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4	Global Optimization
5	of Heat Exchanger Networks. Part I-
6	Stages/Substages Superstructure
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ABSTRACT

We solve globally an extension of the isothermal mixing stages model (Synheat) proposed by Yee and
Grossmann (1990), later extended to non-isothermal mixing by Björk and Weterlund (2002) and solved
globally by Faria et al. (2015). This new extension of that model was recently presented in a Conference
Proceedings (Jongsuwat et al., 2014). The model allows specific structures that are more commonly
accepted in industry than generalized complex structures (Kim and Bagajewicz, 2016) who suffer from
somewhat disorganized branched and subbranches. This stages/substages superstructure has limited
branching and several matches in series in each branch. Our industrial experience shows us that these are
acceptable. The novel contribution of this article is then solving such model globally, adding the control
of temperature differences upon mixing.

1. INTRODUCTION

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The problem of designing heat exchanger networks is perhaps the oldest problem in the discipline of Process Synthesis. A good literature review of heat exchanger network synthesis (HEN) from the 20th century was published by Furman and Sahinidis (2002). Morar and Agachi (2010) also offered a literature review until 2008. Of all this work, we point out the combined use of mathematical programming and superstructures, of which the first generalized superstructure for HEN design was presented by Floudas et al. (1986). This first generalized superstructure consisted of a model that included one heat exchanger between every hot and cold stream, with connections made such that every possible flowsheet is represented. The model was not used in practice for a variety of reasons. First, the MINLP solvers of the time, and the ones of today sometimes, would guarantee at least one local minimum (because the model is non-convex and because many times good initial points are needed) or sometimes did not converge to feasible points if not guided by good initial points. This discouraged researches and practitioners. Second, the model would render some impractical answers, product of several splitting and mixing. Third, many systems that exhibit heat transfer bottlenecks (i.e. tight pinches), require that a pair of streams exchange heat in more than one exchanger, typically two. To ameliorate the issue of solvability and global nature of solutions, we addressed these concerns with a generalized superstructure model that controls temperatures upon mixing, number of splits, etc., in a recent article (Kim and Bagajewicz, 2016). Later, another superstructure model was proposed by Yee and Grossmann, (1990), which makes a series of assumptions: It assumes isothermal mixing and presents several stages where more than one match between streams takes place in parallel with isothermal mixing. What made the model attractive is that the only nonlinearity could be confined to the objective function and what made the model industrially relevant. Further, studies followed where non-isothermal mixing was added (Bjork and Westerlund, 2002 and Huang et al., 2012)

and allowing some different configurations (Huang and Karimi, 2013). Various other approaches for HEN stage superstructure model exist: Konukman et al. (2002), Frausto-Hernandez et al. (2003), Ponce-Ortega et al. (2008), Escobar and Trierweiler (2013), Onishi et al. (2014) and Na et al. (2015). There are also many other recent works for finding local and global optimum of heat exchanger network grassroots models. Laukkanen and Fogelholm (2011) proposed a bilevel optimization method based on grouping streams for simultaneous synthesis of HEN. Bogataj and Kravanja (2012) used a modified outer approximation (OA)/equality relaxation(ER) algorithm for yielding a lower bound close to 1% tolerance gap. Huang et al. (2012) found solutions of an MINLP model based on a hyperstructure of stage-wise stream superstructure of HEN. Haung and Karimi (2012, 2013, 2014) proposed different approaches, including using BARON (Sahinidis, 1996), which proved to be inefficient to solve their model. Finally they used a ad-hoc search strategy of repeatedly using the OA algorithm. Kang et al. (2014) proposed a parallel sequential quadratic programming (SQR) algorithm based on graphic process unit (GPU) acceleration to find solutions on MINLP models of HEN synthesis. Myankooh and Shafiei (2015) found the optimum of an MINLP problem of HEN by using the Ant Colony Optimization for continuous domains (ACO_R) with removing splits in the networks.

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All the aforementioned mathematical programming-based efforts were not able to capture some alternative structures, like several exchangers in series on each branch of each stage. Such a stages model with multiple exchangers in each branch was first presented by Jongsuwat et al. (2014) and solved using an ad-hoc combination of MILP, NLP and MINLP models, but not globally. Here we solve the model globally and compare our methodology (RYSIA), with existing commercial global solvers.

The academic efforts and the available commercial software were reviewed in our previous article (Faria et al., 2015). We only highlight what are the options we pursue in this article: all HEN models contain bilinear terms consisting of flowrates multiplied by temperatures. In addition, for HEN models, the heat transfer equations relating heat transferred with LMTD values are nonconvex. If one uses some rational approximations (Patterson, 1984; Chen, 1987), one can make appropriate substitutions (Manousiouthakis and Sourlas, 1992), to obtain purely quadratic/bilinear models.

In this article, we explore the use of our bound contraction procedure for global optimization (Faria and Bagajewicz, 2011c) to solve the stages/substages model. Like a generalized superstructure model (Kim and Bagajewicz, 2016), the stage/substages-wise model can produce structures that cannot be obtained from the stages model (Yee and Grossmann, 1990). We can produce branches of streams and matches between hot and cold stream pairs using the concept of the sub-stages. In our lower bound, we follow the direct partitioning procedure 1(DPP1) strategy for the relaxation of bilinear terms (Faria and Bagajewicz, 2011c), and we exploit the univariate nature of the LMTD terms (or their rational equivalents), to build relaxations that do not require the addition of new variables. Finally, we also use lifting partitions. The use of lifting partitions with the bound contraction procedure can be generalized by setting the lower and upper limits of total area and total utility usage from the pinch analysis.

This paper is organized as follows: We present the revised stages/substages model first. We follow with the lower bound model. We discuss the bound contraction strategy next, including the introduction of lifting partitions. We then present results.

2. STAGES/SUBSTAGES-WISE SUPERSTRUCTURE MODEL

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The original stage-wise superstructure does not include a case of branch stream which contains two or more exchangers in series and the case of stream bypasses (Yee and Grossmann, 1990). These restrictions may cause the global optimal being excluded in HEN. Thus, the original stage-wise superstructure model may not be suitable in process synthesis and process integration for realistic model. Therefore, in this work modification of the original model is investigated as follows:

mk = 2mk = 1k = 1k = 2k = 3k = 1k = 2k = 3 $Tbh_{i,mk,bh,k}$ i = 1bh = 1 $\overline{Fbh}_{i.mk,bh}$ mk = main stagek = sub stagebh = 2bc = 1i = 1

Figure 1. Stage/Sub-stage wise network superstructure.

