I&EC research
Industrial & Engineering Chemistry Research

Article

pubs.acs.org/IECR

# Global Optimization of Heat Exchanger Networks. Part 1: Stages/Substages Superstructure

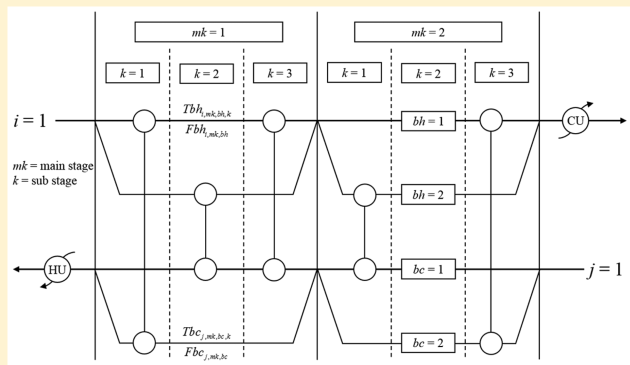
Sung Young Kim,[†] Pitak Jongsuwat,[§] Uthaiporn Suriyapraphadilok,[§] and Miguel Bagajewicz*,[‡]

[†]Department of Chemical Engineering, Kyung Hee University, 1732 Deogyeong-daero, Yongin, 17104, Republic of Korea

[‡]School of Chemical, Biological and Materials Engineering, University of Oklahoma 100 East Boyd Street, T-335, Norman, Oklahoma 73019-0628, United States

[§]Petroleum and Petrochemical College, Chulalongkorn University, 254 Soi Chulalongkorn12, Phayathai Road, Wangmai, Patumwan, Bangkok 10330 Thailand

**ABSTRACT:** We solve globally an extension of the isothermal mixing stages model (Synheat) proposed by Yee and Grossmann, later extended to nonisothermal mixing by Björk and Weterlund and solved globally by Faria et al. This new extension of that model was recently presented in a conference proceedings. The model allows specific structures that are more commonly accepted in industry than generalized complex structures that suffer from somewhat disorganized branched and sub-branches which present several practical challenges. This stages/substages superstructure has limited branching and several matches in series in each branch. Our industrial experience shows us that these are acceptable in practice. The novel contribution of this article is then solving such a model globally, adding the control of temperature differences upon mixing




## 1. INTRODUCTION

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.[6] Morar and Agachi also offered a literature review until 2008.[7] Of all this work, we point out the combined use of mathematical programming and superstrucures, of which the first generalized superstructure for HEN design was presented by Floudas et al.[8] 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 nonconvex 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, a product of several splittings and mixings. 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.[5] Later, another superstructure model was proposed by Yee and Grossmann,[1] 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. Further studies followed where nonisothermal mixing was added[2,9] and some different configurations were allowed.[10] Various other approaches for a HEN stage superstructure model exist: Konukman et al.,[11] Frausto-Hernandez et al.,[12] Ponce-Ortega et al.,[13] Escobar and Trierweiler,[14] Onishi et al.,[15] and Na et al.[16] There are also many other recent works for finding the local and global optimum of heat exchanger network grassroots models. Laukkanen and Fogelholm proposed a bilevel optimization method based on grouping streams for simultaneous synthesis of HEN.[17] Bogataj and Kravanja used a modified outer approximation (OA)/equality relaxation (ER) algorithm for yielding a lower bound close to 1% tolerance gap.[18] Huang et al. found solutions of an MINLP model based on a hyperstructure of stage-wise stream superstructure of HEN.[9]

**Received:** December 3, 2016
**Revised:** February 20, 2017
**Accepted:** April 12, 2017
**Published:** April 12, 2017





DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

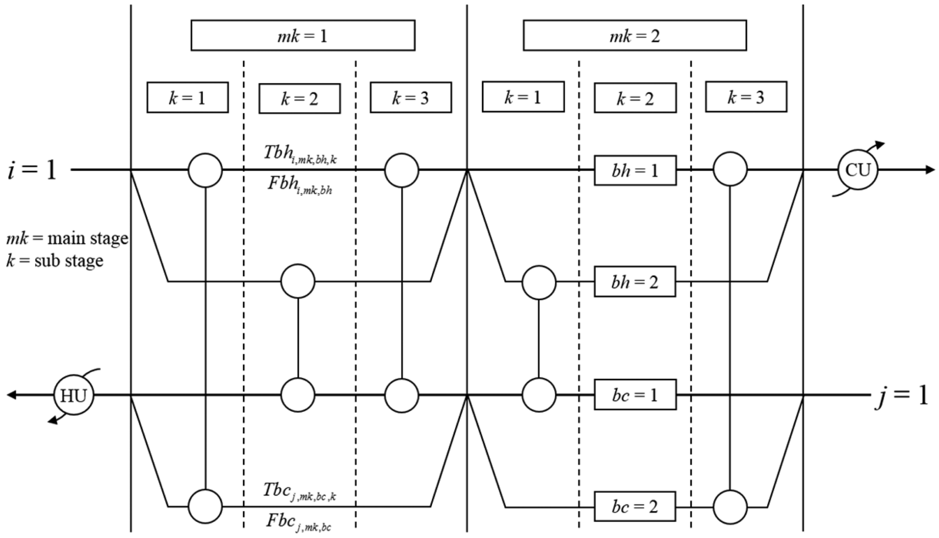



**Figure 1.** Stage/substage wise network superstructure.

Haung and Karimi proposed different approaches[9,10,19] including using BARON,[20] which proved to be inefficient to solve their model. Finally they used an ad-hoc search strategy of repeatedly using the OA algorithm. Kang et al. proposed a parallel sequential quadratic programming (SQR) algorithm based on graphic process unit (GPU) acceleration to find solutions on MINLP models of HEN synthesis.[21] Myankooh and Shafiei 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.[22]

All the aforementioned mathematical programming-based efforts were not able to capture some alternative structures, such as 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.[4] 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),[3,23] with existing commercial global solvers.

The academic efforts and the available commercial software were reviewed in our previous article.[3] We only highlight what are the options we pursue in this article: all HEN models contain bilinear terms consisting of flow rates 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,[24,25] one can make appropriate substitutions,[26] to obtain purely quadratic/bilinear models.

In this article, we explore the use of our bound contraction procedure for global optimization[23] to solve the stages/substages model. Like a generalized superstructure model by Kim and Bagajewicz,[5] the stage/substages-wise model can produce structures that cannot be obtained from the stages model by Yee and Grossmann.[1] We can produce branches of streams and matches between hot and cold stream pairs using the concept of the substages. In our lower bound, we follow the direct partitioning procedure 1(DPP1) strategy for the relaxation of bilinear terms,[23] 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

The original stage-wise superstructure does not include the case of branch stream which contains two or more exchangers in series and the case of stream bypasses.[1] 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 a realistic model. Therefore, in this work modification of the original model is investigated as follows:

The proposed stage/substage-wise superstructure model in Figure 1, a number of substages $k$ 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.

