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Global Optimization of Heat Exchanger Networks. Part 2: Stages/Substages Superstructure with Variable *Cp*

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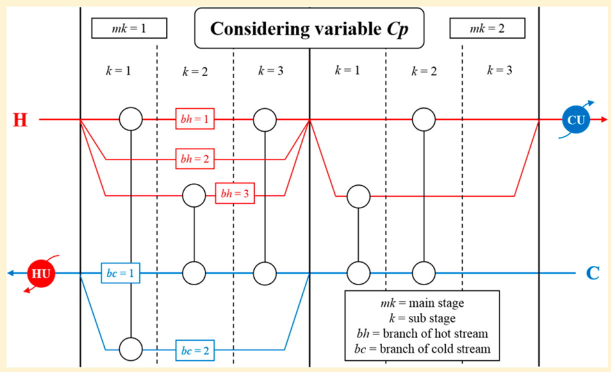
ABSTRACT: We extend the formulation of the stages/substages model described in the first part of this series to account for variable heat capacity with temperature, whose influence on heat exchanger network design was not studied. Variable heat capacity (*Cp*) frequently arises when streams of high molecular weight are used, or when temperature ranges are large, such as in petroleum fractionation, where the range of temperatures in streams spans more than 100 °C. We solve our model globally using RYSIA, a recently developed method bound contraction procedure (*Comput. Chem. Eng.* **2011**, *35*, 446−455; *Ind. Eng. Chem. Res.* **2015**, *54* (5), 1595−1604). 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,[3,4] 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,

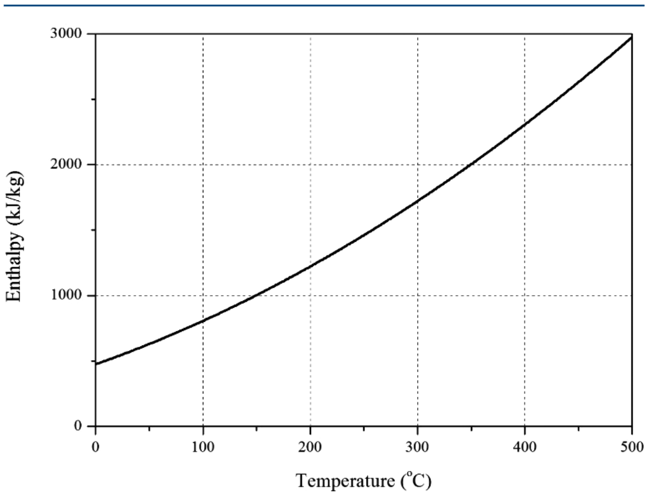


Figure 1. Enthalpy of crude oil (K_w = 11.8).[5]

shows the enthalpy of petroleum (Watson Characterization Factor (K_w) = 11.8)) as a function of temperature.[5] The slope, which is the heat capacity, increases with temperature. This is consistent with mixtures of high molecular weight.

This feature was pointed out and used in several petroleum fractionation design papers.[6−12]

In addition, several methods, especially conceptual design methods, such as the Pinch Design Method (PDM), have inherent inabilities to be extended to consider it.[13,14] We discuss this issue in more detail later.

In dealing with variable *Cp*, Wu et al.[15] extended the stages model to nonisothermal mixing and variable *Cp*. Flow rate fraction variables were used to the establish nonisothermal mixing model, and the heat load of a heat exchanger or a network stage was calculated by an integral in the variable *Cp* model.[15] They did not use the concept of substages and used BARON to solve both models.

In turn, Sreepathi and Rangaiah[16] dealt with variable *Cp*, in single- and multiple-objective retrofitting of heat exchanger networks. For dealing with variable *Cp*, the enthalpy of a stream was expressed as a cubic polynomial of temperature instead of using the step jumps of interval approach.[16] Minimizing the total annual cost was the objective for single-objective retrofitting, and investment cost and utility cost were used in multiple-objective retrofitting of heat exchanger networks.

On the other hand, as pointed out and shown in part 1,[17] the heat exchanger network design problem has been difficult to solve using local solvers, and even some global solvers have recently shown similar convergence difficulties. If one desires to approach in a mathematical programming purist form, one should use a generalized superstructure[18] or its extension to multiple matches.[19] However, the purist approach can render structures that are difficult to implement from the practical point of view.[19] We use RYSIA, a global optimization method recently introduced, which is based on bound contraction without using branch and bound.[20,21]

Received: December 6, 2016
Revised: March 27, 2017
Accepted: April 13, 2017
Published: April 13, 2017

