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SIMULTANEOUS SYNTHESIS OF HEAT EXCHANGER NETWORKS UNDER UNCERTAINTY

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Abstract: *This work presents a computational framework for automatically generating flexible Heat Exchanger Networks (HEN) over a specified range of expected variations in the inlet temperatures and flowrates of the process streams, such that the Total Annual Cost (TAC) as a result of the utility consumption, heat exchanger areas and selection of matches are optimized simultaneously. The proposed framework includes: (i) a multiperiod simultaneous MINLP model to synthesize a flexible HEN configuration, which may be solved using a decomposition technique. This problem is formulated over a discrete set of operating points; (ii) a flexibility analysis to test the feasibility of operation of the given design over the specified range of the uncertain parameters. In this step critical conditions, i.e. points of maximum constraint violation, are identified, which are to be updated in the current set of points in order to resolve the multiperiod design. This computational framework yields a HEN design, which is guaranteed to operate under varying conditions ensuring stream temperature targets and optimal energy integration. The proposed strategy has been successively applied and two numerical examples are used to illustrate the proposed integrated framework.*

Keywords: *heat exchanger network synthesis, process design, uncertainty, flexibility*

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1. Introduction

During the past decades there has been growing awareness both in academia and industry that operability issues need to be considered explicitly at the early stages of process design. It is even more important for heat integrated process, since the economic performance of a process is greatly affected by process variations and the ability of the system to satisfy its operational specifications under external disturbances or inherent modeling uncertainty.

Plant flexibility has been recognized to represent one of the important components in the operability of the production process, since it is related to the capability of a process to achieve feasible operation over a given range of uncertain conditions (Grossmann and Floudas, 1987). Uncertainty is an inherent characteristic of any chemical processes. They may have different sources such as: (*i*) unknown disturbances like uncertainty in the process parameters (operating conditions); (*ii*) uncertain model parameters (kinetic parameters, heat transfer coefficients, etc); (*iii*) Discrete uncertainty (failures, equipment availability, etc).

The incorporation of uncertainty into design may be possible through a deterministic approach using multiperiod optimization problem. In that case the design must be tested to ensure feasibility over the operational range. In this work[1], a computational framework based on a two stage strategy is used in order to develop flexible heat exchangers networks.

In the next section, a deterministic approach for a general process design/synthesis under uncertainty is presented. In Section 3, the mathematical formulation is derived for the specific case of Heat Exchanger Network Synthesis (HENS) and then in section 4 two numerical examples are presented in order to illustrate the whole procedure and some analysis and discussions are made. Finally, some conclusions and final remarks are drawn in section 5.

2. Process Design under uncertainty

An important question is how systematically determine designs that can accomplish a desired degree of flexibility? In a conventional design optimization problem, the design variables must be selected so as to minimize the total cost at some nominal values of the uncertain parameters. When the goal of flexibility is also to be accomplished, there are basically two options: Either (*i*) ensure the flexibility for a fixed parameter range; or (*ii*) maximize the flexibility measure, while at the same time minimizing cost. The latter problem gives rise to a multi-objective optimization problem, which in fact would

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normally be solved by optimizing the cost at different fixed values of the flexibility range (Biegler et al., 1997).

A general representation of a process design under uncertainty is of the following form:

$$\left.\begin{array}{l} \min_{d,z,x} \ \underset{\theta\in T}{E}[C(d,x,z,\theta)] \\ s.t.\ h(d,x,z,\theta)=0 \\ \quad g(d,x,z,\theta)\le 0 \\ d\in D, x\in X, z\in Z, \theta\in T \end{array}\right\} \ (P) \qquad (1)$$

where $d, x,$ and z are the vectors of design, control and state variables, respectively; θ is the vector of uncertain parameters; $E[C(d,x,z,\theta)]$ is the expected cost function for $\theta \in T$; $h(d,x,z,\theta)$ and $g(d,x,z,\theta)$ are the vectors of model equality and inequality constraints describing the process model and specifications.

Most of the previous works use the termed two stage strategy. The first stage is prior to the operation (design phase) where the design variables are chosen. At the second stage the control variables z are adjusted during operation on the realizations of $\theta \in T$. It is made the implicit assumption of "perfect control". It means that the control can be immediately adjusted depending on the realization of θ. No delays in the measurements or adjustments in the control are considered.