- The overall energy balances for each stream

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

$$\sum_{i}\sum_{mk}\sum_{bh}\sum_{bc}\sum_{k} q_{i,j,mk,bh,bc,k} + qhu_j = Fc_j(T_j^{COUT} - T_j^{CIN}) \quad \forall j \tag{2}$$

- The energy balances at each main stage and substage

$$HA_{mk} = CA_{mk} \quad \forall\, mk \tag{3}$$

$$\sum_{i} QHM_{i,mk} = HA_{mk} \quad \forall\, mk \tag{4}$$



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

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

$$\sum_{bh} QH_{i,mk,bh} = QHM_{i,mk} \quad \forall\, i,\, mk \tag{6}$$

$$\sum_{k} qHK_{i,mk,bh,k} = QH_{i,mk,bh} \quad \forall\, i.\, mk,\, bh \tag{7}$$

$$\sum_{j} QCM_{j,mk} = CA_{mk} \quad \forall\, mk \tag{8}$$

$$QCM_{j,mk} = (Tc_{j,mk} - Tc_{j,mk+1})Fc_j \quad \forall\, j,\, mk \tag{9}$$

$$\sum_{bc} QC_{j,mk,bc} = QCM_{j,mk} \quad \forall\, j,\, mk \tag{10}$$

$$\sum_{k} qCK_{i,mk,bc,k} = QC_{j,mk,bc} \quad \forall\, j,\, mk,\, bc \tag{11}$$

From the above equations, each main stage of hot and cold streams are classified into main stages ($HA_{mk}$ and $CA_{mk}$), branch streams ($QHM_{i,mk}$, $QCM_{j,mk}$, $QH_{i,mk,bh}$, $QC_{j,mk,bc}$), and substages ($qHK_{i,mk,bh,k}$, $qCK_{j,mk,bc,k}$), respectively, to reduce the number of dependent variable in each equation as many as possible by introducing intermediate variables.

- Multiple of temperature and heat capacity flow

$$AH_{i,mk,bh,k} = Tbh_{i,mk,bh,k}Fbh_{i,mk,bh} \quad \forall\, i,\, mk,\, bk,\, k \tag{12}$$

$$AC_{j,mk,bc,k} = Tbc_{j,mk,bc,k}Fbc_{j,mk,bc} \quad \forall\, j,\, mk,\, bc,\, k \tag{13}$$

- Substage heat balances

$$\sum_{j}\sum_{bc} q_{i,j,mk,bh,bc,k} = qHK_{i,mk,bh,k} \quad \forall\, i,\, mk,\, bh,\, k \tag{14}$$

$$qHK_{i,mk,bh,k} = AH_{i,mk,bh,k} - AH_{i,mk,bh,k+1} \quad \forall\, i,\, mk,\, bh,\, k \tag{15}$$

$$\sum_{i}\sum_{bh} q_{i,j,mk,bh,bc,k} = qCK_{j,mk,bc,k} \quad \forall\, j,\, mk,\, bh,\, k \tag{16}$$

$$qCK_{j,mk,bc,k} = AC_{j,mk,bc,k} - AC_{j,mk,bc,k+1} \quad \forall\, j,\, mk,\, bc,\, k \tag{17}$$

- Superstructure inlet temperatures

$$Th_{i,1} = T_i^{\mathrm{HIN}} \quad \forall\, i \tag{18}$$

$$\sum_{bh} AH_{i,mk,bh,1} = Fh_i Th_{i,mk} \quad \forall\, i,\, mk \tag{19}$$

$$\sum_{bh} AH_{i,mk,bh,SBNOK+1} = Fh_i Th_{i,mk+1} \quad \forall\, i,\, mk \tag{20}$$

$$Th_{i,mk} = Tbh_{i,mk,bh,1} \quad \forall\, i,\, mk,\, bh \tag{21}$$

$$Tc_{j,NOK+1} = T_j^{\mathrm{CIN}} \quad \forall\, j \tag{22}$$

$$\sum_{bc} AC_{i,mk,bc,1} = Fc_j Tc_{j,mk} \quad \forall\, j,\, mk \tag{23}$$

$$\sum_{bc} AC_{j,mk,bc,SBNOK+1} = Fc_j Tc_{j,mk+1} \quad \forall\, j,\, mk \tag{24}$$

$$Tc_{j,mk+1} = Tbc_{j,mk,bc,SBNOK+1} \quad \forall\, j,\, mk,\, bc \tag{25}$$

- Feasibility of temperatures (monotonic decrease in temperature)

$$Th_{i,mk} \geq Th_{i,mk+1} \quad \forall\, i,\, mk \tag{26}$$

$$Tbh_{i,mk,bh,k} \geq Tbh_{i,mk,bh,k+1} \quad \forall\, i,\, mk,\, bh,\, k \tag{27}$$

$$T_i^{\mathrm{HOUT}} \leq Th_{i,NOK+1} \quad \forall\, i \tag{28}$$

$$Tc_{j,mk} \geq Tc_{j,mk+1} \quad \forall\, j,\, mk,\, bc,\, k \tag{29}$$

$$Tbc_{j,mk,bc,k} \geq Tbc_{j,mk,bc,k+1} \quad \forall\, j,\, mk,\, bc,\, k \tag{30}$$

$$T_j^{\mathrm{COUT}} \geq Tc_{j,1} \quad \forall\, j \tag{31}$$

- Hot and cold utility load

$$(Th_{i,NOK+1} - T_i^{\mathrm{HOUT}})Fh_i = qcu_i \quad \forall\, i \tag{32}$$

$$(T_j^{\mathrm{COUT}} - Tc_{j,1})Fc_j = qhu_j \quad \forall\, j \tag{33}$$

- Logical constraints

$$q_{i,j,mk,bh,bc,k} - \Omega{\cdot}z_{i,j,mk,bh,bc,k} \leq 0 \quad \forall\, i,\, j,\, mk,\, bh,\, bc,\, k \tag{34}$$

$$qcu_i - \Omega{\cdot}zcu_i \leq 0 \quad \forall\, i \tag{35}$$

$$qhu_j - \Omega{\cdot}zhu_j \leq 0 \quad \forall\, j \tag{36}$$

- Maximum matching

$$\sum_{i,bh} z_{i,j,mk,bh,bc,k} \leq 1 \quad \forall\, j,\, mk,\, bc,\, k \tag{37}$$

$$\sum_{j,bc} z_{i,j,mk,bh,bc,k} \leq 1 \quad \forall\, i,\, mk,\, bh,\, k \tag{38}$$

- Mass balances at each main stage

$$\sum_{bh} Fbh_{i,mk,bh} \leq Fh_i \quad \forall\, i,\, mk \tag{39}$$

$$\sum_{bc} Fbc_{j,mk,bc} \leq Fc_j \quad \forall\, i,\, mk \tag{40}$$

- Calculation of approach temperature

$$\Delta Th_{i,j,mk,bh,bc,k} \leq Tbh_{i,mk,bh,k} - Tbc_{j,mk,bc,k} + \Gamma(1 - z_{i,j,mk,bh,bc,k}) \quad \forall\, i,\, j,\, mk,\, bh,\, bc,\, k \tag{41}$$



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

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

$$\Delta Tcu_i \leq Th_{i,NOK+1} - T_{CU}^{OUT} + \Gamma(1 - zcu_i) \quad \forall i \tag{43}$$

$$\Delta Thu_j \leq T_{HU}^{OUT} - Tc_{j,1} + \Gamma(1 - zhu_j) \quad \forall j \tag{44}$$

- Minimum approach temperatures (lower bounds)

$$\Delta Th_{i,j,mk,bh,bc,k} \geq EMAT \quad \forall i, j, mk, bh, bc, k \tag{45}$$

$$\Delta Tc_{i,j,mk,bh,bc,k} \geq EMAT \quad \forall i, j, mk, bh, bc, k \tag{46}$$

$$\Delta Tcu_i \geq EMAT \quad \forall i \tag{47}$$

$$\Delta Thu_j \geq EMAT \quad \forall j \tag{48}$$

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 on area, through a concave function. First, it has been shown that a linear approximation of such a function through the range of appropriate areas, is tight.[27] 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 constraints to calculate them are incorporated.