DOI: 10.1021/acs.iecr.6b04687
Ind. Eng. Chem. Res. 2017, 56, 5958−5969

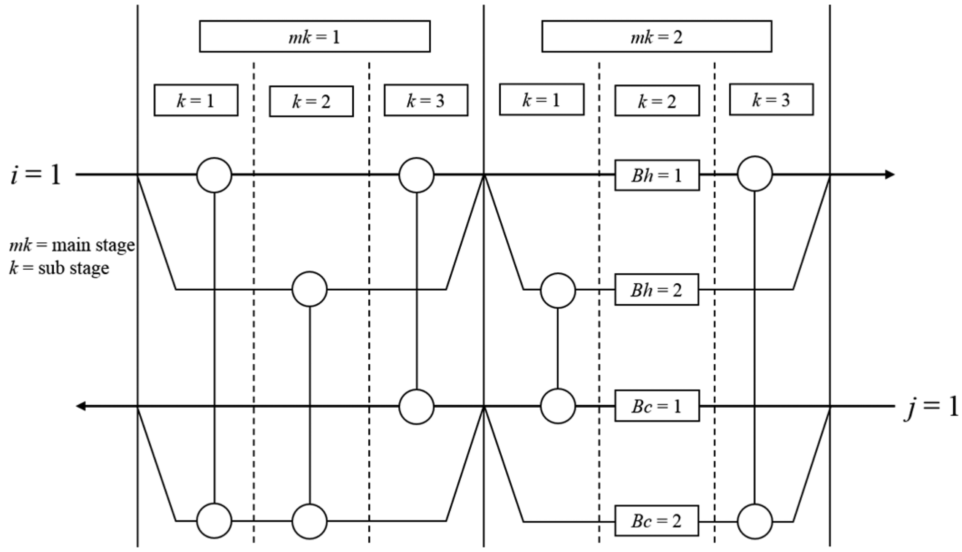


Figure 2. Stage/substages network superstructure.

This paper is organized as follows: We present the revised stages/substages model first, discussing critical aspects (part 1[17]). We follow with the modifications needed for variable *Cp*. We then discuss changes to the fixed *Cp* lower bound model (also shown in part 1[17]). We then discuss the bound contraction strategy next, including the use of lifting partitions. We then present results.

2. STAGES/SUBSTAGES SUPERSTRUCTURE MODEL

The original stagewise superstructure proposed by Yee and Grossmann[22] was extended to multiple substages[23] and solved globally by Kim and Bagajewicz[19] with nonisothermal mixing. The model is based on the stages/substages shown in Figure 2.

Basically, the proposed stage-/substagewise superstructure allows stream branching and the split stream to contain more than one heat exchanger. The original equations for fixed *Cp* are shown in part 1.[17]

3. MODIFICATIONS TO THE STAGES/SUBSTAGES MODEL

We now add the following parameters to the model (see part 1[17]):

$$Cph_i^{IN} = a_i^h + b_i^h T_i^{HIN} + c_i^h (T_i^{HIN})^2 \qquad \forall\ i \tag{1}$$

$$Cph_i^{OUT} = a_i^h + b_i^h T_i^{HOUT} + c_i^h (T_i^{HOUT})^2 \qquad \forall\ i \tag{2}$$

$$Cpc_j^{IN} = a_j^c + b_j^c T_j^{CIN} + c_j^c (T_j^{CIN})^2 \qquad \forall\ j \tag{3}$$

$$Cpc_j^{OUT} = a_j^c + b_j^c T_j^{COUT} + c_j^c (T_j^{COUT})^2 \qquad \forall\ j \tag{4}$$

We also add the following equations:

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

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

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

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

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

4. LOWER BOUND MODEL MODIFICATIONS

The lower bound for constant *Cp* is based on the partition of flow rates 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:

$$ThD_{i,mk,ph} = T_i^{HOUT} + \frac{(ph-1)}{phD}(T_i^{HIN} - T_i^{HOUT}) \quad \forall\ i,\ mk,\ bh,\ k \tag{9}$$

$$TbhD_{i,mk,bh,k,obh} = T_i^{HOUT} + \frac{(obh-1)}{obhD}(T_i^{HIN} - T_i^{HOUT}) \quad \forall\ i,\ mk,\ bh,\ k \tag{10}$$

$$TbcD_{j,mk,pc} = T_j^{CIN} + \frac{(pc-1)}{pcD}(T_j^{COUT} - T_i^{CIN}) \quad \forall\ i,\ mk,\ bh,\ k \tag{11}$$

$$TbcD_{j,mk,bh,k,obc} = T_j^{CIN} + \frac{(obc-1)}{obcD}(T_j^{COUT} - T_j^{CIN}) \quad \forall\ i,\ mk,\ bh,\ k \tag{12}$$

Thus

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

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

DOI: 10.1021/acs.iecr.6b04687
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$$\sum_{pc} TcD_{j,mk,pc} \cdot vTc_{j,mk,pc} \le Tc_{j,mk} \le \sum_{pc} TcD_{j,mk,pc+1} \cdot vTc_{j,mk,pc} \quad \forall\, j, mk \tag{15}$$

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

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

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

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

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

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

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

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

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

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

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

$$QHM_{i,mk} = Fh_i \cdot CphTh_{i,mk} - Fh_i \cdot CphTh_{i,mk+1} \quad \forall\, i, mk \tag{25}$$

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

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

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

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

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

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

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:

$$\sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh} \cdot FbhD_{i,mk,bh,ofh} vTbh_{i,mk,bh,k,obh} \cdot vFbh_{i,mk,bh,ofh} \le AH_{i,mk,bh,k} \le \sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh+1} \cdot FbhD_{i,mk,bh,ofh+1} vTbh_{i,mk,bh,k,obh} vFbh_{i,mk,bh,ofh} \quad \forall\, i, mk, bh, k \tag{29}$$

$$\sum_{obh} CphTbhD_{i,mk,bh,k,obh} vTbh_{i,mk,bh,k,obh} \le CphTbh_{i,mk,bh,k} \le \sum_{obh} CphTbhD_{i,mk,bh,k,obh+1} vTbh_{i,mk,bh,k,obh} \quad \forall\, i, mk, bh, k \tag{30}$$