The proposed stage/substage-wise superstructure model in Figure 1, a number of sub-stages k is added inside the main stage mk and a fixed number of branch bh(bc) is added to both hot(i) and cold(j) stream. Basically, the proposed stage/substage-wise superstructure allows stream branching and the split stream to contain more than one heat exchanger.

1 The overall energy balances for each stream

4

$$2 \qquad \sum_{j} \sum_{mk} \sum_{bh} \sum_{bc} \sum_{k} q_{i,j,mk,bh,bc,k} + qcu_i = Fh_i (T_i^{HIN} - T_i^{HOUT}) \qquad \forall i$$
 (1)

$$3 \qquad \sum_{i} \sum_{mk} \sum_{bh} \sum_{bc} \sum_{k} q_{i,j,mk,bh,bc,k} + qhu_{j} = Fc_{j} (T_{j}^{COUT} - T_{j}^{CIN}) \qquad \forall j$$
 (2)

5 • The energy balances at each main stage and sub-stage

$$6 HA_{mk} = CA_{mk} \forall mk (3)$$

$$7 \sum_{i} QHM_{i,mk} = HA_{mk} \forall mk (4)$$

8
$$QHM_{i,mk} = (Th_{i,mk} - Th_{i,mk+1})Fh_i$$
 $\forall i,mk$ (5)

9
$$\sum_{bh} QH_{i,mk,bh} = QHM_{i,mk} \qquad \forall i, mk$$
 (6)

10
$$\sum_{k} qHK_{i,mk,bh,k} = QH_{i,mk,bh}$$
 $\forall i, mk, bh$ (7)

$$11 \qquad \sum_{j} QCM_{j,mk} = CA_{mk} \qquad \forall mk$$
 (8)

12
$$QCM_{j,mk} = \left(Tc_{j,mk} - Tc_{j,mk+1}\right)Fc_{j} \qquad \forall j,mk$$
 (9)

13
$$\sum_{bc} QC_{j,mk,bc} = QCM_{j,mk}$$
 $\forall j,mk$ (10)

$$14 \qquad \sum_{k} qCK_{i,mk,bc,k} = QC_{j,mk,bc} \qquad \forall j,mk,bc$$
 (11)

- From the above equations, each main stage of hot and cold streams are classified into main stages
- 2 ($\mathit{HA}_{\mathit{mk}}$ and $\mathit{CA}_{\mathit{mk}}$), branch streams ($\mathit{QHM}_{i,\mathit{mk}}$, $\mathit{QCM}_{j,\mathit{mk}}$, $\mathit{QH}_{i,\mathit{mk},\mathit{bh}}$, $\mathit{QC}_{j,\mathit{mk},\mathit{bc}}$), and sub-stages
- 3 ($qHK_{i,mk,bh,k}$, $qCK_{j,mk,bc,k}$) to reduce the number of dependent variable in each equation as many as
- 4 possible by introducing intermediate variables.

6 Multiple of temperature and heat capacity flow

$$7 AH_{i,mk,bh,k} = Tbh_{i,mk,bh,k} Fbh_{i,mk,bh} \forall i,mk,bh,k (12)$$

$$8 AC_{j,mk,bc,k} = Tbc_{j,mk,bc,k} Fbc_{j,mk,bc} \forall j,mk,bc,k (13)$$

9 Sub-stage heat balances

10
$$\sum_{i} \sum_{bc} q_{i,j,mk,bh,bc,k} = qHK_{i,mk,bh,k}$$
 $\forall i,mk,bh,k$ (14)

11
$$qHK_{i,mk,bh,k} = AH_{i,mk,bh,k} - AH_{i,mk,bh,k+1} \qquad \forall i,mk,bh,k$$
 (15)

12
$$\sum_{i} \sum_{bh} q_{i,j,mk,bh,bc,k} = qCK_{j,mk,bc,k} \qquad \forall j,mk,bc,k$$
 (16)

13
$$qCK_{j,mk,bc,k} = AC_{j,mk,bc,k} - AC_{j,mk,bc,k+1} \qquad \forall j,mk,bc,k$$
 (17)

■ Superstructure inlet temperatures

$$Th_{i,1} = T_i^{HIN}$$
 $\forall i$ (18)

$$1 \qquad \sum_{bh} AH_{i,mk,bh,1} = Fh_i Th_{i,mk}$$

$$\forall i, mk \tag{19}$$

$$2 \qquad \sum_{bh} AH_{i,mk,bh,SBNOK+1} = Fh_i Th_{i,mk+1}$$

$$\forall i, mk$$
 (20)

$$3 Th_{i,mk} = Tbh_{i,mk,bh,1}$$

$$\forall i, mk, bh$$
 (21)

$$4 Tc_{j,NOK+1} = T_j^{CIN}$$

$$\forall j$$
 (22)

$$5 \qquad \sum_{bc} AC_{i,mk,bc,1} = Fc_{j}Tc_{j,mk}$$

$$\forall j, mk$$
 (23)

$$6 \qquad \sum_{bc} AC_{j,mk,bc,SBNOK+1} = Fc_j Tc_{j,mk+1}$$

$$\forall j, mk$$
 (24)

$$7 Tc_{j,mk+1} = Tbc_{j,mk,bc,SBNOK+1}$$

$$\forall j, mk, bc$$
 (25)

8 Feasibility of temperatures (monotonic decrease in temperature)

9
$$Th_{i.mk} \geq Th_{i.mk+1}$$

$$\forall i, mk$$
 (26)

$$10 Tbh_{i,mk,bh,k} \ge Tbh_{i,mk,bh,k+1}$$

$$\forall i, mk, bh, k$$
 (27)

$$11 T_i^{HOUT} \le Th_{i,NOK+1}$$

$$\forall i$$
 (28)

$$12 \qquad Tc_{j,mk} \ge Tc_{j,mk+1}$$

$$\forall j, mk$$
 (29)

$$13 Tbc_{j,mk,bc,k} \ge Tbc_{j,mk,bc,k+1}$$

$$\forall j, mk, bc, k$$
 (30)

$$14 T_j^{COUT} \ge Tc_{j,1}$$

$$\forall j$$
 (31)

1 Hot and cold utility load

$$(Th_{i,NOK+1} - T_i^{HOUT})Fh_i = qcu_i$$

$$\forall i$$
 (32)

$$3 \qquad \left(T_{j}^{COUT} - Tc_{j,1}\right)Fc_{j} = qhu_{j}$$

$$\forall j$$
 (33)