- Logarithmic mean temperature difference (LMTD) (Chen[25])

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

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

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

- Area calculation

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

$$qcu_i - Acu_iU_{CUi}LMTD_{CUi} = 0 \quad \forall\, i \tag{53}$$

$$qhu_j - Ahu_jU_{HUj}LMTD_{HUj} = 0 \quad \forall\, j \tag{54}$$

- Objective function

$$\min\{\sum_i qcu_i\cdot CU\text{cost} + \sum_j qhu_j\cdot HU\text{cost} + C_{\text{var}}(\sum_{i,j,mk,bh,bc,k} A_{i,j,mk,bh,bc,k} + \sum_i Acu_i + \sum_j Ahu_j)/n + C_{fixed}(\sum_{i,j,mk,bh,bc,k} z_{i,j,mk,bh,bc,k} + \sum_i zcu_i + \sum_j zhu_j)/n\} \tag{55}$$

where $n$ is the number of years used to annualized the capital cost.

## 3. LOWER BOUND MODEL

In the bilinear terms (eqs 12 and 13), we choose branched flow rate 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,[5] resulting in eight equations containing bilinear and quadratic terms and six new variables. It was shown that it is less efficient than the partitioning proposed by Faria et al.[3] which results in one new variable and three more equations.

The partitioned variables are the branched flow rate differences in this case. In the case of image partitioning, we partition the temperature differences, as done by Faria et al.[3]

### 3.1. Bilinear Terms.

Equations 12 and 13 are considered for this decomposition.

- Partitioning $Fbh_{i,mk,bh}$ variable with $o$ partitions

$$\sum_o FbhD_{i,mk,bh,o} \times vFbhD_{i,mk,bh,o} \leq Fbh_{i,mk,bh} \leq \sum_o FbhD_{i,mk,bh,o+1} \times vFbhD_{i,mk,bh,o} \quad \forall\, i, mk, bh \tag{56}$$

$$\sum_o vFbhD_{i,mk,bh,o} = 1 \quad \forall\, i, mk, bh \tag{57}$$

We partition flow rates $Fbh_{i,mk,bh}$ using $o$ partitions. Then $AH_{i,mk,bh,k}$ is bounded by the following relations.

$$AH_{i,mk,bh,k} \geq \sum_o FbhD_{i,mk,bh,o} \times TbhB_{i,mk,bh,k,o} \quad \forall i, mk, bh, k \tag{58}$$


DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

$$AH_{i,mk,bh,k} \le \sum_o FbhD_{i,mk,bh,o+1} \times TbhB_{i,mk,bh,k,o} \quad \forall\ i,\ mk,\ bh,\ k \tag{59}$$

The variable $TbhB_{i,mk,bh,k,o}$ is introduced to replace the product of the partitioned flow rates and binary variables. According to the direct partitioning procedures (DPP1) of (Faria and Bagajewicz[28]), $TbhB_{i,mk,bh,k,o}$ has the following equations.

$$TbhB_{i,mk,bh,k,o} \ge 0 \quad \forall\ i,\ mk,\ bh,\ k,\ o \tag{60}$$

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

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

$$Tbh_{i,mk,bh,k} - TbhB_{i,mk,bh,k,o} \ge 0 \quad \forall i,\ mk,\ bh,\ k,\ o \tag{63}$$

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

**3.2. Nonlinear Function.** Equation 52 is considered for this decomposition.

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

$$\sum_l \Delta TD_{i,j,mk,bh,bc,k,l} \times YHX_{i,j,mk,bh,bc,k,l} \le \Delta Th_{i,j,mk,bh,bc,k} \le \sum_l \Delta TD_{i,j,mk,bh,bc,k,l+1} \times YHX_{i,j,mk,bh,bc,k,l} \tag{64}$$

$$\sum_n \Delta TD_{i,j,mk,bh,bc,k+1,n} \times YHX_{i,j,mk,bh,bc,k+1,n} \le \Delta Tc_{i,j,mk,bh,bc,k} \le \sum_n \Delta TD_{i,j,mk,bh,bc,k+1,n+1} \times YHX_{i,j,mk,bh,bc,k+1,n} \tag{65}$$

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

$$\sum_n YHX_{i,j,mk,bh,bc,k+1,n} = z_{i,j,mk,bh,bc,k} \tag{67}$$

Now we rewrite the area calculation as follows; $\forall i,j,mk,bh,bc,k$:

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

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 eq 68 with new positive continuous variable ($H_{i,j,mk,bh,bc,k,l,n}$):

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

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

$$\sum_l H_{i,j,mk,bh,bc,k,l,n} - \Omega YHX_{i,j,mk,bh,bc,k+1,n} \le 0 \quad \forall i,\ j,\ mk,\ bh,\ bc,\ k,\ n \tag{70}$$

$$\sum_n H_{i,j,mk,bh,bc,k,l,n} - \Omega YHX_{i,j,mk,bh,bc,k,l} \le 0 \quad \forall i,\ j,\ mk,\ bh,\ bc,\ k,\ l,\ n \tag{71}$$

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

$$\sum_l \sum_n H_{i,j,mk,bh,bc,k,l,n} = A_{i,j,mk,bh,bc,k} \quad \forall\ i,\ j,\ mk,\ bh,\ bc,\ k \tag{73}$$

A similar procedure can be applied to eqs 53 and 54.

## 4. LIFTING PARTITIONING

To help increasing (lifting) the lower bound value, we resort to partitioning of variables that participate in the objective function (Kim and Bagajewicz[5]). For these we introduce new variables for total heat of heating utilities and total area.

$$\sum_j Q_j^{HU} = TQH \tag{74}$$

$$\sum_{i,j,mk,bh,bc,k} A_{i,j,mk,bh,bc,k} + \sum_i Acu_i + \sum_j Ahu_j = TA \tag{75}$$

