# Synthesis of Energy-Optimal HEN Structures with Specified Flexibility Index through Simultaneous MILP Formulation

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**Abstract –** The synthesis of minimum-utility Heat-Exchanger Network (HEN) structures satisfying a given flexibility-index target is accomplished through a one-stage, non-iterative, superstructure-based-simultaneous-MILP formulation. The formulation assumes that the feasible region defined by the reduced inequality constraints is convex in uncertain parameters, so that the solution lies at any of the vertices of the polyhedral region of uncertainty. With this formulation, the standard definition of the HEN-synthesis problem is extended such that it now includes a flexibility-index specification for the potential HEN structure.

*Keywords:* Heat-exchanger network, synthesis with flexibility target, superstructure, MILP

## INTRODUCTION

One of the extensively studied synthesis problems in chemical engineering is the synthesis of Heat-Exchanger Networks (HENs). The works in this area have been concentrated mostly around the standard definition of the HEN-synthesis problem, which can be stated as: *"Given hot/cold streams to be cooled/heated from specified (nominal) supply temperatures to specified target temperatures, and hot/cold utility specifications, synthesize a HEN such that the resulting HEN has minimum total cost."* Most of the heuristic/algorithmic and mathematical-programming (MP) based HEN-synthesis techniques originating from the standard definition of the HEN-synthesis problem use nominal values of parameters, and thus, do not incorporate any measure of flexibility directly into the synthesis step. The assessment of flexibility of the resulting HEN is done indirectly by testing its flexibility, which is defined as the measure of the size of the region of feasible operation in the space of desired or undesired deviations from nominal values of the parameters. The retrofit design of HENs for improving flexibility has been studied systematically through MP techniques, however, mostly for fixed network topologies and operating conditions (fixed parameters). The retrofit of HENs with fixed topologies but varying parameters are handled mostly deterministically through definition of an uncertainty-range of parameters; by incorporating the flexibility-index (or flexibility-test) of Swaney and Grossmann (1985) into mostly two-stage iterative MP formulations. A review of the subjects mentioned above can be found in Papalexandri and Pistikopoulos (1993).

Compared to the works done on HEN-synthesis around its standard definition and HEN-retrofitting for fixed network topologies, the problem of incorporating flexibility considerations in the synthesis of HENs has received limited attention. Floudas and Grossmann (1986, 1987) have developed a two-stage procedure (as iterations between a multiperiod synthesis problem and a flexibility-analysis step) for synthesizing HENs, featuring maximum energy recovery but not necessarily minimum total cost, that can tolerate a specified range of uncertain source-stream temperatures and flowrates. Papalexandri and Pistikopoulos (1993), for the synthesis or retrofit of HENs possessing a specified flexibility index at the minimum total annualized cost, have integrated the iterative scheme of Floudas and Grossmann into a two-stage iterative scheme, without decomposition to the multiperiod case. Bahri et al. (1997), by considering disturbances as multiperiod operations, presented an approach for the synthesis of flexible and controllable plants, which also involves a two-stage iterative MP, termed as "back-off calculation". These MP-based techniques

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require the solution of large MINLPs, where the integer variables denote existence/absence of units (exchangers) or streams embedded in hyper-/superstructure representation of the process (HEN).

In this work, the synthesis of minimum-utility HEN structures possessing a desired flexibility (satisfying the given flexibility-index target) is accomplished through a one-stage, non-iterative, superstructure-based-simultaneous-MILP formulation. The formulation assumes that the feasible region defined by the reduced inequality constraints is convex –or, one-dimensional-quasi-convex (Swaney and Grossmann, 1985)– in uncertain parameters (here, considered as source-stream temperatures), so that the solution lies at any of the vertices of the polyhedral region of uncertainty.

With this formulation, the standard definition of the HEN-synthesis problem is extended such that it now includes a flexibility-index specification for the potential HEN structure and can be stated as follows: "*Given hot/cold streams to be cooled/heated from specified (nominal) supply temperatures to specified target temperatures, hot/cold utility specifications, and a desired flexibility index (expected disturbance space), synthesize a HEN such that it has minimum utility consumption under nominal operating conditions and remains feasible against deviations in source-stream temperatures as long as the maximum magnitude of the deviations is less than or equal to the specified flexibility index.*"

An example HEN problem is solved for different values of the desired flexibility index, and the resulting HEN structures are analyzed in terms of flexibility, structural grouping, and utility-consumption level.