4 Logical constraints

5
$$q_{i,j,mk,bh,bc,k} - \Omega \cdot z_{i,j,mk,bh,bc,k} \le 0$$

$$\forall i, j, mk, bh, bc, k$$
 (34)

6
$$qcu_i - \Omega \cdot zcu_i \leq 0$$

$$\forall i$$
 (35)

$$7 \qquad qhu_j - \Omega \cdot zhu_j \le 0$$

$$\forall j$$
 (36)

8 Maximum matching

$$9 \qquad \sum_{i,bh} z_{i,j,mk,bh,bc,k} \leq 1$$

$$\forall j, mk, bc, k \tag{37}$$

$$10 \qquad \sum_{j,bc} z_{i,j,mk,bh,bc,k} \le 1$$

$$\forall i, mk, bh, k \tag{38}$$

■ Mass balances at each main stage

$$12 \qquad \sum_{hh} Fbh_{i,mk,bh} \le Fh_i$$

$$\forall i, mk$$

$$13 \qquad \sum_{bc} Fbc_{j,mk,bc} \le Fc_j$$

$$\forall j, mk \tag{40}$$

(39)

■ Calculation of approach temperature

$$1 \qquad \Delta T h_{i,j,mk,bh,bc,k} \leq T b h_{i,mk,bh,k} - T b c_{j,mk,bc,k} + \Gamma \left(1 - z_{i,j,mk,bh,bc,k} \right) \qquad \qquad \forall i,j,mk,bh,bc,k \tag{41}$$

$$2 \qquad \Delta Tc_{i,j,mk,bh,bc,k} \leq Tbh_{i,mk,bh,k+1} - Tbc_{j,mk,bc,k+1} + \Gamma\left(1 - z_{i,j,mk,bh,bc,k}\right) \qquad \forall i,j,mk,bh,bc,k \tag{42}$$

$$3 \qquad \Delta T c u_i \leq T h_{i,NOK+1} - T_{CU}^{OUT} + \Gamma \left(1 - z c u_i \right)$$
 $\forall i$ (43)

$$4 \qquad \Delta Thu_{j} \leq T_{HU}^{OUT} - Tc_{j,1} + \Gamma \left(1 - zhu_{j} \right) \qquad \qquad \forall j \tag{44}$$

5 Minimum approach temperatures (lower bounds)

6
$$\Delta Th_{i,j,mk,bh,bc,k} \ge EMAT$$
 $\forall i,j,mk,bh,bc,k$ (45)

7
$$\Delta Tc_{i,i,mk,bh,bc,k} \ge EMAT$$
 $\forall i, j, mk, bh, bc, k$ (46)

$$8 \qquad \Delta T c u_i \ge E M A T \qquad \qquad \forall i \tag{47}$$

9
$$\Delta Thu_{j} \geq EMAT$$
 $\forall j$ (48)

The areas of heat exchangers are used explicitly in the objective function (The original Synheat model uses the ratio of the heat transferred to the log mean temperature difference). The area costs are assumed to be linearly dependent on the areas, thus making the objective function linear. It can be argued that the costs are nonlinearly dependent of area, through a concave function. First, it has been shown that a linear approximation of such function through the range of appropriate areas, is tight (Barbaro and Bagajewicz, 2005). Finally, if one insists on using the concave function, one can underestimate it in our lower bound using piecewise linear functions.

- Because the areas of heat exchangers are explicitly defined in the objective function, new
- 2 constraints to calculate them are incorporated.
- 3 Logarithmic mean temperature difference (LMTD) (Chen, 1987)

$$4 \qquad LMTD_{i,j,mk,bh,bc,k} = \left[\Delta Th_{i,j,mk,bh,bc,k} \Delta Tc_{i,j,mk,bh,bc,k} \frac{\Delta Th_{i,j,mk,bh,bc,k} + \Delta Tc_{i,j,mk,bh,bc,k}}{2} \right]^{1/3} \forall i,j,mk,bh,bc,k \quad (49)$$

$$LMTD_{CUi} = \left[\Delta Tcu_i \left(T_i^{HOUT} - T_{CU}^{IN} \right) \frac{\Delta Tcu_i + \left(T_i^{HOUT} - T_{CU}^{OUT} \right)}{2} \right]^{1/3} \qquad \forall i$$
 (50)

$$LMTD_{HUj} = \left[\Delta Thu_j \left(T_{HU}^{IN} - T_j^{CIN} \right) \frac{\Delta Thu_j + \left(T_{HU}^{IN} - T_j^{CIN} \right)}{2} \right]^{1/3} \qquad \forall j$$
 (51)

7 Area calculation

$$8 q_{i,j,mk,bh,bc,k} - A_{i,j,mk,bh,bc,k} U_{i,j} LMTD_{i,j,mk,bh,bc,k} = 0 \forall i,j,mk,bh,bc,k (52)$$

$$9 qcu_i - Acu_i U_{CU_i} LMTD_{CU_i} = 0 \forall i (53)$$

$$10 qhu_j - Ahu_j U_{HUj} LMTD_{HUj} = 0 \forall j (54)$$

$$Min \left\{ \sum_{i} qcu_{i} \cdot CU \operatorname{cost} + \sum_{j} qhu_{j} \cdot HU \operatorname{cost} + C_{\operatorname{var}} \left(\sum_{i,j,mk,bh,bc,k} A_{i,j,mk,bh,bc,k} + \sum_{i} Acu_{i} + \sum_{j} Ahu_{j} \right) \middle/ n + C_{\operatorname{fixed}} \left(\sum_{i,j,mk,bh,bc,k} z_{i,j,mk,bh,bc,k} + \sum_{i} zcu_{i} + \sum_{j} zhu_{j} \right) \middle/ n \right\}$$

$$(55)$$

1 3. LOWER BOUND MODEL

- In the bilinear terms (Equations 12 and 13), we choose branched flowrate to be the partitioned variable. In turn the area equations are treated using the image partitioning model. One can reformulate such equation by adding variables and reduce the whole model to a set of equations containing bilinear expressions only and follow by dealing with the bilinear terms the usual way. One example of this reformulation was shown and evaluated by Kim and Bagajewicz (2016), resulting in 8 equations containing bilinear and quadratic terms and 6 new variables. It was shown that it is less efficient than the partitioning proposed by Faria et al. (2015) which results in one new variable and 3 more equations.
- 9 The partitioned variables are the branched flowrate differences in this case. In the case of image 10 partitioning, we partition the temperature differences, as done by Faria et al.(2015).