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:

$$\sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh} \cdot FbhD_{i,mk,bh,ofh} WTbhFbh_{i,mk,bh,k,obh,ofh} \le AH_{i,mk,bh,k} \le \sum_{obh} \sum_{ofh} CphTbhD_{i,mk,bh,k,obh+1} \cdot FbhD_{i,mk,bh,ofh+1} WTbhFbh_{i,mk,bh,k,obh,ofh} \qquad \forall\, i, mk, bh, k \tag{31}$$

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

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

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

We do the same for cold streams. We relax the equation as follows:

$$\sum_{obc} \sum_{ofc} CpcTbcD_{j,mk,bc,k,obc} \cdot FbcD_{j,mk,bc,ofc} vTbc_{j,mk,bc,k,obc} vFbc_{j,mk,bc,ofc} \le AC_{j,mk,bc,k} \le \sum_{obc} \sum_{ofc} CpcTbcD_{j,mk,bc,k,obc+1} \cdot FbcD_{j,mk,bc,ofc+1} vTbc_{j,mk,bc,k,obc} vFbc_{j,mk,bc,ofc} \qquad \forall\, j, mk, bc, k \tag{35}$$

$$\sum_{obc} CpcTbcD_{j,mk,bc,k,obc} vTbc_{j,mk,bc,k,obc} \le CpcTbc_{j,mk,bc,k} \le \sum_{obc} CpcTbcD_{j,mk,bc,k,obc+1} vTbc_{j,mk,bc,k,obc} \quad \forall\, j, mk, bc, k \tag{36}$$

DOI: 10.1021/acs.iecr.6b04687
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Table 1. Data for Example 1

Stream	F [kg/s]	T_{in} [°C]	T_{out} [°C]	h [KW/m²·°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 [$/unit]
Variable cost for heat exchanger area	550 [$/m²]

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:

$$\sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc}\cdot FbcD_{j,mk,bc,ofc}WTbcFbc_{j,mk,bc,k,obc,ofc} \le AC_{j,mk,bc,k} \le \sum_{obc}\sum_{ofc} CpcTbcD_{j,mk,bc,k,obc+1}\cdot FbcD_{j,mk,bc,ofc+1}WTbcFbc_{j,mk,bc,k,obc,ofc} \quad \forall\ j,\ mk,\ bc,\ k \tag{37}$$

$$WTbcFbc_{j,mk,bc,k,obc,ofc} \le vTbc_{j,mk,bc,k,obc} \quad \forall\ j,\ mk,\ bc,\ k,\ obc,\ ofc \tag{38}$$

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}

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	29 min 22 s

$$WTbcFbc_{j,mk,bc,k,obc} \le vFbc_{j,mk,bc,ofc} \quad \forall\ j,\ mk,\ bc,\ k,\ obc,\ ofc \tag{39}$$

$$WTbcFbc_{j,mk,bc,k,obc,ofc} \ge vTbc_{j,mk,bc,k,obc} + vFbc_{j,mk,bc,ofc} - 1 \quad \forall\ j,\ mk,\ bc,\ k,\ obc,\ ofc \tag{40}$$

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

$$\sum_{bh} AH_{i,mk,bh,1} = Fh_i CphTh_{i,mk} \quad \forall\ i,\ mk \tag{41}$$

$$\sum_{bh} AH_{i,mk,bh,SBNOK+1} = Fh_i CphTh_{i,mk+1} \quad \forall\ i,\ mk \tag{42}$$