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

$$\sum_m (TQHD_m \cdot vTQH_m) \le TQH \le \sum_m (TQHD_{m+1} \cdot vTQH_m) \tag{76}$$

$$\sum_m vTQH_m = 1 \tag{77}$$



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944–5957

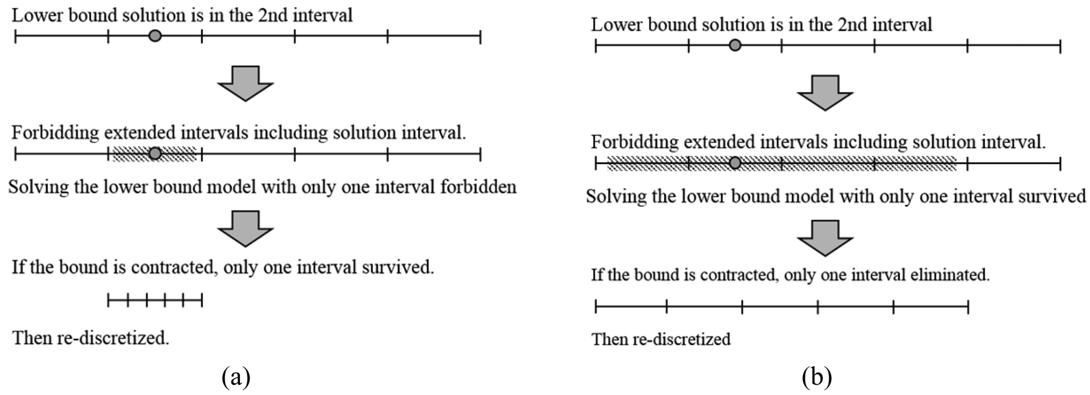



**Figure 2.** (a) single partition forbidding, (b) extended partition forbidding.

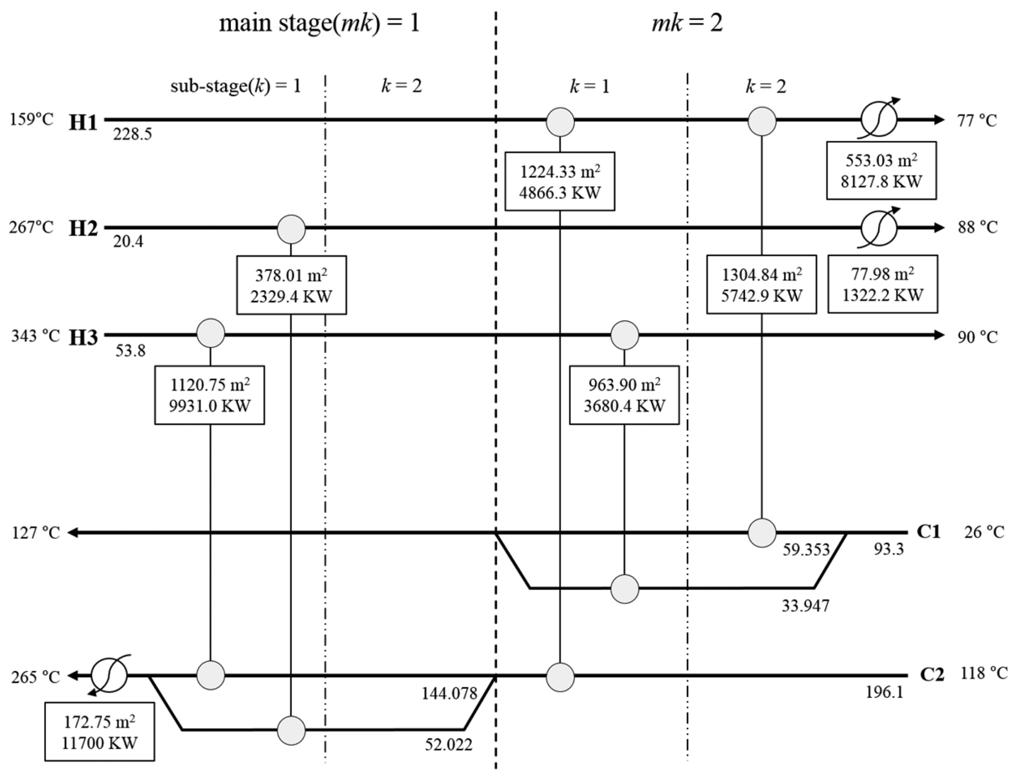



**Figure 3.** Solution network for example 1 with 2 main stages and 2 substages.

$$\sum_p (TAD_p \cdot vTA_p) \le TA \le \sum_p (TAD_{p+1} \cdot vTA_p) \quad (78)$$

$$\sum_p vTA_p = 1 \quad (79)$$

$TAD_p$ 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 flow rates 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


DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

lifting), and branch and bound variables, which are the variables for which a branch and bound procedure is tried (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 first. Then we use the result of the lower bound model as initial values for the upper bound model. We proceed to perform bound contraction on all variables as explained below.

**5.1. Bound Contraction.** The bound contraction procedure is used by RYSIA in the partition elimination strategy presented by Faria and Bagajewicz[28,29] and Faria et al.[3] We summarized the basic strategy in this section. 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 flow rates).
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 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.
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.[3,28,29] 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.

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 in a previous paper[3] that it is more time-consuming, especially if we use bound contracting at each node.

## 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.[30]) and solved using CPLEX (version 12.3) as the MIP solver and DICOPT (Viswanathan and Grossmann[31]) as the MINLP solver on a PC machine (i7 3.6 GHz, 8GB RAM).

Our model shares the same features as the original stages model; that is, there is no general a priori rule to decide how many stages are needed. In practice, one can start with any number of stages and keep increasing them until little change is seen in the objective function. This may lead to several suboptimal solutions. We do not explore this issue in this article.

**6.1. Example 1.** The first example is an example to find the optimum HEN design, which consists of three hot streams and two cold streams. We illustrate the proposed approach in detail using this example, which is adapted from Nguyen et al.[32] The data are presented in Tables 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 $550/m$^2$. We solved using two main stages and two substages model and compared with a 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 | $F_{cp}$ [KW/C] | $C_p$ [KJ/kg·°C] | $T_{in}$ [°C] | $T_{out}$ [°C] | h [KW/m$^2$·°C] |
|---|---|---|---|---|---|
| H1 | 228.5 | 1 | 159 | 77 | 0.4 |
| H2 | 20.4 | 1 | 267 | 88 | 0.3 |
| H3 | 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 |

**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 $\Delta T$ in the area calculations using two 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. For this analysis, we calculated the minimum utility using a temperature approximation equal to our EMAT. The minimum area was obtained using vertical heat transfer, which is a feature of the method.

The globally optimal solution has an annualized cost of $1,783,257 and was obtained in the root node of the seventh iteration satisfying the 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[20]) and after 10 h running, we obtained an upper bound value of $2,574,980 with 77% gap. ANTIGONE (version 1.1) (Misener and Floudas[33]) could not find an upper bound value.

**Table 3. Global Optimal Solution Using 2 Main Stages and 2 Substages**

| no. of starting partitions | objective value ($) (upper bound) | gap | no. of iterations | no. of partitions at convergence | CPU time |
|---|---|---|---|---|---|
| 2 | 1,783,257 | 0.6% | 7 | 4 | 9 m, 40 s |

We found alternative solutions with a different number of substages in Table 4 (Figure 4). The purpose of showing these is to point out that the problem has several solutions



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

**Table 4. Global Optimal Solutions with a Different Number of Substages**

| no. of substages | no. of starting partitions | objective value (upper bound) | gap | no. of iterations | no. of partitions at convergence | CPU time |
|---|---|---|---|---|---|---|
| 1 | 2 | $1,797,826 | 0.8% | 21 | 9 | 1 h, 33 m, 55 s |
| 3 | 2 | $1,780,505 | 0.5% | 11 | 7 | 1 h, 34 m, 27 s |
| 4 | 2 | $1,780,505 | 0.5% | 3 | 2 | 5 m, 57 s |

