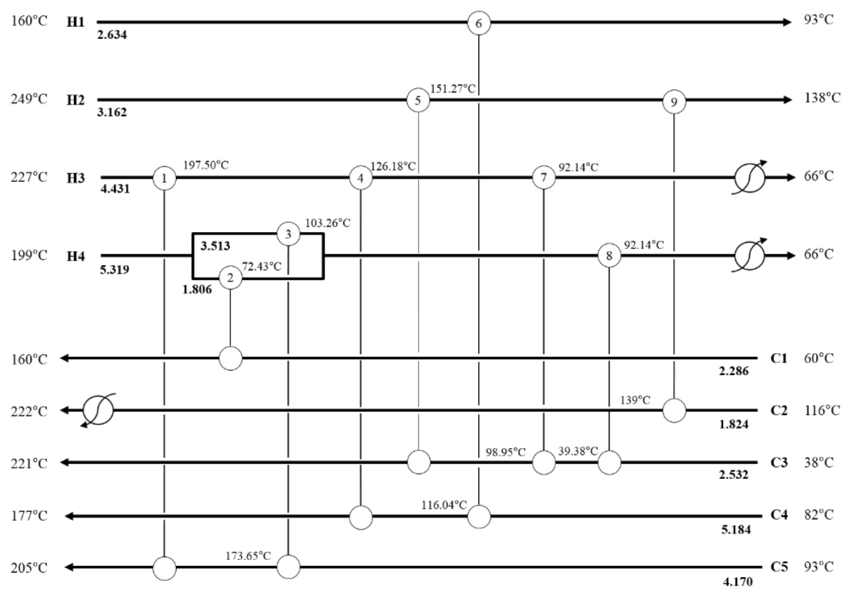
	Area (m^2)	Q (KW)
HX1	89.332	79.18
HX2	52.390	33.45
HX3	20.630	13.93
HX4	291.435	321.14
HX5	672.873	305.64
HX6	467.992	328.15
HX7	243.635	159.56
HX8	43.989	24.92
HX9	213.117	145.74
HX10	209.611	124.51
HX11	136.632	137.21
CU1	193.731	144.37
CU2	219.394	114.90
HU1	206.147	151.00

Table 10. Comparing the variable Cp model when Cp=1 and the fixed Cp model from the generalized superstructure model (Kim and Bagajewicz, 2016).

	Objective value ($)	Gap	# of iterations	# of partitions at convergence	CPU Time
Variable Cp model (when Cp=1)	99,629,274	0.01%	8	2	17m 34s
Fixed Cp model (superstructure model)	99,636,825	0.9%	3	2	22m 41s



(a)



(b)

Figure 7. Optimal solution networks for example 2 (a) when Cp=1 with for variable Cp (b) when the fixed Cp used for the generalized superstructure model (Kim and Bagajewicz, 2016).

6.3. Example 3: The third example consisting of 11 hot and 2 cold streams corresponds to a crude fractionation unit. The data is given in Table 11 and 12. This example was solved using 2 main stages and 2 sub-stages superstructure model. We assumed a minimum temperature approach of $EMAT_{i,j}$ =10 ºC. We also assumed that 4 branched streams are possible in cold stream and no branching on hot stream. The fixed cost of units is 250,000$, and the area cost coefficient is 550 $/m^2. The lower limits of total area and total heat of heating utilities in the lifting partitioning are used for 8636 m^2 and 23566 kW, respectively calculated using pinch analysis.

Table 11. Data for example 3

Stream		F [kg/s]	T_{in} [C]	T_{out} [C]	H [KW/m^2·C]
H1	TCR	46.30	140.2	39.5	0.26
H2	LGO	12.70	248.8	110	0.72
H3	KEROSENE	14.75	170.1	60	0.45
H4	HGO	9.83	277	121.9	0.57
H5	HVGO	55.08	250.6	90	0.26
H6	MCR	46.03	210	163	0.33
H7	LCR	82.03	303.6	270.2	0.41
H8	VR1	23.42	360	241.4	0.47
H9	LVGO	19.14	178.6	108.9	0.6
H10	SR-Quench	7.66	359.6	280	0.47
H11	VR2	23.42	241.4	280	0.47
C1	Crude	96.41	30	130	0.26
C2	Crude	96.64	130	350	0.72
HU			500	499	0.53
CU			20	40	0.53

Table 12. Cost data for example 3.

Heating utility cost	100 [$/KJ]
Cooling utility cost	10 [$/KJ]
Fixed cost for heat exchangers	250,000 [$/unit]
Variable cost for heat exchanger area	550 [$/m^2]

Flows, temperature and ΔT were partitioned into 2 intervals and the extended interval forbidding was used for bound contracting. We produced the value of parameters *a*, *b* and *c* in Table 13 for variable Cp by varying with temperature so that the amount of heat is the same for each stream.