3.1. Bilinear terms

- 13 Equations (12-13) are considered for this decomposition.
- Partitioning $Fbh_{i,mk,bh}$ variable with o partitions

$$15 \qquad \sum_{o} FbhD_{i,mk,bh,o} \times vFbhD_{i,mk,bh,o} \le Fbh_{i,mk,bh} \le \sum_{o} FbhD_{i,mk,bh,o+1} \times vFbhD_{i,mk,bh,o} \quad \forall i,mk,bh$$
 (56)

$$16 \qquad \sum_{o} vFbhD_{i,mk,bh,o} = 1 \qquad \qquad \forall i,mk,bh \tag{57}$$

- 1 We partition flowrates $Fbh_{i,mk,bh}$ using o partitions. Then $AH_{i,mk,bh,k}$ is bounded by the following
- 2 relations.

$$3 \qquad AH_{i,mk,bh,k} \ge \sum_{o} FbhD_{i,mk,bh,o} \times TbhB_{i,mk,bh,k,o} \qquad \forall i,mk,bh,k$$
 (58)

$$4 \qquad AH_{i,mk,bh,k} \leq \sum_{o} FbhD_{i,mk,bh,o+1} \times TbhB_{i,mk,bh,k,o} \qquad \forall i,mk,bh,k$$
 (59)

- 5 $TbhB_{i,mk,bh,k,o}$ is introduced to replace the product of the partitioned flowrates and binary variables.
- 6 According to the direct partitioning procedures (DPP1) of (Faria and Bagajewicz, 2011a), $TbhB_{i,mk,bh,k,o}$
- 7 has the following equations.

$$8 \quad TbhB_{i,mk,bh,k,o} \ge 0 \qquad \forall i,mk,bh,k,o \qquad (60)$$

9
$$TbhB_{i,mk,bh,k,o} - T_i^{HIN} \times vFbhD_{i,mk,bh,o} \le 0$$
 $\forall i,mk,bh,k,o$ (61)

10
$$(Tbh_{i,mk,bh,k} - TbhB_{i,mk,bh,k,o}) - T_i^{HIN} \times (1 - vFbhD_{i,mk,bh,o}) \le 0$$
 $\forall i, mk, bh, k, o$ (62)

11
$$Tbh_{i,mk,bh,k} - TbhB_{i,mk,bh,k,o} \ge 0$$
 $\forall i,mk,bh,k,o$ (63)

12 A same procedure is applied to partition $Fbc_{j,mk,bc}$.

14 3.2. Nonlinear function

13

15 Equation (52) are considered for this decomposition.

Partition temperature differences $\forall i, j, mk, bh, bc, k$

$$1 \qquad \sum_{l} \Delta TD_{i,j,mk,bh,bc,k,l} \times YHX_{i,j,mk,bh,bc,k,l} \leq \Delta Th_{i,j,mk,bh,bc,k} \leq \sum_{l} \Delta TD_{i,j,mk,bh,bc,k,l+1} \times YHX_{i,j,mk,bh,bc,k,l}$$
(64)

$$2 \qquad \sum_{n} \Delta TD_{i,j,mk,bh,bc,k+1,n} \times YHX_{i,j,mk,bh,bc,k+1,n} \leq \Delta Tc_{i,j,mk,bh,bc,k} \leq \sum_{n} \Delta TD_{i,j,mk,bh,bc,k+1,n+1} \times YHX_{i,j,mk,bh,bc,k+1,n}$$
(65)

$$3 \qquad \sum_{l} YHX_{i,j,mk,bh,bc,k,l} = z_{i,j,mk,bh,bc,k} \tag{66}$$

$$4 \sum_{n} YHX_{i,j,mk,bh,bc,k+1,n} = z_{i,j,mk,bh,bc,k} (67)$$

6 Now we rewrite area calculation as follow:

5

 $\forall i, j, mk, bh, bc, k$

$$\frac{q_{i,j,mk,bh,bc,k}}{U_{i,j}} - A_{i,j,mk,bh,bc,k} \sum_{l} \sum_{n} YHX_{i,j,mk,bh,bc,k,l} YHX_{i,j,mk,bh,bc,k+1,n} \\
\times \sqrt[3]{\Delta TD_{i,j,mk,bh,bc,k,l+1} \Delta TD_{i,j,mk,bh,bc,k+1,n+1}} \frac{(\Delta TD_{i,j,mk,bh,bc,k,l+1} + \Delta TD_{i,j,mk,bh,bc,k+1,n+1})}{2} \le 0$$
(68)

- substituting the product of binaries $(YHX_{i,j,mk,bh,bc,k,l}, YHX_{i,j,mk,bh,bc,k+1,n})$ and area $(A_{i,j,mk,bh,bc,k})$ in equation
- 9 (68) with new positive continuous variable $(H_{i,j,mk,bh,bc,k,l,n})$:

$$\frac{q_{i,j,mk,bh,bc,k}}{U_{i,j}} - \sum_{l} \sum_{n} H_{i,j,mk,bh,bc,k,l,n} \\
\times \sqrt[3]{\Delta T D_{i,j,mk,bh,bc,k,l+1} \Delta T D_{i,j,mk,bh,bc,k+1,n+1}} \frac{(\Delta T D_{i,j,mk,bh,bc,k,l+1} + \Delta T D_{i,j,mk,bh,bc,k+1,n+1})}{2} \le 0$$
(69)

11 To complement the above substitution valid, the following constraints are needed:

12
$$\sum_{l} H_{i,j,mk,bh,bc,k,l,n} - \Omega YHX_{i,j,mk,bh,bc,k+1,n} \le 0 \qquad \forall i,j,mk,bh,bc,k,n$$
 (70)

$$\sum_{n} H_{i,j,mk,bh,bc,k,l,n} - \Omega YHX_{i,j,mk,bh,bc,k,l} \le 0 \qquad \forall i,j,mk,bh,bc,k,l$$
 (71)

$$2 \qquad H_{i,j,mk,bh,bc,k,l,n} - A_{i,j,mk,bh,bc,k} + \left(2 - YHX_{i,j,mk,bh,bc,k,l} - YHX_{i,j,mk,bh,bc,k+1,n}\right) \ge 0 \qquad \forall i,j,mk,bh,bc,k,l,n$$
 (72)

$$\sum_{l} \sum_{n} H_{i,j,mk,bh,bc,k,l,n} = A_{i,j,mk,bh,bc,k} \qquad \forall i,j,mk,bh,bc,k$$
 (73)

4 A similar procedure can be applied to equations (53) and (54).

4. LIFTING PARTITIONING

5

- 7 To help increasing (lifting) the lower bound value, we resort to partitioning of variables that
- 8 participate in the objective function (Kim and Bagajewicz, 2016). For these we introduce new variables
- 9 for total heat of heating utilities and total area including utilities.