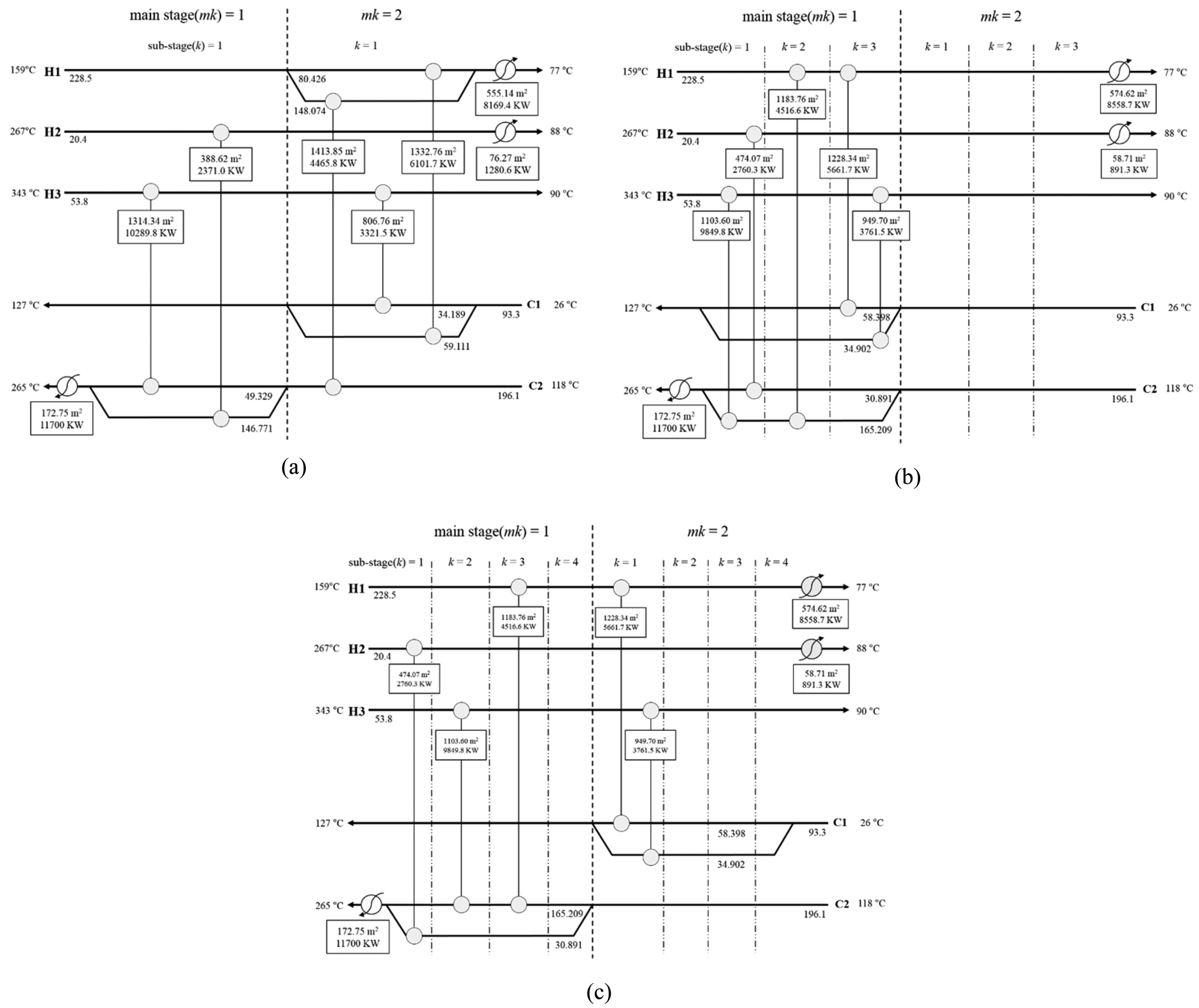



**Figure 4.** Networks for example 1 with a different number of substages: (a) $k$ = 1, (b) $k$ = 3, (c) $k$ = 4.

within a small gap. One of these solutions was also obtained by Kim and Bagajewicz[5] using a new generalized superstructure solved using RYSIA. There are other suboptimal solutions shown in the aforementioned article indicating the computational difficulty that this problem presents close to low gaps. We note also that two of the solutions shown have the same objective and the same matches, except that they take place in different stages/substages. This issue affects the computational performance because it forces the binary associated branch and bound procedure to check the same structure twice. Finally, we note that the discrepancy in the computational time when more substages are added merits further analysis in future work.

We notice that in our solutions more than one exchanger is in each branch, something that, as explained, cannot be obtained using other models, like the popular stage model (Yee and Grossmann[1]).

**6.2. Example 2.** The second example consisting of 11 hot and 2 cold streams corresponds to a crude fractionation unit. The data are given in Tables 5 and 6. This example was solved using a two main stages and two substages superstructure model. We assumed a minimum temperature approach of $EMAT_{i,j}$ = 10 °C. We also assumed that four branched streams are possible in cold stream and no branching on hot stream. This assumption is consistent with industrial practice in crude units, where more branches than four are considered impractical. We note that the possibility of better solutions using a larger number of branches exists and can be explored using the current model. One might obtain lower area and even lower energy consumption. One can also


DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

**Table 5. Data for Example 2**

| stream | | $F_{Cp}$ [KW/°C] | $C_p$ [KJ/kg·°C] | $T_{in}$ [°C] | $T_{out}$ [°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 |
| H3 | 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 |
| H6 | MCR | 166.7 | 2.5 | 210 | 163 | 0.33 |
| H7 | LCR | 291.7 | 2.9 | 303.6 | 270.2 | 0.41 |
| H8 | VR1 | 84.3 | 1.7 | 360 | 290 | 0.47 |
| H9 | 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 [$/unit] |
| variable cost for heat exchanger area | 550 [$/m²] |

see migrations of certain exchangers in series in one branch to another branch. Such an exercise corresponds to a practitioner solving a specific problem as no general conclusions can be made. The fixed cost of units is $250,000, and the area cost coefficient is $550/m². The lower limits of total area and total heat of heating utilities in the lifting partitioning are used for 8636 m² and 23566 kW, respectively, calculated using pinch analysis.

We started to solve this example using two partitions for the chosen partitioning variables (flow and $\Delta T$) and used extended partition forbidding for the bound contraction when the number of partitions was larger than 2. We found that it took more than 6 h to solve the lower bound model. We also ran BARON (version 14.4) (Sahinidis[20]), which after 10 h 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[33]) could not find a feasible solution of the upper bound value.

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

$$\sum_{i,j,mk,bh,bc,k} z_{i,j,mk,bh,bc,k} + \sum_i zcu_i + \sum_j zhu_j = TU \tag{80}$$

$$\sum_m (TUD_m \cdot vTU_m) \leq TU \leq \sum_m (TUD_{m+1} \cdot vTU_m) \tag{81}$$

$$\sum_m vTU_m = 1 \tag{82}$$

where $vTU_m$ is the binary variable for $TU$ and $TUD_m$ is the 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.