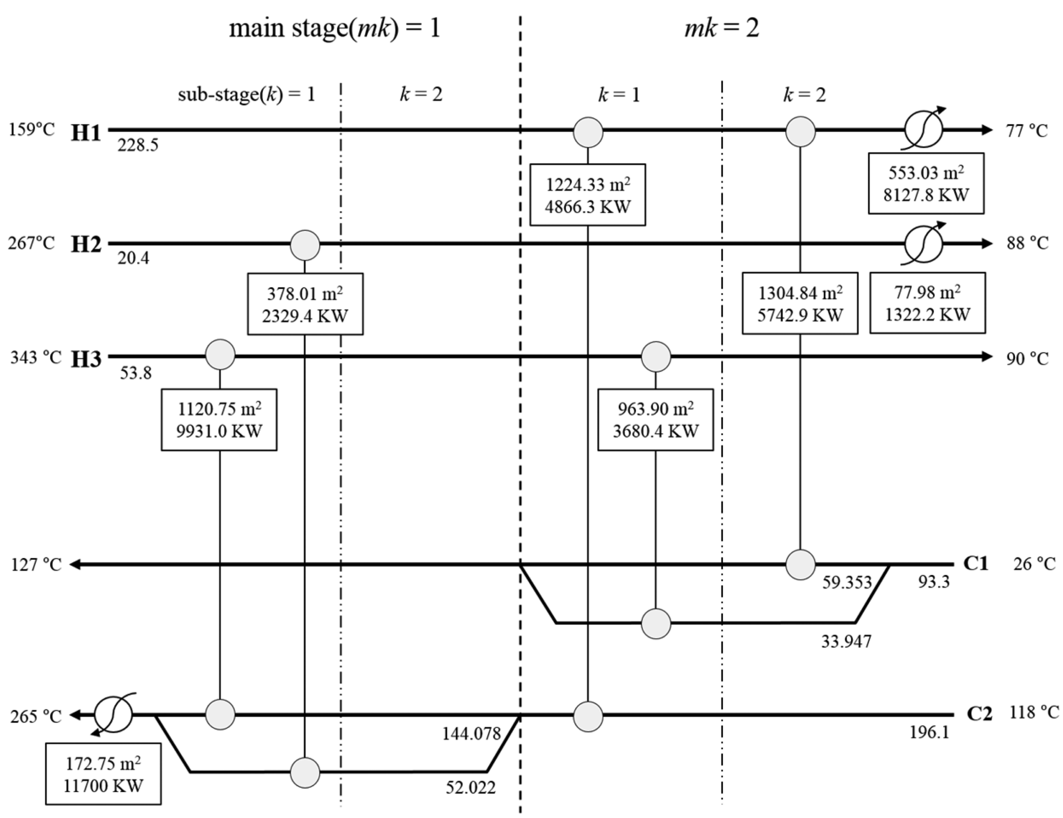

Figure 3. Solution network for example 1 with 2 main stages and 2 substages.

DOI: 10.1021/acs.iecr.6b04687
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$$\sum_{bc} AC_{i,mk,bc,1} = Fc_j CpcTc_{j,mk} \qquad \forall\ j,\ mk \qquad (43)$$

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

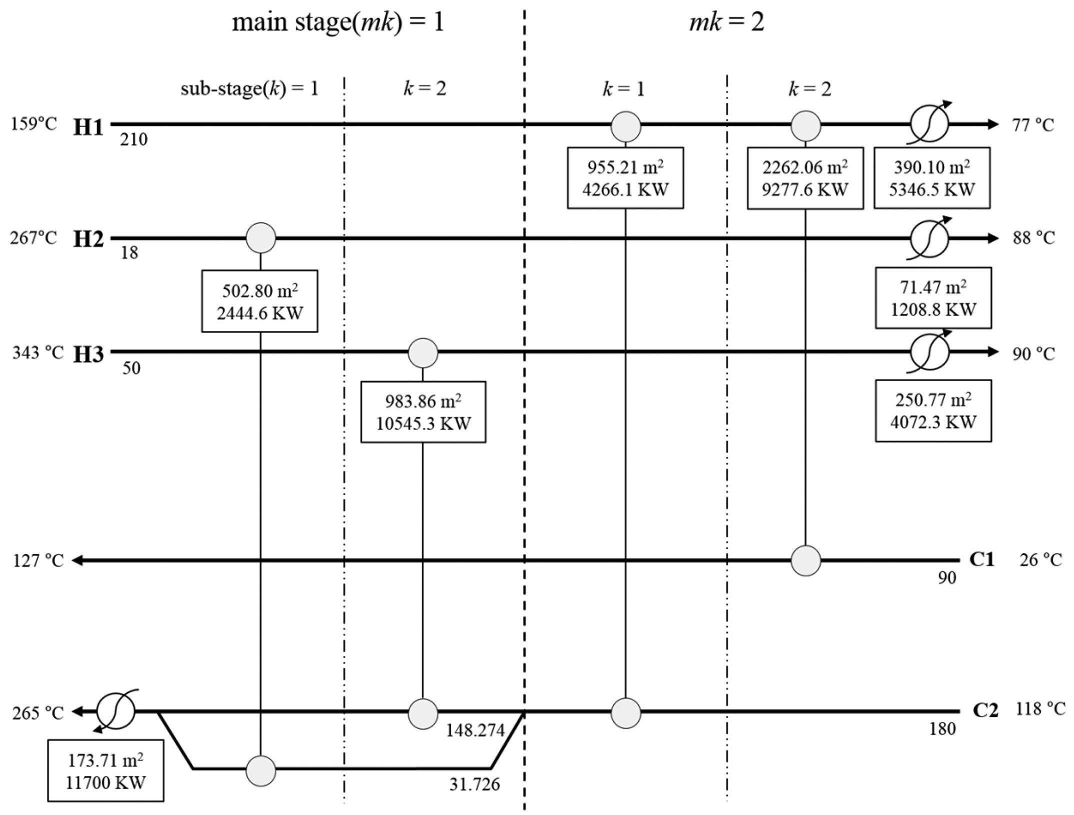

Figure 4. Solution network of example 1 for variable *Cp*.