## FORMULATION

The general MINLP formulation for the problem of superstructure-based simultaneous HEN synthesis and flexibility targeting can be described by Eq.1, where **d** is the vector of design variables (exchanger areas), **x** is the vector of state variables (outlet temperatures), **z** is the vector of binary variables (denoting potential existence/absence of exchangers embedded in the superstructure), **u** is the vector of control/free variables (heater/cooler loads), **p** is the vector of fixed parameters, and $\boldsymbol{\theta}$ is the vector of uncertain parameters (source temperatures). Eq.(1a) is the objective function and can be formulated in terms of total annualized cost or total utility consumption. For a synthesis problem, the vector **d** is dropped from the set of decision variables. Eqs.(1b-1c) are the vector of equality and inequality constraints, respectively. If the vector of states, **x**, can be eliminated using Eq.(1b), then Eq.(1c) can be written as the vector of reduced inequalities. Eq.(1d) describes the range of the uncertain parameters as deviations from nominal values, $\boldsymbol{\theta}^o$, where $\Delta\boldsymbol{\theta}^-$ and $\Delta\boldsymbol{\theta}^+$ are the scaled deviations from $\boldsymbol{\theta}^o$, and the non-negative scalar, $\delta$, is the targeted flexibility index. The region $R(\delta)$ describes the scaled hyperrectangle which is required to be within the feasible region defined by Eqs.(1b-1c). For a fixed HEN topology and design (known **z** and **d**), the flexibility index defined by Swaney and Grossmann (1985) is the maximum of scalar $\delta$. This problem (Eq.1) is very difficult to solve directly since, due to Eq.(1d), it involves a max-min-max constraint that leads to a nondifferentiable global-optimization problem (Halemane and Grossmann, 1983). The problem can be solved indirectly with a two-stage procedure (as iterations between a multiperiod synthesis problem and a flexibility-analysis step) (Papalexandri and Pistikopoulos, 1993), however, this technique requires the solution of large MINLPs through the Generalized Benders Decomposition in each iteration.

$$\min_{\mathbf{d},\mathbf{x},\mathbf{u},\mathbf{z}} \ \Phi(\mathbf{d},\mathbf{x},\mathbf{u},\mathbf{z},\mathbf{p},\boldsymbol{\theta}) \qquad (1a)$$

$$\text{s.t.} \quad \mathbf{h}(\mathbf{d},\mathbf{x},\mathbf{u},\mathbf{z},\mathbf{p},\boldsymbol{\theta}) = \mathbf{0} \qquad (1b)$$

$$\mathbf{g}(\mathbf{d},\mathbf{x},\mathbf{u},\mathbf{z},\mathbf{p},\boldsymbol{\theta}) \le \mathbf{0} \qquad (1c)$$

$$\boldsymbol{\theta} \in R(\delta) = \left\{\boldsymbol{\theta} \middle| \left(\boldsymbol{\theta}^o - \delta\Delta\boldsymbol{\theta}^-\right) \le \boldsymbol{\theta} \le \left(\boldsymbol{\theta}^o + \delta\Delta\boldsymbol{\theta}^+\right)\right\} \qquad (1d)$$

In this work, the synthesis of minimum-utility HEN structures satisfying a given flexibility-index target through one-stage, non-iterative, superstructure-based formulation is accomplished with the assumption that the feasible region defined by the reduced inequality constraints is convex in uncertain parameters (source-stream temperatures), so that the solution lies at any of the vertices of the polyhedral region of uncertainty. The general vertex-solution can be described by Eq.2, which is a reformulation of Eq.1 using the approach named as "Algorithm I" by Halemane and Grossmann (1983). Eq.(2a) is the objective function that is evaluated at the nominal operating point, *n=0*. Eqs.(2b-2c) are the vector of equality and inequality constraints that are evaluated at the nominal operating point and augmented for each vertex point ($n=1,...,2^N$). Eq.(2d) constraints the vector $\boldsymbol{\theta}$ to take only $2^N$ vertex values, $\boldsymbol{\theta}^n$, scaled by the scalar flexibility index, $\delta$, as $\pm$ directed deviations from the nominal

$$\min_{\mathbf{x}^n,\mathbf{z}^o,\mathbf{u}^n} \ \Phi(\mathbf{d}^o,\mathbf{x}^o,\mathbf{u}^o,\mathbf{z}^o,\mathbf{p},\boldsymbol{\theta}^o) \qquad n = 0, 1, ..., 2^N \qquad (2a)$$