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

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

$$\sum_m (QAD_m \cdot vQA_m) \leq QA \leq \sum_m (QAD_{m+1} \cdot vQA_m) \tag{84}$$

$$\sum_m vQA_m = 1 \tag{85}$$

where $vQA_m$ is the binary variable for $QA$ and $QAD_m$ is the discrete point of the total exchanged heat of 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 an objective value of $3,499,599 and 3.5% tolerance gap after 15 iterations using 12 h 29 m 10 s CPU time. The solution network is presented in Figure 6.

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

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

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

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 1 m 57 s CPU time (Table 8). This optimal solution was found in the first iteration (Figure 7). We found the optimal solution using less CPU time than our generalized superstructure model (Kim and Bagajewicz[5]). The results are summarized in Table 9.

**Table 7. Optimal Solution Network with an Additional Lifting Partitioning**

| no. of starting partitions | objective value ($) (upper bound) | gap | no. of iterations | no. of partitions at convergence | CPU time |
|---|---|---|---|---|---|
| 2 | 3,527,430 | 4.3% | 18 | 7 | 13 h, 14 m, 26 s |



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

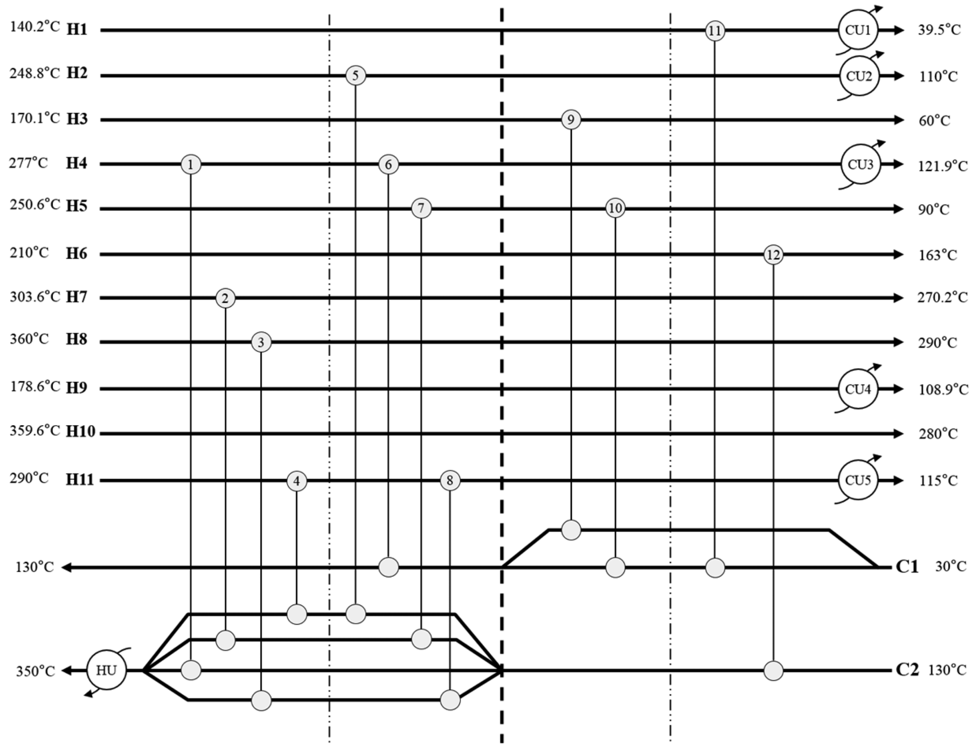



**Figure 5.** Solution for example 2 with lifting partitioning of the number of units.

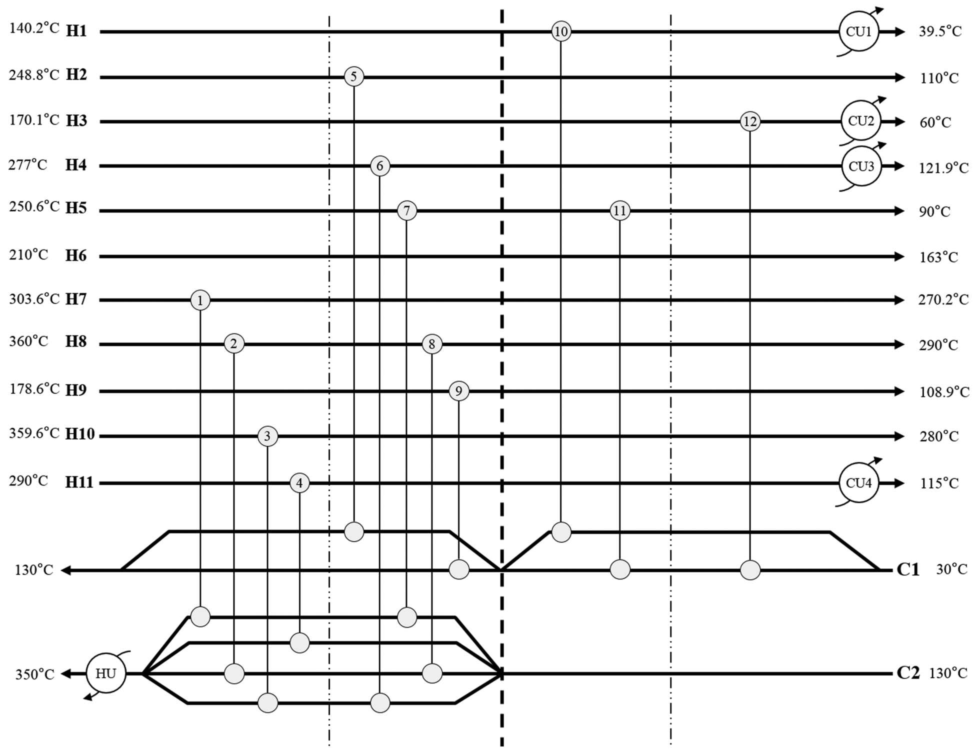



**Figure 6.** Solution networks for example 2 adding lifting partitioning (units and heat exchanged).

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 Tables 7, 8, and 9 since the bound contraction was slow. If we assumed that three branches is the maximum possible for cold streams, the objective value was $3,586,052 with 5.9% gap using 1 h 20 min 27 s of CPU time. (Figure 8)

This solution showed a higher objective value than the generalized superstructure model (Kim and Bagajewicz[5]) because the stages/substages model has the limitation of branching compared to the generalized superstructure model.

If we did not use the liftings including eqs 86 and 87 in the model, it was the same result without these equations but it took more than 6 h to solve the lower bound model. In



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

**Table 8. Optimal Solution Network with Lifting Partitioning of the Number of Units, The Total Heat Exchangers Duty and the Sub-Stages Heat Balances**

| no. of starting partitions | objective value ($) (Upper Bound) | gap | no. of iterations | no. of partitions at convergence | CPU time |
|---|---|---|---|---|---|
| 2 | 3,456,649 | 2.3% | 1 | 2 | 1 m, 57 s |

addition, BARON (version 14.4) (Sahinidis[20]) obtained an upper bound value of $10^{51}$ (clearly infinity) and a lower bound of $1,903,050 after 24 h running, and ANTIGONE (version 1.1) (Misener and Floudas[33]) 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 eqs 86 and 87: the objective value was $3,598,373 with 6.2% gap after 11 h 28 min 48 s 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

The stages/substages model (Jonguswat et al.[4]) was fully described in detail in this paper incorporating details that Jonguswat et al.[4] did not present. Instead of the ad-hoc method used by Jonguswat et al.,[4] 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[5]) to improve the lower bound value as well as its computational time. Our two examples proved to be computationally very challenging as several suboptimal 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[20]) and