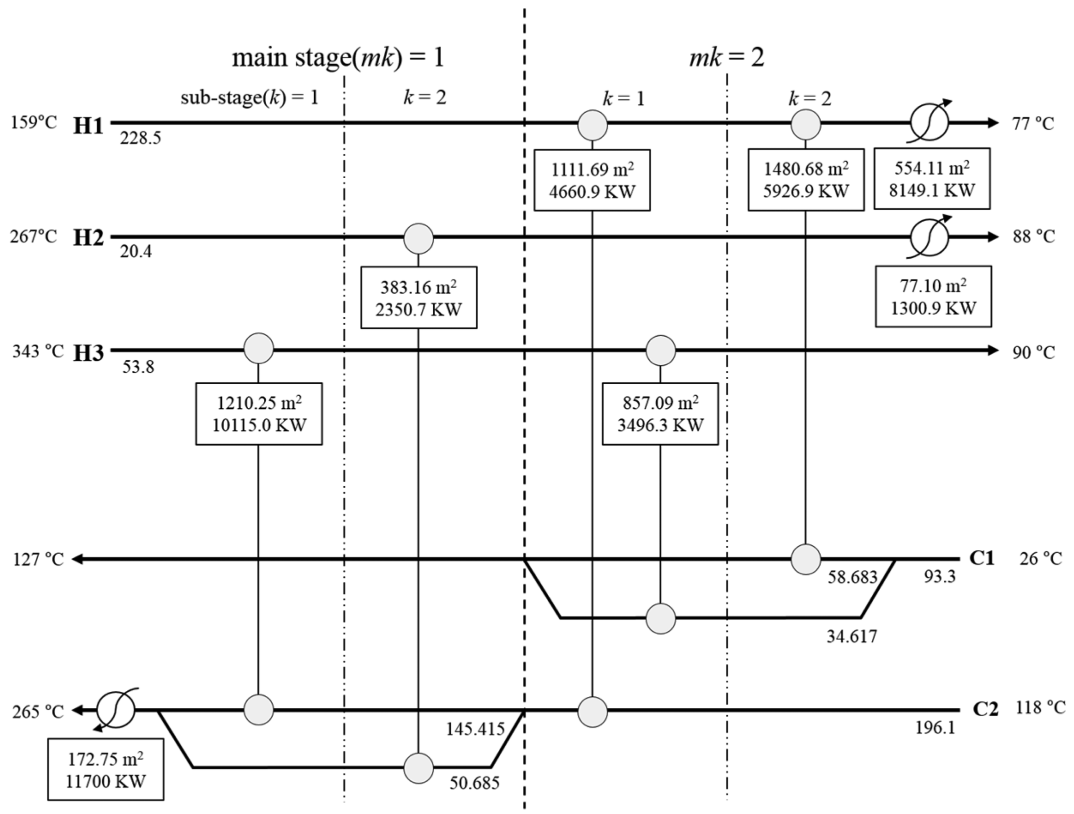

Figure 5. Solution network of example 1 for $Cp = 1$.

DOI: 10.1021/acs.iecr.6b04687
Ind. Eng. Chem. Res. 2017, 56, 5958–5969

$CphTh_{i,mk}$ and $CpcTc_{j,mk}$ are already relaxed in eqs 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 1.[17]

6. EXAMPLES

Our examples were implemented in GAMS (version 23.7)[24] and solved using CPLEX (version 12.3) as the MIP solver and DICOPT[25] as the MINLP solver on a PC machine (i7 3.6 GHz, 8GB RAM). For each example, we choose a low number of stages and substages. We already showed in part 1[17] what are the effects of using a larger number of stages: as this number increases, one may eventually find better solutions, or the same solution with matches taking place in different stages/substages but essentially corresponding to the same network.

We also compare with fixed *Cp* solutions. To make the comparison fair, we change the *Cp* of each stream from constant to variable in such a manner that each stream undergoes the same enthalpy change.

Finally, we use pinch technology to obtain the minimum energy consumption corresponding to each minimum temperature approach and the minimum area. These two calculations are rigorous. In addition, we do not use any information based on the pinch design method.

6.1. Example 1. The first example consists of three hot streams and two cold streams, and it is adapted from Nguyen et al.[26] The data are presented in Table 1 and 2. We used a minimum temperature approach of 10 °C, a fixed cost of units of $250,000, and an area cost coefficient of $550/m.[1,2] We solved using a two main stages and two substages model. We assumed that the limit of the number of branched streams for hot and cold streams was 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 the seventh iteration, satisfying a 1% gap between UB and LB. The optimal solution network is presented in Figure 3. We showed alternative solutions with a different number of substages in part 1[17] using the fixed *Cp* model. One of these solutions was also obtained by Kim and Bagajewicz[19] using a new generalized superstructure solved using RYSIA.

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

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 the 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.

Table 5. Data for Example 2

Stream	F [kg/s]	T_{in} [°C]	T_{out} [°C]	h [kJ/s·m^2·°C]
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]

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}

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	17 min 34 s

The globally optimal solution for variable *Cp* has an annualized cost of $1,783,727 using 9 iterations and a 29 min 22 s 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.

We obtained a globally optimal solution of 1,786,076 with 0.79% gap using 4 iterations and a 5 min 10 s 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)[27] and ANTIGONE (version 1.1)[28] using their default parameter choices. None of them rendered a feasible solution.

6.2. Example 2. The second example is 10SP1.[29] This example consists of four hot and five cold streams, and the data are given in Tables 5 and 6. We assumed a minimum temperature approach of 10 °C. The fixed cost of units is $5,291.9, and the area cost coefficient is $77.79/m^2. We solved using the two main stages and two substages model. We assumed that