$$\text{s.t.} \quad \mathbf{h}^n(\mathbf{d}^o,\mathbf{x}^n,\mathbf{z}^o,\mathbf{u}^n,\mathbf{p},\boldsymbol{\theta}) = \mathbf{0} \qquad n = 0, 1, ..., 2^N \qquad (2b)$$

$$\mathbf{g}^n(\mathbf{d}^o,\mathbf{x}^n,\mathbf{z}^o,\mathbf{u}^n,\mathbf{p},\boldsymbol{\theta}) \le \mathbf{0} \qquad n = 0, 1, ..., 2^N \qquad (2c)$$

$$\boldsymbol{\theta} - \boldsymbol{\theta}^o - \delta\boldsymbol{\theta}^n = \mathbf{0} \qquad n = 1, ..., 2^N \qquad (2d)$$

$$\boldsymbol{\theta} - \boldsymbol{\theta}^o = \mathbf{0} \qquad n = 0 \qquad (2e)$$

$$\boldsymbol{\theta}^n \in R_o(\delta) = \left\{\boldsymbol{\theta}^n \middle| \boldsymbol{\theta}^n \text{ is a vertex of } R(\delta),\ n = 1,...,2^N\right\} \qquad (2f)$$

values, $\theta^o$. Eq.(2e) denotes that at n=0, $\delta$ is considered to be zero. The set $R_o(\delta)$ describes the vertices of the scaled hyperrectangle which is required to be within the feasible region defined by Eqs.(2b-2c).

The basis of this work is the superstructure-based simultaneous-MINLP formulation developed by Yee and Grossmann (1990) as a solution to the standard HEN-synthesis problem (see Zamora and Grossmann (1998) for a recent development). The original MINLP formulation (a nonlinear total-cost function as objective and a set of linear constraints) is based on a stagewise superstructure representation that considers potential exchanges between any pair of hot and cold streams within a stage via binary decision variables. In this work, the model of Yee and Grossmann is reformulated as MILP and the set of linear constraints is augmented such that the resulting structure satisfies expected deviations in source-stream temperatures in every combination of disturbance directions (vertex directions), identified by an additional index *n*. The nominal operating condition (operation under zero disturbance in source-stream temperatures) is identified by *n=0*. For a HEN problem with $N_H$ hot streams and $N_C$ cold streams, there are $N=2^{(N_H+N_C)}$ vertices (+ and − directed simultaneous disturbance directions) besides the nominal operating point (zero-disturbance direction). Overall heat balances for each stream, heat balances at each stage of the superstructure, assignment of superstructure inlet temperatures, equations for the feasibility of temperatures, hot/cold-utility load equations, logical constraints, approach-temperature equations forming the set of linear constraints in the original formulation of Yee and Grossmann are written for each of the $2^{(N_H+N_C)}$ vertices as well as the nominal point. Source-stream temperatures are perturbed for each vertex by a scalar $\delta$; the desired flexibility index. Thus, satisfaction of the linear constraints is required for each vertex as well as the nominal point. The target temperatures specified by the HEN problem are required to be matched exactly for each vertex direction by variable (vertex-direction-dependent) heater/cooler loads. The objective function is the minimization of the total utility consumption at the nominal operating point; *n=0*. Thus, the whole problem becomes MILP for which the superstructure-dependent global solution can be obtained using the software package GAMS. To preserve the linearity of the constraints, the isothermal-mixing assumption of Yee and Grossmann (which is rigorous if the resulting HEN does not involve stream splits but may lead to overestimation of the area cost in the case of stream splits) is retained. The original nonlinear total-cost function of Yee and Grossmann is not used in this work.

*Objective function:*

$$\min_{\substack{t_{i,k,n},\ t_{j,k,n},\ z_{i,j,k,n=0},\\ zcu_{i,n=0},\ zhu_{j,n=0},\\ qcu_{i,n},\ qhu_{j,n},q_{i,j,k,n}}} \sum_{i\in HP} qcu_{i,n=0} + \sum_{j\in CP} qhu_{j,n=0} \quad (3)$$