$$\sum_{j} Q_{j}^{HU} = TQH \tag{74}$$

11
$$\sum_{i,j,mk,bh,bc,k} A_{i,j,mk,bh,bc,k} + \sum_{i} Acu_{i} + \sum_{j} Ahu_{j} = TA$$
 (75)

- These new variables TQH and TA are partitioned using m and p partitions. We use binary variables
- 13 $vTQH_m$ for TQH and vTA_p for TA.

$$\sum_{m} \left(TQHD_{m} \cdot vTQH_{m} \right) \le TQH \le \sum_{m} \left(TQHD_{m+1} \cdot vTQH_{m} \right) \tag{76}$$

$$\sum_{m} vTQH_{m} = 1 \tag{77}$$

$$\sum_{p} \left(TAD_{p} \cdot vTA_{p} \right) \le TA \le \sum_{p} \left(TAD_{p+1} \cdot vTA_{p} \right) \tag{78}$$

$$\sum_{p} vTA_{p} = 1 \tag{79}$$

 TAD_n and $TQHD_m$ are discrete points of the total area and exchanged heat of heater.

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. The partitioning methodology generates linear models that guarantee to be lower bounds of the problems. Upper bounds are needed for the bound contraction procedure. These upper bounds are usually obtained using the original MINLP model often initialized by the results from the lower bound model. When this fails, alternatives can be constructed. For example, one can freeze the binary variables with values given by the lower bound and try to solve as NLP; one can also add freezing the flowrates with the values given by the lower bound. In this latter case, optimization is rather trivial, and reduces to calculating heat exchanged and temperatures. We remind the reader that an upper bound solution does not have to be a local optimum; any feasible solution qualifies.

We defined different variables: partitioning variables, which are used to construct linear relaxations of bilinear and nonconvex terms, bound contracted variables, which are also partitioned, but

- only for the purpose of performing their bound contraction (these are those that participate in the lifting),
- and branch and bound variables, which are the variables for which a branch and bound procedure is tried
- 3 (they need not be the same set as the other two variables).
- The global optimization strategy is now summarized as follows: We run the lower bound model
- 5 first. Then we use the result of the lower bound model as initial values for the upper bound model. We
- 6 proceed to perform bound contraction on all variables as explained below.

5.1. Bound contraction

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- The bound contraction procedure used by RYSIA in the partition elimination strategy presented
- 9 by Faria and Bagajewicz (2011a, b) and Faria et al (2015). We summarized the basic strategy in this section.
- 10 Further details of different strategies can be found in the original paper.
 - 1. Run the lower bound model to calculate a lower bound(LB) of the problem and identify the partitions containing the solution of the lower bound model.
 - 2. Run the original MINLP initialized by the solution of the lower bound model to find an upper bound (UB) solution. If there is failure use the alternatives discussed above (Freezing some binaries and eventually flowrates).
 - 3. Calculate the gap between the upper bound solution and the lower bound solution. If the gap is lower than the tolerance, the solution was found. Otherwise go to the step 4.
 - 4. Run the lower bound model
 - forbidding one of the partitions identified in step 1, or
 - forbidding all the partitions including the one identified in step 1, except the most distant.

If the solution is infeasible or if it is feasible but larger than the upper bound, then all the partitions that have not been forbidden for this variable, are eliminated. The surviving region between the new bounds is re-partitioned.

If the solution is feasible but lower than the upper bound, we cannot bound contract.

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

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

The detailed illustration of the partition elimination using the bound contraction procedures was introduced in our previous publications using examples (Faria and Bagajewicz, 2011a,b; Faria, et al., 2015). In those papers, different options for bound contracting have been introduced: One-pass partition elimination, cyclic elimination, single and extended partitions forbidding (Figure 2), etc., all of which are detailed in the article referenced.

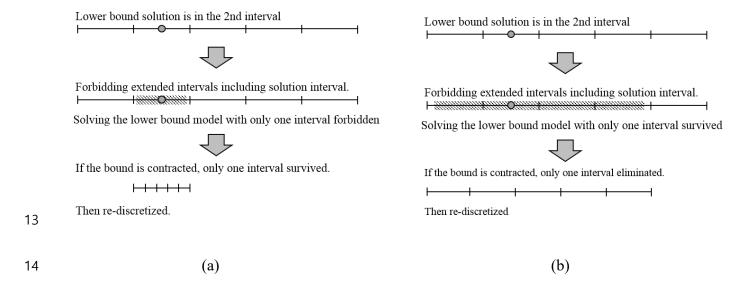


Figure 2. (a) single partition forbidding, (b) extended partition forbidding

The process is repeated with new bounds until convergence or until the bounds cannot be contracted anymore. If the bound contraction does not occur anymore, we suggest to increase the number of partitions and start over. An alternative is branch and bound but we already showed that is more time consuming, especially if we use bound contracting at each node in a previous paper (Faria et al., 2015).

6. EXAMPLES

Two examples of different sizes of networks are presented in this section. The 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 using this example, which is adapted from Nguyen et al. (2010). The data are presented in Table 1 and 2. We assumed a minimum temperature approach of 10° C. The fixed cost of units is 250,000\$, and the area cost coefficient is 550\$/m². We solved using two main stages and two sub-stages model and compared with different number of substages 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	Fcp [KW/C]	Cp [KJ/Kg·°C]	Tin [C]	Tout [°C]	$h [KW/m^2.^{o}C]$
H1	228.5	1	159	77	0.4
H2	20.4	1	267	88	0.3
Н3	53.8	1	343	90	0.25
C1	93.3	1	26	127	0.15
C2	196.1	1	118	265	0.5
HU		1	500	499	0.53
CU		1	20	40	0.53

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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	$550 [\$/m^2]$

We partitioned flows in the bilinear terms of the energy balances and ΔT in the area calculations

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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 7

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The globally optimal solution 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 results are summarized in Table 3 and the optimal solution network is presented in Figure 3. We also run BARON (version 14.4) (Sahinidis,

the lifting partitioning are used for 5590 m² and 11700 kW calculated using pinch analysis.

- 1 1996) and after 10 hours running, we obtained an upper bound value of \$2,574,980 with 77% gap.
- 2 ANTIGONE (version 1.1) (Misener and Floudas, 2014) could not find an upper bound value.

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Table 3. Global optimal solution using 2 main stages and 2 sub-stages.