Table 13. Parameters of variable Cp for example 3.

	a	b	c
H1	1.27	0.011	-3.54×10^{-5}
H2	1.70	0.004	-6.29×10^{-6}
H3	1.28	0.008	-1.93×10^{-5}
H4	1.87	0.003	-4.54×10^{-6}
H5	1.94	0.003	-6.02×10^{-6}
H6	-0.20	0.013	-2.05×10^{-5}
H7	-1.41	0.015	-1.74×10^{-5}
H8	-0.31	0.006	-5.95×10^{-6}
H9	0.89	0.010	-2.01×10^{-5}
H10	1.89	0.004	-4.06×10^{-6}
H11	1.01	0.003	-4.03×10^{-6}
C1	0.89	0.014	-4.75×10^{-5}
C2	2.48	0.001	-2.38×10^{-6}

We found the solution with a 1.4% gap between the UB and LB in Table 14. The results are summarized in Table 15. The optimum solution, presented in Figure 8, has an annualized cost of $3,451,585.

Table 14. Global optimal solution of example 1 for variable Cp.

# of starting partitions	Objective value ($) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	3,451,585	1.4%	2	2	24m 48s

Table 15. Heat exchanger results for example 3.

		Area (m^2)	Q (KW)
HX1		515.97	1834.6
HX2		343.83	3277.9
HX3		2904.71	12761.9
HX4		482.84	5405.4
HX5		993.55	7933.0
HX6		67.59	2782.5
HX7		334.78	3327.8
HX8		594.63	6037.0
HX9		29.58	529.9
HX10		57.27	1948.9
HX11		208.98	4409.6
CU1		1086.88	10721.7
CU2		11.27	1893.9
CU3		464.76	8461.1
CU4		30.69	923.8
HU1		408.63	23566.0