*Overall heat balance for each stream and for each vertex, n:*

$$\left(T^{in}{}_{i,n} - T^{out}{}_{i,n}\right)F_i = \sum_{k\in ST}\sum_{j\in CP} q_{i,j,k,n} + qcu_{i,n} \qquad i\in HP,\ n=0,1,...,N \quad (4)$$

$$\left(T^{out}{}_{j,n} - T^{in}{}_{j,n}\right)F_j = \sum_{k\in ST}\sum_{i\in HP} q_{i,j,k,n} + qhu_{j,n} \qquad j\in CP,\ n=0,1,...,N \quad (5)$$

*Heat balance at each stage and for each vertex, n:*

$$\left(t_{i,k,n} - t_{i,k+1,n}\right)F_i = \sum_{j\in CP} q_{i,j,k,n} \qquad k\in ST,\ i\in HP,\ n=0,1,...,N \quad (6)$$

$$\left(t_{j,k,n} - t_{j,k+1,n}\right)F_j = \sum_{i\in HP} q_{i,j,k,n} \qquad k\in ST,\ j\in CP,\ n=0,1,...,N \quad (7)$$

*Assignment of inlet temperatures for each vertex, n, for the specified $\delta$:*

$$T^{in}{}_{i,n} = T^{in,o}{}_i + r_{i,n}\,\delta \qquad i\in HP,\ n=0,1,...,N \quad (8)$$

$$T^{in}{}_{j,n} = T^{in,o}{}_j + r_{j,n}\,\delta \qquad j\in CP,\ n=0,1,...,N \quad (9)$$

*Assignment of superstructure inlet temperatures for each vertex, n:*

$$T^{in}{}_{i,n} = t_{i,1,n} \qquad n=0,1,...,N \quad (10)$$

$$T^{in}{}_{j,n} = t_{j,ST+1,n} \qquad n=0,1,...,N \quad (11)$$

*Feasibility of temperatures for each vertex, n:*

$$t_{i,k,n} \ge t_{i,k+1,n} \qquad k\in ST,\ i\in HP,\ n=0,1,...,N \quad (12)$$

$$t_{j,k,n} \ge t_{j,k+1,n} \qquad k\in ST,\ j\in CP,\ n=0,1,...,N \quad (13)$$

$$T^{out}{}_{i,n} \le t_{i,ST+1,n} \qquad i\in HP,\ n=0,1,...,N \quad (14)$$

$$T^{out}{}_{j,n} \ge t_{j,1,n} \qquad j\in CP,\ n=0,1,...,N \quad (15)$$

*Hot and cold utility loads for each vertex, n:*

$$\left(t_{i,ST+1,n} - T^{out}{}_{i,n}\right)F_i = qcu_{i,n} \qquad i\in HP,\ n=0,1,...,N \quad (16)$$

$$\left(T^{out}{}_{J,n} - t_{j,1,n}\right)F_j = qhu_{j,n} \qquad j\in CP,\ n=0,1,...,N \quad (17)$$

*Logical constraints for each vertex, n:*

$$q_{i,j,k,n} - \Omega\, z_{i,j,k,n=0} \le 0 \qquad k\in ST,\ i\in HP,\ j\in CP,\ n=0,1,...,N \quad (18)$$

$$qcu_{i,n} - \Omega\, zcu_{i,n=0} \le 0 \qquad i\in HP,\ n=0,1,...,N \quad (19)$$

$$qhu_{j,n} - \Omega\, zhu_{j,n=0} \le 0 \qquad j\in CP,\ n=0,1,...,N \quad (20)$$

$$z_{i,j,k,n=0}, zcu_{i,n=0}, zhu_{j,n=0} = 0,1 \qquad n=0 \quad (21)$$

*Approach temperature settings for each vertex, n:*

$$dt_{i,j,k,n=0} \ge \Delta T_{min} \qquad i\in HP,\ j\in CP,\ n=0 \quad (22)$$

$$dt_{i,j,k,n\ne 0} \ge 0 \qquad i\in HP,\ j\in CP,\ n=1,...,N \quad (23)$$

The explicit MILP formulation, based on the MINLP formulation of Yee and Grossmann, is given by Eqs.(3-27), where the index *n* is the vertex identifier. The objective (Eq.3) is the minimization of the cold (**qcu**) and hot (**qhu**) utility (energy) consumption at the nominal condition, *n=0*. The binary decision-variable vectors, **z**, **zcu**, and **zhu**, that denote existence of stream matches, cold- and hot-utility heat exchanges, respectively, are defined only for the nominal operating conditions *n=0* (common for each vertex), since the potential structure is based on the nominal condition and, with this single structure, the constraints should be satisfied at every vertex by the control/free variables (heater/cooler loads). The vector of states, **t**, is the temperatures at the inlet and outlet of each stage in the superstructure for each vertex direction.