DOI: 10.1021/acs.iecr.6b04687
Ind. Eng. Chem. Res. 2017, 56, 5958−5969

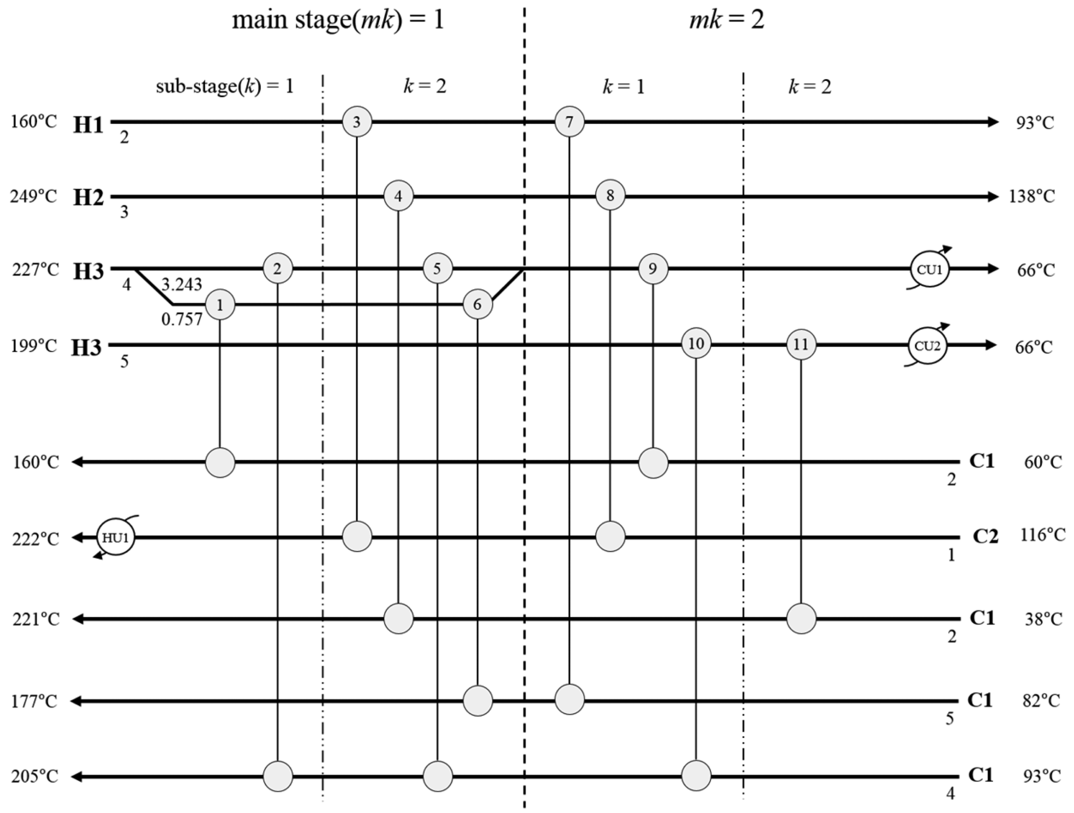

Figure 6. Solution Network of Example 2 for Variable *Cp*.

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

the limit of the number of branched streams for hot and cold streams was 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.[2] Upper limits are 50% higher values than lower limits. If the answer falls between bounds, one can accept it. However, if it falls on the upper bound, one may want to run again with larger upper bound(s). We produced the values 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.

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

We also tested with fixed *Cp*, and we obtained a globally optimal solution of $99,369,753 with 0.2% gap using 15 min 24 s of 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)[27] and ANTIGONE (version 1.1)[28] using the default parameter options. None of them rendered a feasible solution.

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 Tables 11 and 12. This example was solved using a 2 main stages and 2 substages superstructure model. We assumed a minimum temperature approach ($EMAT_{ij}$) of 10 °C. We also assumed that 4 branched streams are possible in the cold stream and no branching of the hot stream. The fixed cost of units is $250,000, and the area

Table 10. Comparing the Variable *Cp* Model Setting *Cp* = 1 and the Fixed Cp Model from the Generalized Superstructure Model[19]

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

DOI: 10.1021/acs.iecr.6b04687
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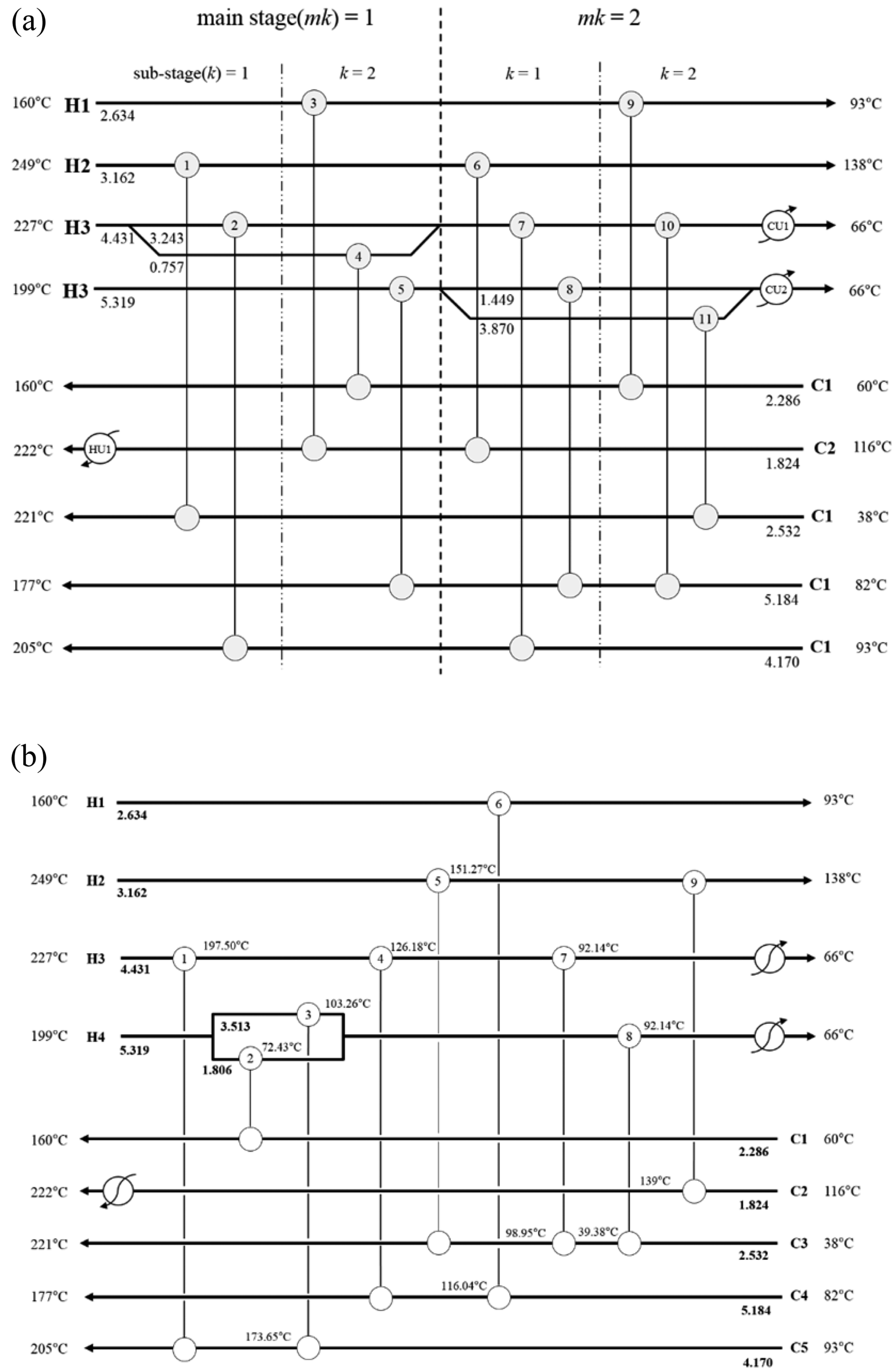