# of starting partitions	Objective value (\$) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	1,783,257	0.6%	7	4	9m 40s

We found alternative solutions with a different number of sub-stages in Table 4 (Figure 4). The purpose of showing these is to point out that the problem has several solutions within a small gap. One of these solutions was also obtained by Kim and Bagajewicz (2015) using a new generalized superstructure solved using RYSIA. There are other sub-optimal solutions shown in the aforementioned article indicating the computational difficulty that this problem presents close to low gaps.

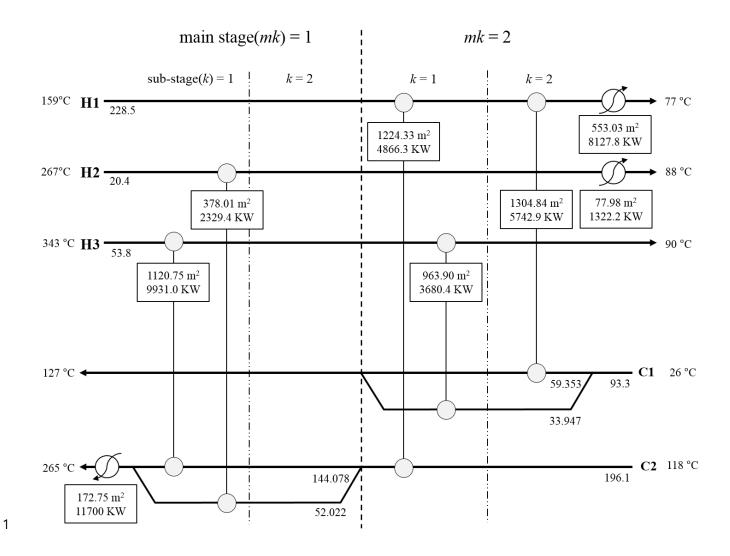
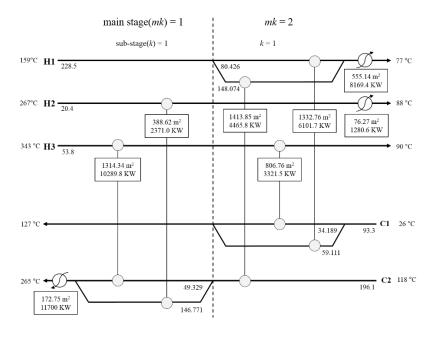


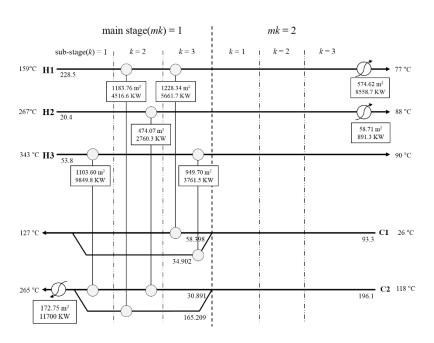
Figure 3. The solution network for example 1 with 2 main stages and 2 sub-stages.

Table 4. Global optimal solutions with a different number of sub-stages.

# of sub- stages	# of starting partitions	Objective value (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
1	2	\$1,797,826	0.8%	21	9	1h 33m 55s
3	2	\$1,780,505	0.5%	11	7	1h 34m 27s
4	2	\$1,780,505	0.5%	3	2	5m 57s



3 (a)



5 (b)

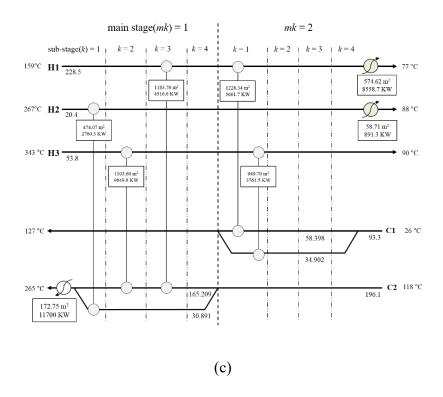


Figure 4. Networks for example 1 with a different number of sub-stages. (a) k=1, (b) k=3, (c) k=4

We notice that in our solutions more than one exchanger in each branch, something that, as explained, cannot be obtained using other models, like the popular stage model (Yee and Grossmann, 1990).

6.2. Example 2: The second example consisting of 11 hot and 2 cold streams corresponds to a crude fractionation unit. The data is given in Table 5 and 6. This example was solved using 2 main stages and 2 sub-stages superstructure model. We assumed a minimum temperature approach of $EMAT_{i,j} = 10 \, ^{\circ}\text{C}$. We also assumed that 4 branched streams are possible in cold stream and no branching on hot stream. The

- 1 fixed cost of units is 250,000\$, and the area cost coefficient is 550 $\$/m^2$. The lower limits of total area and
- 2 total heat of heating utilities in the lifting partitioning are used for 8636 m² and 23566 kW, respectively
- 3 calculated using pinch analysis.

Table 5. Data for example 2

Stream		F _{Cp} [KW/C]	Cp [KJ/Kg·C]	T _{in} [C]	Tout [C]	H [KW/m²⋅C]
H1	TCR	166.7	2.3	140.2	39.5	0.26
H2	LGO	45.8	2.5	248.8	110	0.72
Н3	KEROSENE	53.1	2.3	170.1	60	0.45
H4	HGO	35.4	2.5	277	121.9	0.57
H5	HVGO	198.3	2.4	250.6	90	0.26
Н6	MCR	166.7	2.5	210	163	0.33
H7	LCR	291.7	2.9	303.6	270.2	0.41
Н8	VR1	84.3	1.7	360	290	0.47
Н9	LVGO	68.9	2.5	178.6	108.9	0.6
H10	SR-Quench	27.6	3.2	359.6	280	0.47
H11	VR2	84.3	1.7	290	115	0.47
C1	Crude	347.1	2.1	30	130	0.26
C2	Crude	347.9	3.0	130	350	0.72
HU			1	500	499	0.53
CU			1	20	40	0.53

Table 6. Cost data for example 2.

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

We started to solve this example with using 2 partitions for the chosen partitioning variables (flow and ΔT) and used extended partition forbidding for the bound contraction when the number of partitions is larger than 2. We found that it took more than 6 hours to solve the lower bound model. We also run BARON (version 14.4) (Sahinidis, 1996), which after 10 hours running obtained an upper bound value of 10^{50} (clearly infinity) and a lower bound of \$1,919,460. In turn, ANTIGONE (version 1.1) (Misener and Floudas, 2014) could not find a feasible solution of the upper bound value.