*Calculation of approach temperatures for each vertex, n:*

$$dt_{i,j,k,n} \le t_{i,k,n} - t_{j,k,n} + \Gamma\left(1 - z_{i,j,k,n=0}\right) \qquad k \in ST,\ i \in HP,\ j \in CP,\ n=0,1,...,N \quad (24)$$

$$dt_{i,j,k+1,n} \le t_{i,k+1,n} - t_{j,k+1,n} + \Gamma\left(1 - z_{i,j,k,n=0}\right) \qquad k \in ST,\ i \in HP,\ j \in CP,\ n=0,1,...,N \quad (25)$$

$$dtcu_{i,n} \le t_{i,ST+1,n} - T^{out}{}_{CU,n} + \Gamma\left(1 - zcu_{i,n=0}\right) \qquad i \in HP,\ n=0,1,...,N \quad (26)$$

$$dthu_{j,n} \le T^{out}{}_{HU,n} - t_{j,1,n} + \Gamma\left(1 - zhu_{j,n=0}\right) \qquad j \in CP,\ n=0,1,...,N \quad (27)$$

## EXAMPLE AND RESULTS

The example HEN problem with two hot and two cold streams and the two-stage superstructure is shown in Fig.1. With two hot and two cold source streams, there are 16 vertices, and together with the nominal operation point, the original constraints of Yee and Grossmann are repeated for 17 different source-stream temperatures as indicated by Eqs.(8-9), where, $r_n$ is assigned to all 16 combinations of –1 and +1, except the nominal condition at which $r_n$ is assigned to zero.

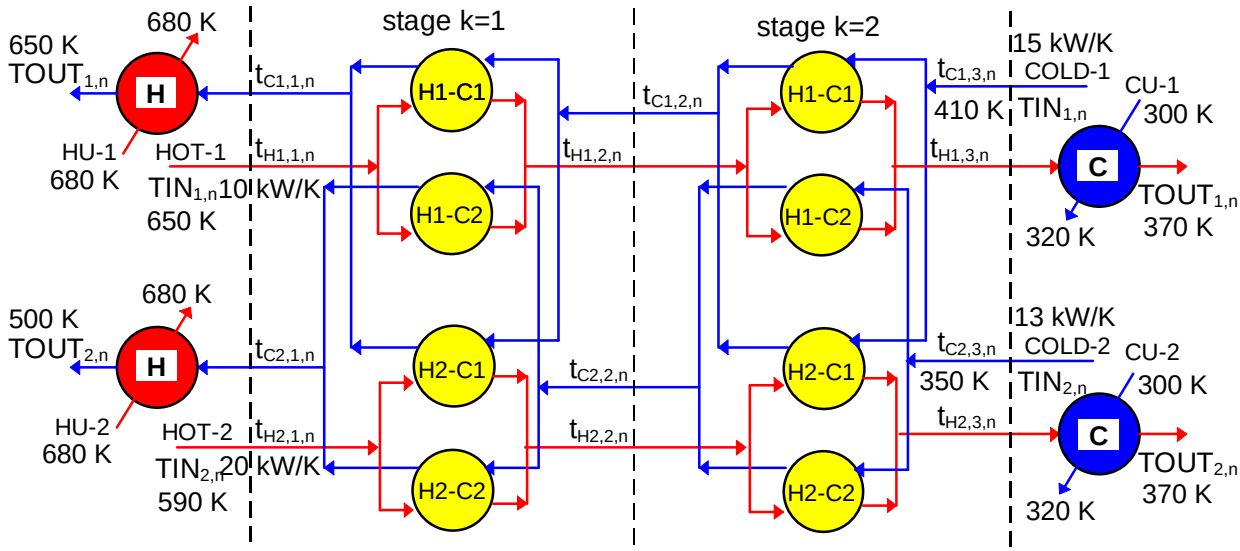



Figure 1. Stream data and the two-stage superstructure of Yee and Grossmann (1990).