Figure 7. Optimal solution networks for example 2 (a) when Cp = 1 for variable Cp and (b) when the fixed Cp was used for the generalized superstructure model.[19]

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.

Flows, temperature, and ΔT were partitioned into 2 intervals, and the extended interval forbidding was used for bound contracting. We produced the values of the 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.

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.

We obtained similar objective values as those of the fixed Cp model (part 1[17]) and the generalized superstructure model,[19] but we obtained a different solution network (Figure 8). We tried to solve this problem using BARON (version 14.4)[27] and ANTIGONE (version 1.1)[28] using the default parameter

DOI: 10.1021/acs.iecr.6b04687
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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	290	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	290	115	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]

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}

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	24 min 48 s

options. None of them rendered a feasible solution after 24 h of running.

7. DISCUSSION

We start by remarking that the objective functions of the variable *Cp* and fixed *Cp* are similar, even though the structures can be different. One might think then that it is not worth solving using variable *Cp* because of such similar cost. We now explain why the similarities in cost arise: As we stated above, to make the comparison with a constant *Cp* case, we adjusted the coefficients to keep the overall heat released or absorbed by each stream the same. If the same EMAT is used, under conditions where the energy cost is dominant, then the likelihood of the temperature difference being equal to EMAT in at least one exchanger is very high. Under these conditions, both networks, the one with variable *Cp* and the one with fixed *Cp*, will have the same energy consumption (a minimum corresponding to HRAT = EMAT). In addition, an optimal solution for each of the networks will show a pattern as close as possible to vertical heat transfer (using pinch design terminology). Thus, the costs are very likely going to be similar. Yet the structure may not be. This was already discussed by Bagajewicz and Valtinson.[14] In a nutshell, the structure obtained is likely to be different because pinch technology considers an average *Cp* and therefore at the end there is a violation of the minimum approach. The difficulties of the pinch design method are further explored by Bagajewicz et al.[13]

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

8. CONCLUSIONS

We extend the stages/substages model in part 1[17] to include variable heat capacity with temperature in the heat exchanger network model and to solve globally using RYSIA, a newly developed global optimization procedure based on bound contraction (without resorting to branch and bound). Considering variable *Cp* is needed to build a stages/substages model in which all streams have temperature-dependent heat capacities. 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,[19] and lower values of total area and total heat of heating utilities for lifting partitions from pinch analysis (examples 1 and 3) and our previous research[2] (example 2) are used to improve the lower bound value as well as its computational time. Our examples proved that variable *Cp* can be adopted in the stages/substages model and can be solved with similar computational difficulty to that of the fixed *Cp* model (in part 1[17]). 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