To address the difficulty, we added lifting partitioning equations for total number of units as follows:

$$\sum_{i,j,mk,bh,bc,k} z_{i,j,mk,bh,bc,k} + \sum_{i} zcu_i + \sum_{j} zhu_j = TU$$
(80)

$$\sum_{m} (TUD_{m} \cdot vTU_{m}) \le TU \le \sum_{m} (TUD_{m+1} \cdot vTU_{m})$$
(81)

$$\sum_{m} vTU_{m} = 1 \tag{82}$$

where, vTU_m is the binary variable for TU and TUD_m is discrete point of the total number of unit. With these equations, we found the solution with a 4.3% gap (Table 7). The optimal solution network presented in Figure 5, has an annualized cost of \$3,527,430.

Table 7. Optimal solution network with an additional lifting partitioning.

# of starting partitions	Objective value (\$) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	3,527,430	4.3%	18	7	13h 14m 26s

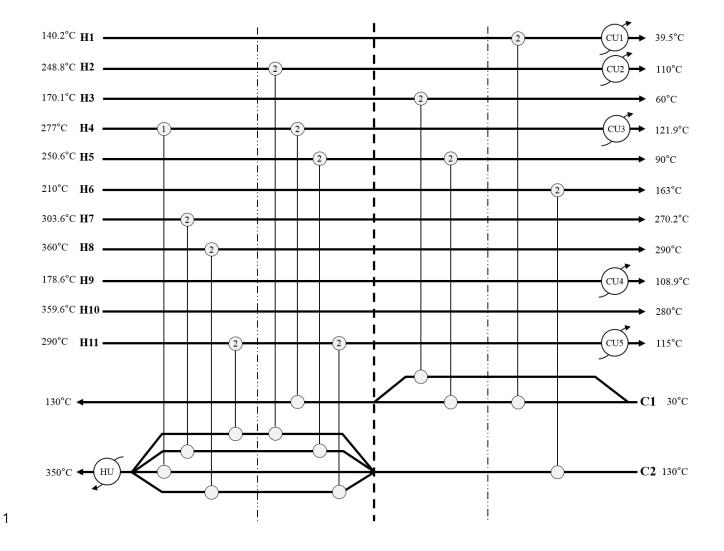


Figure 5. Solution for example 2 with lifting partitioning of the number of units.

We added lifting partitioning of the total heat exchanged by heat exchangers in addition to the partition of total utility usage, as follows:

$$\sum_{i,j,mk,bh,bc,k} q_{i,j,mk,bh,bc,k} = QA \tag{83}$$

$$\sum_{m} (QAD_{m} \cdot vQA_{m}) \leq QA \leq \sum_{m} (QAD_{m+1} \cdot vQA_{m})$$
(84)

$$\sum_{m} vQA_{m} = 1 \tag{85}$$

- 1 where vQA_m is the binary variable for QA and QAD_m is discrete point of the total exchanged heat of
- 2 heat exchangers. When we used both the total number of units and total exchanged heat in the lifting
- partitioning we obtained a slightly better result with objective value of \$3,499,599 and 3.5% tolerance gap
- 4 after 15 iterations using 12h 29m 10s cpu time. The solution network is presented in Figure 6.

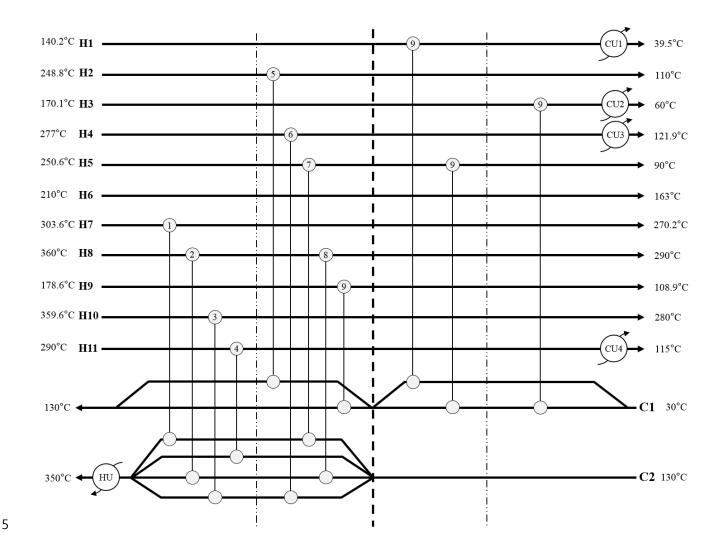


Figure 6. The solution networks for example 2 adding lifting partitioning (units and heat exchanged).

Finally, we added sub-stage heat balance constraints. Using the definition of AH and AC, we write $QH_{i,mk,bh}$ and $QC_{j,mk,bc}$ in equations (6) and (8) as follows:

$$QH_{i,mk,bh} = AH_{i,mk,bh,"1"} - AH_{i,mk,bh,"SBNOK+1"} \quad \forall i,mk,bh$$
(86)

$$QC_{j,mk,bc} = AC_{j,mk,bc,"1"} - AC_{j,mk,bc,"SBNOK+1"} \quad \forall j,mk,bc$$
 (87)

After adding these equations to all the previous lifting constraints we obtained an objective value of \$3,456,649 with 2.3% tolerance gap after using 1m 57s cpu time (Table 8). This optimal solution was found in the 1st iteration (Figure 7). We found the optimal solution using less cpu time than our generalized superstructure model (Kim and Bagajewicz, 2016). The result is summarized in Table 9.

Table 8. Optimal solution network with lifting partitioning of the number of units, the total heat exchangers duty and the sub-stages heat balances.

# of starting partitions	Objective value (\$) (Upper Bound)	Gap	# of iterations	# of partitions at convergence	CPU Time
2	3,456,649	2.3%	1	2	1m 57s

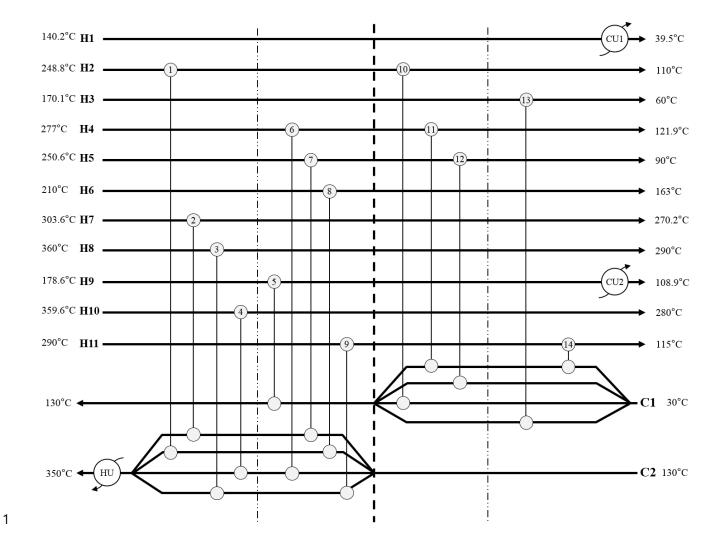


Figure 7. Solution for example 2 with lifting partitioning of the number of units, the total heat exchangers duty and the sub-stages heat balances.