**Table 9. Heat Exchanger Results for Example 2 with Equations 80−87**

| | area ($m^2$) | 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 | |

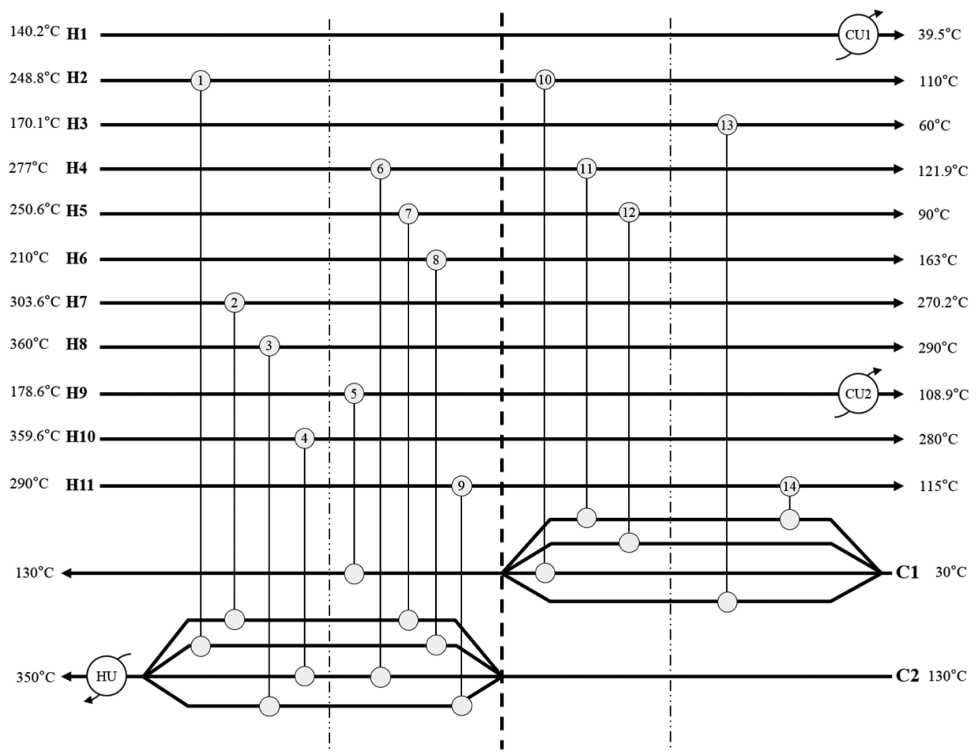



**Figure 7.** Solution for example 2 with lifting partitioning of the number of units, the total heat exchangers duty and the substages heat balances.



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

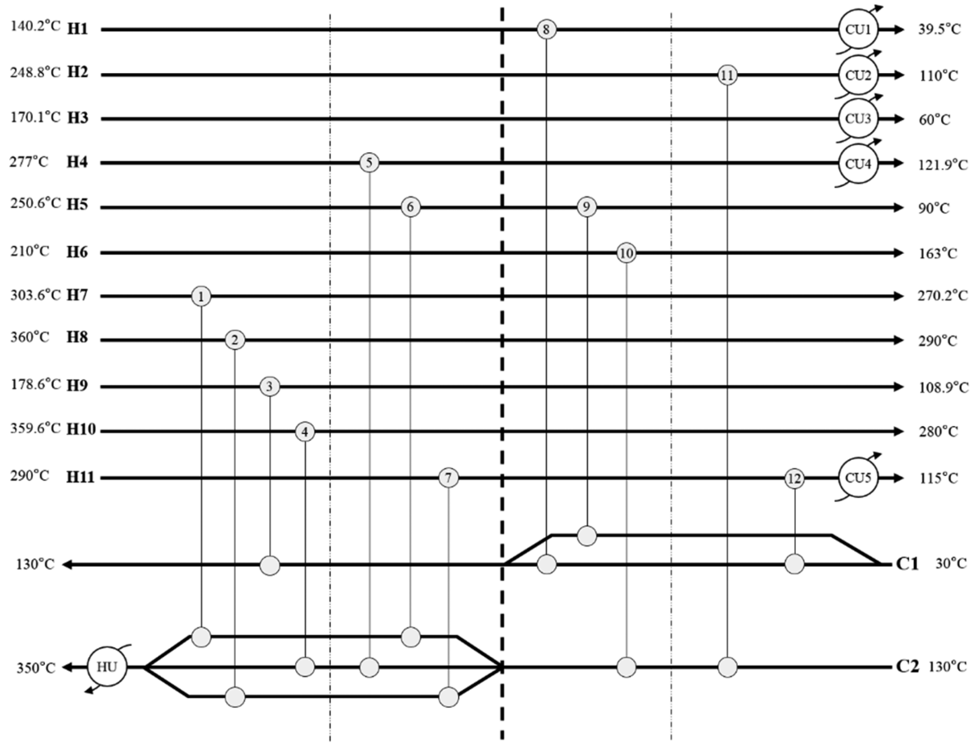



**Figure 8.** Solution network of the stages/substages model.

ANTIGONE (Misener and Floudas[33]) 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.

## ■ AUTHOR INFORMATION


### Corresponding Author

*E-mail: bagajewicz@ou.edu, Tel.:+1-405-325-5458.

### ORCID

Miguel Bagajewicz: 0000-0003-2195-0833


### 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
$o$ = heat capacity flow rate partitioning point
$n1$ = hot side temperature differences partitioning point
$n2$ = 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
$CUcost$ = cold utility cost
$HUcost$ = hot utility cost
$EMAT$ = exchanger minimum approach different
$FbhD_{i,mk,bh,o}$ = discrete point of the partitioned flow rate of substage hot stream
$FbcD_{j,mk,bc,o}$ = discrete point of the partitioned flow rate of substage cold stream
$ThD_{i,j,mk,bh,bc,k,n1}$ = discrete point of temperature differences in hot side of heat exchanger
$TcD_{i,j,mk,bh,bc,k,n2}$ = discrete point of temperature differences in cold side of heat exchanger
$\Gamma$ = maximum temperature differences
$\Omega$ = maximum area or maximum heat

### 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
$vFbhD_{i,mk,bh,o}$ = binary variable related to the partitioned hot stream substage flow rate
$Yh_{i,j,mk,bh,bc,k,n1}$ = binary variable related to the partitioned hot side temperature differences
$Yc_{i,j,mk,bh,bc,k,n2}$ = 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 $mk$



DOI: 10.1021/acs.iecr.6b04686
Ind. Eng. Chem. Res. 2017, 56, 5944−5957

$QHM_{i,mk}$ = 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 $fbc_{j,mk,bc}$
$Th_{i,mk}$ = 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 $mk$
$Fbh_{i,mk,bh}$ = 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
$\Delta Tcu_i$ = cold utility temperature difference
$\Delta Thu_j$ = hot utility temperature difference