When the MILP formulation is solved for the fixed values of the desired flexibility index, δ (± directed deviations in source-stream temperatures), ranging from δ=0K to δ=150K (150K is the maximum value of δ that can be tolerated for the problem specifications) Fig.2 can be constructed. There are four plateaus of total utility requirement levels at the nominal operating point, *n=0*. Each plateau corresponds to one or more (but finite number) of different HEN structures synthesized by solving the MILP for the given value of δ. The HEN with structure A consumes 2550 kW total utility at the nominal operating point and at the same time tolerates an uncertainty ±36.9K (0K≤δ≤36.9K) in source-stream temperatures (i.e., with structure A, the largest hyperrectangle that can be inscribed within the feasible region has vertices at ±36.9K as measured from the nominal point at the center). The second plateau corresponding to 3750 kW total utility consumption contains structures B3, B2, B4, B1, B5=B7, and B6, which can tolerate uncertainties of 0K≤δ≤70.6K, 0K≤δ≤74.2K, 0K≤δ≤84.2K, 0K≤δ≤90.0K, 0K≤δ≤90.0K, and 0K≤δ≤90.0K, respectively. Structures B5 and B7 are actually identical flowsheets however they appear in either the stage k=1 or stage k=2 of the superstructure as reflections of each other. The third plateau corresponding to 4250 kW total utility consumption contains structures C1, and C2=C3=C4, which can

tolerate uncertainties of 0K≤δ≤91.5K, 0K≤δ≤120K, 0K≤δ≤120K, and 0K≤δ≤120K, respectively. Similarly, structures C2, C3, and C4 are actually identical flowsheets. The fourth plateau corresponding to 8850 kW total utility consumption contains structures D1 and D2, both of which can tolerate uncertainties of ±150K (0K≤δ≤150K). Thus, Fig.2 reveals the trade-off between flexibility and total utility consumption clearly, and the final decision can be made after computing the total (area plus utility) cost for the structures embedded in the desired flexibility range, if there are multiple structures.

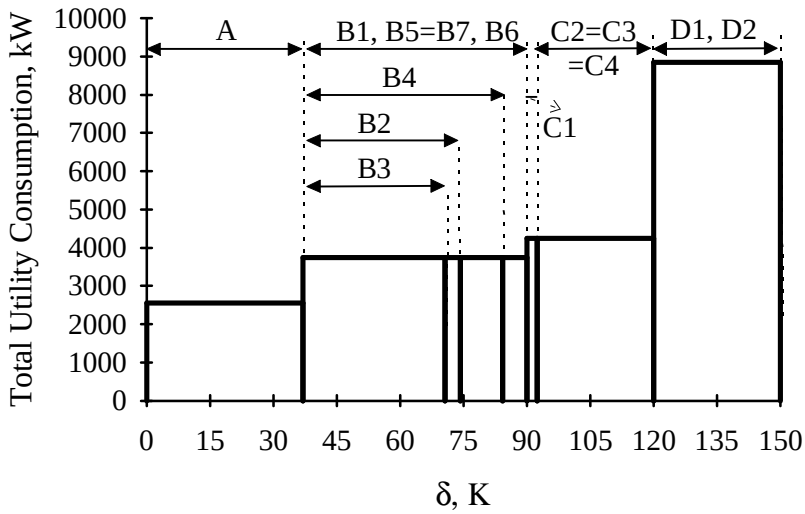



Figure 2. Total utility consumption at the nominal operating condition versus the flexibility index for structures A through D2.

As an example, Fig.3 shows the HEN structure B1 obtained from the superstructure as a result of the solution of the MILP formulation with the desired flexibility of δ=90K (the structure B1 tolerates a flexibility range 0K≤δ≤90K). For this structure, the heating, cooling, and total utility requirements are 1050 kW, 2700 kW, and 3750 kW, respectively.