DOI: 10.1021/acs.iecr.6b04687
Ind. Eng. Chem. Res. 2017, 56, 5958−5969

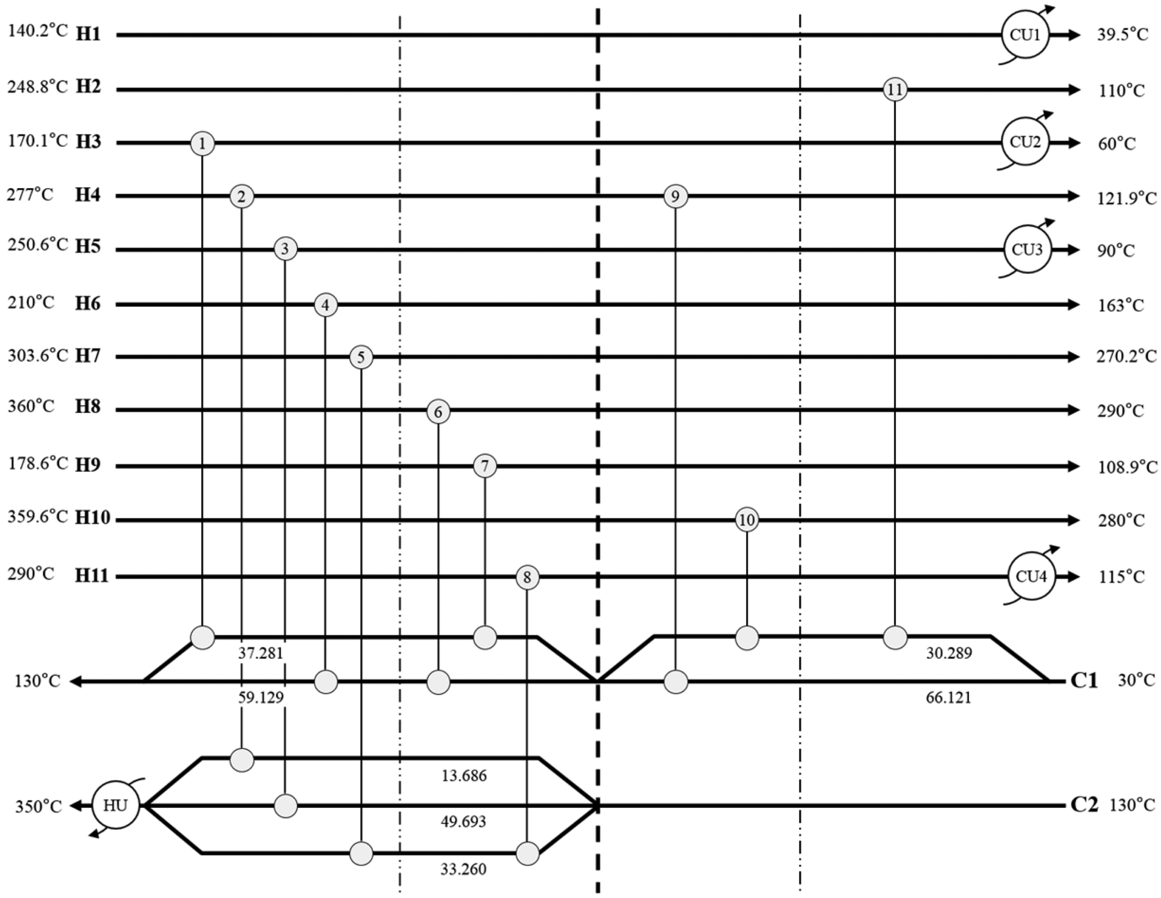

Figure 8. Solution network of example 3 for variable *Cp*.

convergence when a small gap is achieved, research that is left for future work.

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Notes

The authors declare no competing financial interest.

■ NOMENCLATURE

Sets

- *i* Hot process stream
- *j* Cold process stream
- *mk* Stage
- *bh* Hot stream branch
- *bc* Cold stream branch
- *k* Substage
- *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* Substage temperature partitioning point for hot stream
- *obc* Substage 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
- Cph_i^{IN} Variable heat capacity of inlet temperature of hot stream
- Cph_i^{OUT} Variable heat capacity of outlet temperature of hot stream
- Cpc_j^{IN} Variable heat capacity of inlet temperature of cold stream
- Cpc_j^{OUT} Variable heat capacity of outlet temperature of cold stream
- $C_{var.}$ Variable cost coefficients for heat exchangers
- C_{fixed} Fixed cost coefficients for heat exchangers
- *CUcost* Hot utility cost
- *HUcost* 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

DOI: 10.1021/acs.iecr.6b04687
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$TcD_{j,mk,pc}$	Discrete point of the partitioned temperature of main-stage cold stream
$TbhD_{i,mk,bh,obh}$	Discrete point of the partitioned temperature of substage hot stream
$TbcD_{j,mk,bc,k,obc}$	Discrete point of the partitioned temperature of substage cold stream
$CphThD_{i,mk,ph}$	Discrete point of the partitioned $CphTh_{i,mk}$
$CpcTcD_{i,mk,pc}$	Discrete point of the partitioned $CpcTc_{i,mk}$
$CphTbhD_{i,mk,bh,k,obh}$	Discrete point of the partitioned $CphTbh_{i,mk,bh,k}$
$CpcTbcD_{i,mk,bc,k,obc}$	Discrete point of the partitioned $CpcTbc_{i,mk,bc,k}$
$ThD_{i,j,mk,bh,bc,k,lhx}$	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 substage flow rate
$vFbcD_{j,mk,bc,ofc}$	Binary variable related to the partitioned cold stream substage 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 substage temperature
$vTbcD_{j,mk,bc,k,obc}$	Binary variable related to the partitioned cold stream substage temperature
$YHX_{i,j,mk,bh,bc,k,lhx}$	Binary variable related to the partitioned hot side temperature differences
$YHX_{i,j,mk,bh,bc,k,nhx}$	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 substage 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 substage 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 substage 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 substage
$Cpcb_{i,mk,bc,k}$	Variable hear capacity of cold stream for substage
$Th_{i,mk}$	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
$Tbc_{i,mk,bc,k}$	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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