## ■ REFERENCES


(1) Yee, T. F.; Grossmann, I. E. Simultaneous optimization model for heat integration – II. Heat exchanger network synthesis. *Comput. Chem. Eng.* **1990**, *14*, 1165–1184.
(2) Björk, K.; Westerlund, T. Global optimization of heat exchanger network synthesis problems with and without the isothermal mixing assumption. *Comput. Chem. Eng.* **2002**, *26*, 1581–1593.
(3) Faria, D.; Kim, S. Y.; Bagajewicz, M. J. Global optimization of the stage-wise superstructure model for heat exchanger networks. *Ind. Eng. Chem. Res.* **2015**, *54* (5), 1595–1604.
(4) Jongsuwat, P.; Suriyapraphadilok, U.; Bagajewicz, M. New Heat Exchanger Network Design Model. *17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction*, August 2014, 23–27.
(5) Kim, S. Y.; Bagajewicz, M. Global Optimization of Heat Exchanger Networks using a New Generalized Superstructure. *Chem. Eng. Sci.* **2016**, *147* (22), 30–46.
(6) Furman, K. C.; Sahinidis, N. V. A critical review and annotated bibliography for heat exchanger network synthesis in the 20th century. *Ind. Eng. Chem. Res.* **2002**, *41* (10), 2335–2370.
(7) Morar, M.; Agachi, P. S. Review: Important contributions in development and improvement of the heat integration techniques. *Comput. Chem. Eng.* **2010**, *34*, 1171–1179.
(8) Floudas, C.; Ciric, A.; Grossmann, I. E. Automatic synthesis of optimum heat exchanger network configurations. *AIChE J.* **1986**, *32* (2), 276–290.
(9) Huang, K. F.; Al-mutairi, E. M.; Karimi, I. A. Heat exchanger network synthesis using a stagewise superstructure with non-isothermal mixing. *Chem. Eng. Sci.* **2012**, *73*, 30–43.
(10) Huang, K. F.; Karimi, I. A. Simultaneous synthesis approaches for cost-effective heat exchanger networks. *Chem. Eng. Sci.* **2013**, *98*, 231–245.
(11) Konukman, A. E. S.; Camurdan, M. C.; Akman, U. Simultaneous flexibility targeting and synthesis of minimum-utility heat-exchanger networks with superstructure-based MILP formulation. *Chem. Eng. Process.* **2002**, *41*, 501–518.
(12) Frausto-Hernandez, S.; Rico-Ramirez, V.; Jimenez-Gutierrez, A.; Hernandez-Castro, S. MINLP synthesis of heat exchanger networks considering pressure drop effects. *Comput. Chem. Eng.* **2003**, *27* (8–9), 1143–1152.
(13) Ponce-Ortega, J. M.; Jimenez-Gutierrez, A.; Grossmann, I. E. Optimal synthesis of heat exchanger networks involving isothermal process streams. *Comput. Chem. Eng.* **2008**, *32* (8), 1918–1942.
(14) Escobar, M.; Trierweiler, J. O. Optimal heat exchanger network synthesis: A case study comparison. *Appl. Therm. Eng.* **2013**, *51* (1–2), 801–826.
(15) Onishi, V. C.; Ravagnani, M. A. S. S.; Caballero, J. A. MINLP model for the synthesis of heat exchanger networks with handling pressure of process streams. *Comput.-Aided Chem. Eng.* **2014**, *24*, 163–168.
(16) Na, J.; Jung, J.; Park, C.; Han, C. Simultaneous synthesis of a heat exchanger network with multiple utilities using utility substages. *Comput. Chem. Eng.* **2015**, *79*, 70–79.
(17) Laukkanen, T.; Fogelholm, C. A bilevel optimization method for simultaneous synthesis of medium-scale heat exchanger networks based on grouping of process streams. *Comput. Chem. Eng.* **2011**, *35*, 2389–2400.
(18) Bogataj, M.; Kravanja, Z. An alternative strategy for global optimization of heat exchanger networks. *Appl. Therm. Eng.* **2012**, *43*, 75–90.
(19) Huang, K. F.; Karimi, I. A. Efficient algorithm for simultaneous synthesis of heat exchanger networks. *Chem. Eng. Sci.* **2014**, *105*, 53–68.
(20) Sahinidis, N. V. BARON: A general purpose global optimization software package. *J. Glob. Optim.* **1996**, *8*, 201–205.
(21) Kang, L.; Liu, Y.; Ren, Y.; Tang, Y. Optimal design of heat exchanger networks by using SQP algorithm based on GPU acceleration. *Comput.-Aided Chem. Eng.* **2014**, *33*, 295–300.
(22) Pourfarhady Myankooh, Y.; Shafiei, S. Application of $ACO_R$ to find optimal no stream splitting heat exchanger networks for pre-designed heat exchanger network. *Chem. Eng. Res. Des.* **2015**, *96*, 158–171.
(23) Faria, D.; Bagajewicz, M. Novel Bound Contraction Procedure for Global Optimization of Bilinear MINLP Problems with Applications to Water Management Problems. *Comput. Chem. Eng.* **2011**, *35*, 446–455.
(24) Paterson, W. R. A replacement for the logarithmic mean. *Chem. Eng. Sci.* **1984**, *39*, 1635–1636.
(25) Chen, J. J. J. Comments on improvements on a replacement for the logarithmic mean. *Chem. Eng. Sci.* **1987**, *42*, 2488–2489.
(26) Manousiouthakis, V.; Sourlas, D. A global optimization approach to rationally constrained rational programming. *Chem. Eng. Commun.* **1992**, *118*, 127–147.
(27) Barbaro, A.; Bagajewicz, M. J. New rigorous one-step MILP formulation for heat exchanger network synthesis. *Comput. Chem. Eng.* **2005**, *29*, 1945–1976.
(28) Faria, D.; Bagajewicz, M. A New Approach for Global Optimization of a Class of MINLP Problems with Applications to Water Management and Pooling Problems. *AIChE J.* **2012**, *58* (8), 2320–2335.
(29) Faria, D.; Bagajewicz, M. Global Optimization of Water Management Problems Using Linear Relaxations and Bound Contraction Methods. *Ind. Eng. Chem. Res.* **2011**, *50* (7), 3738–3753.
(30) Brooke, A.; Kendrick, D.; Meeraus, D.; Raman, R. *GAMS–A User Guide*; GAMS Development Corporation: Washington, DC, 2007.
(31) Viswanathan, J.; Grossmann, I. E. A combined Penalty Function and Outer Approximation Method for MINLP Optimization. *Comput. Chem. Eng.* **1990**, *14*, 769–782.
(32) Nguyen, D. Q.; Barbaro, A.; Vipanurat, N.; Bagajewicz, M. All-at-once and step-wise detailed retrofit of heat exchanger networks using an MILP model. *Ind. Eng. Chem. Res.* **2010**, *49*, 6080–6103.



DOI: 10.1021/acs.iecr.6b04686
*Ind. Eng. Chem. Res.* 2017, 56, 5944–5957

(33) Misener, R.; Floudas, C. A. ANTIGONE: Algorithms for continuous/integer global optimization of nonlinear equations. *J. Glob. Optim* **2014**, *59*, 503−526.

## ■ NOTE ADDED AFTER ASAP PUBLICATION

After this paper was published ASAP May 9, 2017, a correction was made to eq 4. The corrected version was reposted May 10, 2017.



DOI: 10.1021/acs.iecr.6b04686
*Ind. Eng. Chem. Res.* 2017, 56, 5944−5957