Table 9. Heat exchanger results for example 2 with equations (80-87).

	Area (m2)	Duty [KW]
EX1	186.20	1364.9
EX2	840.90	7848.3
EX3	230.58	2786.7
EX4	166.18	1952.6

EX5	477.45	2276.2	
EX6	388.69	3153.2	
EX7	2093.75	12017.2	
EX8	1081.76	5440.7	
EX9	744.95	5652.7	
EX10	204.84	3048.9	
EX11	109.53	659.1	
EX12	1385.12	9214.1	
EX13	566.16	3734.6	
EX14	108.71	1314.0	
CU1	1087.17	10724.5	
CU2	32.70	1058.9	
HU	426.45	23566.0	
Total annual cost	\$ 3,456,649		

When we used 10 partitions for partitioning variables instead of 2, the cpu time was increased and did not show better results than those in Table 7, 8 and 9 since the bound contraction was slow. If we assumed that 3 branches is the maximum possible for cold streams, the objective value was \$3,586,052 with 5.9% gap using 1 hr 20min 27sec of cpu time. (Figure 8)

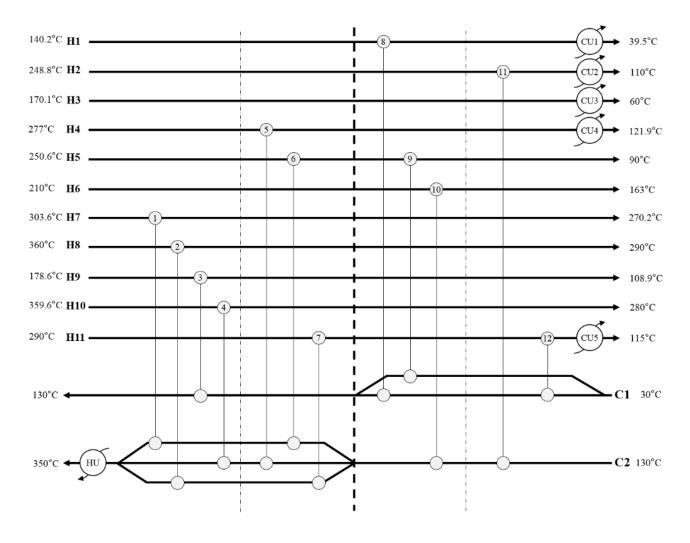


Figure 8. The solution network of the stages/substages model.

This solution showed higher objective value than the generalized superstructure model (Kim and Bagajewicz, 2015) because the stages/substages model has the limitation of branching compared to the generalized superstructure model.

If we did not use the liftings including equations (86) and (87) in the model, it was the same result without these equations that it took more than 6 hours to solve the lower bound model. In addition,

1 BARON (version 14.4) (Sahinidis, 1996) obtained an upper bound value of 10⁵¹ (clearly infinity) and a

2 lower bound of \$1,903,050 after 24 hours running and ANTIGONE (version 1.1) (Misener and Floudas,

3 2014) could not find a feasible solution of the upper bound value. We also tested using a branch and a

bound method with the lifting partitioning and lifting equations (86) and (87), the objective value was

\$3,598,373 with 6.2% gap after 11 hr 28 min 48 sec of cpu time.

Aside from the fact that this example is bigger than example 1 and therefore does not solve using the same approach needing additional lifting constraints, there are similarities in the sense that as soon as a small gap is achieved, several alternative solutions exist, complicating the search for a smaller gap global optimum.

7. CONCLUSION

We solve globally a new stages/substages HEN model proposed by Jonguswat et al. (2014). The stages/substages model (Jonguswat et al., 2014) was fully described in detail in this paper incorporating details that Jonguswat et al. (2014) did not present. Instead of the ad-hoc method used by Jonguswat et al. (2014), we used RYSIA, a newly developed global optimization procedure based on bound contraction (without resorting to branch and bound). We discussed new options of RYSIA in the examples and compared their efficiencies. 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 (Sahinidis, 1996) and ANTIGONE (Misener and Floudas, 2014) had serious difficulties. 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

13 mk : Stage

bh : Hot stream branch

bc : Cold stream branch

k : Sub-stage

o : Heat capacity flow rate partitioning point

*n*l : Hot side temperature differences partitioning point

*n*2 : Cold side temperature differences partitioning point

PARAMETERS

NOK : Number of main stages

2 SBNOK : Number of sub stages

 Fh_i : Heat capacity flow rate for hot stream

 Fc_i : Heat capacity flow rate for cold stream

 T_i^{HIN} : Inlet temperature of hot stream

 T_i^{HOUT} : Outlet temperature of hot stream

 T_i^{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

CUcost : Hot utility cost

*HU*cost : Cold utility cost

17 EMAT : Exchanger minimum approach different

 $FbhD_{i,mk,bh,o}$: Discrete point of the partitioned flow rate of sub-stage hot stream

 $FbcD_{j,mk,bc,o}$: Discrete point of the partitioned flow rate of sub-stage cold stream

 $ThD_{i,i,mk,bh,bc,k,n1}$: Discrete point of temperature differences in hot side of heat exchanger

 $T_{CD_{i,j,mk,bh,bc,k,n2}}$: Discrete point of temperature differences in cold side of heat exchanger

3 Γ : Maximum temperature differences

 Ω : Maximum area or maximum heat

BINARY VARIABLES

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

 zcu_i : Binary variable to denote a cold utility

 zhu_i : Binary variable to denote a hot utility

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

 $Yh_{i,j,mk,bh,bc,k,n1}$: Binary variable related to the partitioned hot side temperature differences

 $Y_{C_{i,j,mk,bh,bc,k,n2}}$: Binary variable related to the partitioned cold side temperature differences

15 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_i : 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
- $QCM_{i.mk}$: Total exchanged heat for cold stream j in stage mk
- $QC_{i,mk,bc}$: 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 $Fbc_{j,mk,bc}$
- $Th_{i,mk}$: 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
- $Fbh_{imk\ bh}$: 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
- $\Delta T c u_i$: Cold utility temperature difference
- ΔThu_i : Hot utility temperature difference

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