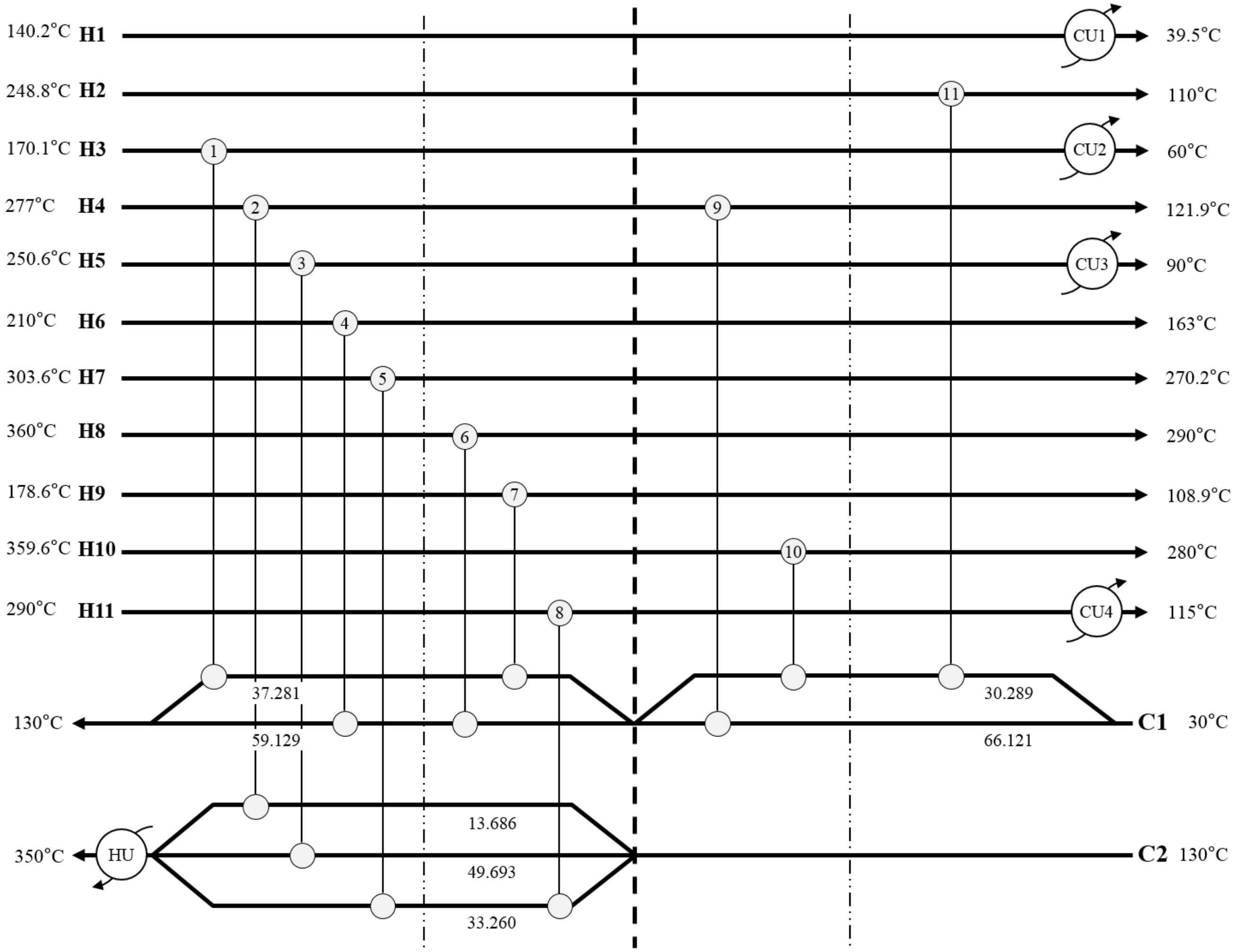


Figure 8. The solution network of example 3 for variable Cp.

We obtained the similar objective values with the fixed Cp model (Part I of this paper) and the generalized superstructure model (Kim and Bagajewicz, 2016), but we obtained the different solution network (Figure 8). We tried to solve this problem using BARON (version 14.4) (Sahinidis, 1996), and ANTIGONE (version 1.1) (Misener and Floudas, 2014). None of them rendered a feasible solution after 24 hours of running.

7. CONCLUSIONS

We use a new stages/substages model proposed by Jonguswat et al. (2014) to solve globally heat exchanger network problems. We used RYSIA, a newly developed global optimization procedure based on bound contraction (without resorting to branch and bound). For the lower bound, we use relaxations based on partitioning one variable of bilinear terms. We also partition domain and images of monotone functions, a methodology that avoids severe reformulation to obtain bilinear terms when such reformulation is possible. We also use recently introduced lifting partitioning constraints (Kim and Bagajewicz, 2016) to improve the lower bound value as well as its computational time. Our two examples proved to be computationally very challenging as several sub-optimal solutions exist within a small gap between lower and upper bound. We also found that our method is able to obtain results when BARON and ANTIGONE had serious difficulties (they do not obtain a feasible solution). Finally, there is a need for a new set of methods to accelerate convergence when a small gap is achieved, research that is left for future work.

NOMENCLATURE

SETS

i	: Hot process stream
j	: Cold process stream
mk	: Stage
bh	: Hot stream branch
bc	: Cold stream branch
k	: Sub-stage
ofh	: Heat capacity flow rate partitioning point for hot stream

ofc	: Heat capacity flow rate partitioning point for cold stream
ph	: Main-stage temperature partitioning point for hot stream
pc	: Main-stage temperature partitioning point for cold stream
obh	: Sub-stage temperature partitioning point for hot stream
obc	: Sub-stage temperature partitioning point for cold stream
lhx	: Hot side temperature differences partitioning point
nhx	: Cold side temperature differences partitioning point

PARAMETERS

NOK	: Number of main stages
$SBNOK$	: Number of sub stages
Fh_i	: Heat capacity flow rate for hot stream
Fc_j	: Heat capacity flow rate for cold stream
T_i^{HIN}	: Inlet temperature of hot stream
T_i^{HOUT}	: Outlet temperature of hot stream
T_j^{CIN}	: Inlet temperature of cold stream
T_j^{COUT}	: Outlet temperature of cold stream
T_{CU}^{IN}	: Inlet temperature of cold utility
T_{CU}^{OUT}	: Outlet temperature of cold utility
T_{HU}^{IN}	: Inlet temperature of hot utility
T_{HU}^{OUT}	: Outlet temperature of hot utility
C_{var}	: Variable cost coefficients for heat exchangers

C_{fixed} : Fixed cost coefficients for heat exchangers

$CU\text{cost}$: Hot utility cost

$HU\text{cost}$: Cold utility cost

$EMAT$: Exchanger minimum approach different

$FbhD_{i,mk,bh,ofh}$: Discrete point of the partitioned flow rate of hot stream

$FbcD_{j,mk,bc,ofc}$: Discrete point of the partitioned flow rate of cold stream

$ThD_{i,mk,ph}$: Discrete point of the partitioned temperature of main-stage hot stream

$TcD_{j,mk,pc}$: Discrete point of the partitioned temperature of main-stage cold stream

$TbhD_{i,mk,bh,obh}$: Discrete point of the partitioned temperature of sub-stage hot stream

$TbcD_{j,mk,bc,k,obc}$: Discrete point of the partitioned temperature of sub-stage cold stream

$CphThD_{i,mk,ph}$: Discrete point of the partitioned $CphTh_{i,mk}$

$CpcTcD_{j,mk,pc}$: Discrete point of the partitioned $CpcTc_{j,mk}$

$CphTbhD_{i,mk,bh,k,obh}$: Discrete point of the partitioned $CphTbh_{i,mk,bh,k}$