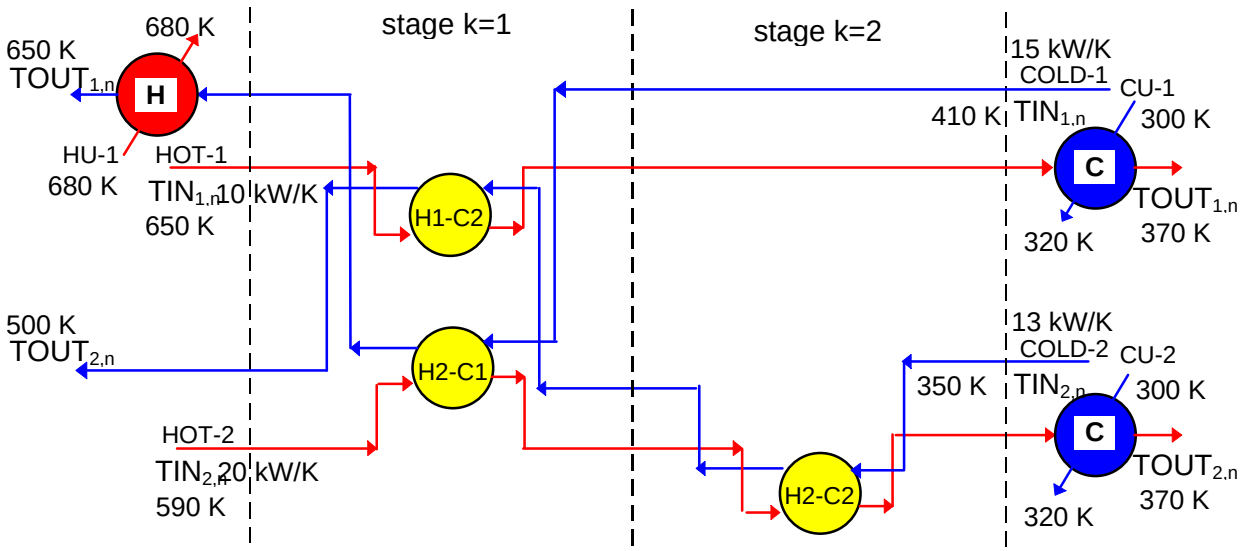



Figure 3. Structure B1 reduced from the superstructure for δ=90K.

## CONCLUSIONS

The synthesis of minimum-utility HEN structures satisfying a given flexibility target was accomplished through one-stage, non-iterative, superstructure-based-simultaneous-MILP formulation with the assumption of convex feasible region. The source-stream temperatures were considered to be the uncertain parameters. With this formulation, that achieved simultaneous minimum-utility-structure synthesis and flexibility-index targeting, the standard definition of the HEN-synthesis problem was extended such that it now includes a flexibility-index specification for the HEN structure potentially present in the superstructure. An example application of the formulation revealed the trade-off between flexibility and total utility consumption for the reduced structures embedded in the desired flexibility range.

## ACKNOWLEDGMENT

Financial supports provided by TÜBÝTAK (The Scientific and Technical Research Council of Turkey) (Project No: MÝSAG-83) and the Boðaziçi University Research Foundation (Project No: 99A503) are gratefully acknowledged.

## NOTATION

| | |
|---|---|
| CP | cold process stream |
| **d** | vector of design variables |
| $dt_{i,j,k,n}$ | temperature approach for match i and j in stage k at vertex n |
| $dtcu_{i,n}$ | temperature approach for match i and cold utility at vertex n |
| $dthu_{j,n}$ | temperature approach for match j and hot utility at vertex n |
| F | heat-capacity-flowrate |
| **g** | vector of inequality constraints |
| **h** | vector of equality constraints |
| HP | hot process stream |
| n | vertex-direction identifier (subscript or superscript) |
| N | total number of vertices |
| **p** | vector of fixed parameters |
| $q_{i,j,k,n}$ | heat exchanged between stream i and j in stage k at vertex n |
| $qcu_{i,n}$ | heat exchanged between stream i and cold utility at vertex n |
| $qhu_{j,n}$ | heat exchanged between stream j and hot utility at vertex n |
| $r_n$ | N combinations of −1 and +1 |
| ST | stage |
| $t_{i,k,n}$ | temperature of stream i at hot end of stage k at vertex n |
| $t_{j,k,n}$ | temperature of stream j at hot end of stage k at vertex n |
| T | temperature |
| **u** | vector of free/control variables |
| **z** | vector of binary variables |
| $z_{i,j,k}$ | binary variable for existence of unit for match i and j in stage k |
| $zcu_i$ | binary variable for existence of unit for match i and cold utility in stage k |
| $zhu_j$ | binary variable for existence of unit for match j and hot utility in stage k |

*Greek Letters*

| | |
|---|---|
| $\delta$ | flexibility index (scalar) |
| $\Phi$ | objective function |
| $\Gamma$ | upper bound for temperature difference |
| $\theta$ | vector of uncertain parameters |
| $\Omega$ | upper bound for heat exchange |

*Subscripts*

| | |
|---|---|
| i | hot process stream |
| j | cold process stream |
| k | index for superstructure stage |

*Superscripts*

| | |
|---|---|
| in | inlet |
| o | value at nominal operating condition |
| out | outlet |

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