$CpcTbcD_{j,mk,bc,k,obc}$: Discrete point of the partitioned $CpcTbc_{j,mk,bc,k}$

$ThD_{i,j,mk,bh,bc,k,lhx}$: Discrete point of temperature differences in hot side of heat exchanger

$TcD_{i,j,mk,bh,bc,k,nhx}$: Discrete point of temperature differences in cold side of heat exchanger

BINARY VARIABLES

$z_{i,j,mk,bh,bc,k}$: Binary variable to denote a heat exchanger

zcu_i : Binary variable to denote a cold utility

zhu_j : Binary variable to denote a hot utility

$vFbhD_{i,mk,bh,ofh}$: Binary variable related to the partitioned hot stream sub-stage flow rate

$vFbcD_{j,mk,bc,ofc}$: Binary variable related to the partitioned cold stream sub-stage flow rate

$vThD_{i,mk,ph}$: Binary variable related to the partitioned hot stream main-stage temperature

$vTcD_{j,mk,pc}$: Binary variable related to the partitioned cold stream main-stage temperature

$vTbhD_{i,mk,bh,k,obh}$: Binary variable related to the partitioned hot stream sub-stage temperature

$vTbcD_{j,mk,bc,k,obc}$: Binary variable related to the partitioned cold stream sub-stage temperature

$YHX_{i,j,mk,bh,bc,k,lhx}$: Binary variable related to the partitioned hot side temperature differences

$YHX_{i,j,mk,bh,bc,k+1,nhx}$: Binary variable related to the partitioned cold side temperature differences

VARIABLES

$q_{i,j,mk,bh,bc,k}$: Exchanged heat for (i, j) match in stage *mk* on sub-stage *k*

qcu_i : Cold utility demand for stream *i*

qhu_j : Hot utility demand for stream *j*

HA_{mk} : Total exchanged heat in stage *mk*

$QHM_{i,mk}$: Total exchanged heat for hot stream *i* in stage *mk*

$QH_{i,mk,bh}$: Total exchanged heat for branch *bh* of hot stream *i* in stage *mk*

$qHK_{i,mk,bh,k}$: Exchanged heat for branch *bh* of hot stream *i* in stage *mk* on sub-stage *k*

$AH_{i,mk,bh,k}$: Product of $Tbh_{i,mk,bh,k}$ and $Fbh_{i,mk,bh}$

CA_{mk} : Total exchanged heat in stage *mk*

$QCM_{j,mk}$: Total exchanged heat for cold stream *j* in stage *mk*

$QC_{j,mk,bc}$: Total exchanged heat for branch *bc* of cold stream *j* in stage *mk*

$qCK_{j,mk,bc,k}$: Exchanged heat for branch *bc* of cold stream *j* in stage *mk* on sub-stage *k*

$AC_{j,mk,bc,k}$: Product of $Tbc_{j,mk,bc,k}$ and $Fbc_{j,mk,bc}$

$Cph_{i,mk}$: Variable heat capacity of hot stream for main-stage

$Cpc_{j,mk}$: Variable heat capacity of cold stream for main-stage

$Cphb_{i,mk,bh,k}$: Variable heat capacity of hot stream for sub-stage

$Cpcb_{j,mk,bc,k}$: Variable hear capacity of cold stream for sub-stage

$Th_{i,mk}$: Temperature of hot stream i on the hot side of main stage mk

$Tc_{j,mk}$: Temperature of cold stream j on the cold side of main stage mk

$Tbh_{i,mk,bh,k}$: Temperature of branch hot stream i on the hot side of stage mk

$Tbc_{j,mk,bc,k}$: Temperature of branch cold stream j on the cold side of stage mk

$CphTh_{i,mk}$: Product of $Th_{i,mk}$ and $Cph_{i,mk}$

$CpcTc_{j,mk}$: Product of $Tc_{j,mk}$ and $Cpc_{j,mk}$

$CphTbh_{i,mk,bh,k}$: Product of $Tbh_{i,mk,bh,k}$ and $Cphb_{i,mk,bh,k}$

$CpcTbc_{j,mk,bc,k}$: Product of $Tbc_{j,mk,bc,k}$ and $Cpcb_{j,mk,bc,k}$

$Fbh_{i,mk,bh}$: Heat capacity flow rate of branch hot stream on the stage mk

$Fbc_{j,mk,bc}$: Heat capacity flow rate of branch cold stream on the stage mk

$\Delta Th_{i,j,mk,bh,bc,k}$: Hot side temperature difference

$\Delta Tc_{i,j,mk,bh,bc,k}$: Cold side temperature difference

ΔTcu_{i} : Cold utility temperature difference

ΔThu_{j} : Hot utility temperature difference

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