If a finite number of points in T is replaced by a discrete set of points, which are somehow specified. The original design problem P can be reformulated as a multiperiod optimization problem (P') that is used to approximate the solution of the optimal design under uncertainty

$$\left.\begin{array}{l} \min_{d,x^p,z^p} \sum_{p=1}^{N} w_p C(d,x^p,z^p,\theta^p) \\ s.t.\ h^p(d,x^p,z^p,\theta^p)=0 \\ \quad g^p(d,x^p,z^p,\theta^p)\le 0 \\ \quad p=1,\dots,N \end{array}\right\} \ (P') \qquad (2)$$

The two stage strategy is depicted in Fig. 1. For the selected N periods the multiperiod optimization problem P' is solved. The flexibility/feasibility of the multiperiod design must be tested over the space T. If the design is feasible, the procedure terminates; otherwise, the critical point obtained from the flexibility evaluation is included in the current set of θ points, and a new multiperiod formulation is performed. Computational experience has shown that commonly few major iteration must be performed to achieve the feasibility with this method (Biegler et al., 1997).

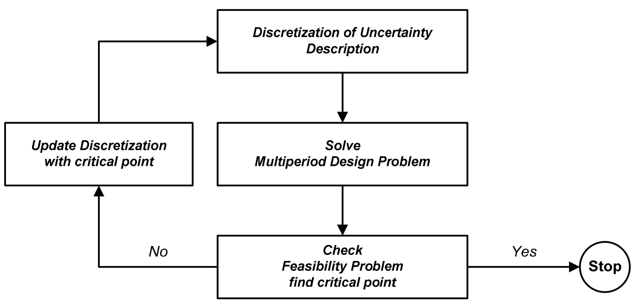

Fig. 1. Two stage strategy for optimal design under uncertainty.

3. Mathematical Formulation for HENS

3.1 Problem Statement

The problem to be addressed in this work can be stated as follows:

Given are: (***i***) Stream Integration data; (***ii***) A specified range for disturbances, inlet temperatures and flowrates, addressed as uncertain parameters, where the flexibility of the network is desired (flexibility target); and (***iii***) A minimum temperature approach (ΔT_{min});

The objective is then the following: synthesize a heat exchanger network with minimum Total Annual Cost (operating and capital investment cost) able to operate feasibly under the specified disturbance range.

Nomenclature

Sets	
CP	*set of cold process stream j*
CU	*set of cold utility*
HP	*set of hot process stream i*
HU	*set of hot utility*
ST	*set of stages in the superstructure*
I	*set of equality constraints*
J	*set of inequality constraints*
V	*set of vertices k*

Parameters		
δ		*scalar factor*
δ^k		*scalar factor at vertex k or active set k*
θ		*vector of uncertain parameters*
θ^L		*vector of lower bounds for uncertain parameters*
θ^N		*vector of nominal values for uncertain parameters*
θ^U		*vector of upper bounds for uncertain parameters*
$\Delta\theta^+$		*vector of positive expected deviation for uncertain parameters*
$\Delta\theta^-$		*vector of negative expected deviation for uncertain parameters*
$\Delta\theta^k$		*vector of values for uncertain parameters at vertex k*
w_i/w_j	$[kW/K]$	*flow capacity of hot stream i / cold stream j*
N_T	-	*number of stages*
T_i^{in}	$[K]$	*inlet temperature of hot stream i*
T_j^{in}	$[K]$	*inlet temperature of cold stream j*
T_i^{out}	$[K]$	*outlet temperature of hot stream i*
T_j^{out}	$[K]$	*outlet temperature of cold stream j*
U		*upper bound for slack variables*
s_j		*slack variable for inequality j*
n_z		*number of control variables*
N_p		*number of uncertain parameters*

Variable	
d, x, z	*vector of design, state and control variables respectively*
u	*auxiliary variable for parametric function*
$\chi(d)$	*feasibility measure for given design variable*
$\psi(d,\theta)$	*Parametric function for a given design and realization of uncertain parameters*

λ_j		*Lagrangean multiplier for inequality constraint j*
μ_i		*Lagrangean multiplier for equality constrain i*
dt_{ijk}	$[K]$	*temperature approach between hot stream i, cold stream j, at location k*
dt_{cui}	$[K]$	*temperature approach between hot stream i, and cold utility*
dt_{huj}	$[K]$	*temperature approach between cold stream j, and hot utility*
q_{ijk}	$[kW]$	*heat load between hot stream i and cold stream j at stage k*
q_{cui}	$[kW]$	*heat load between hot stream i and cold utility*
q_{huj}	$[kW]$	*heat load between cold stream j and hot utility*
t_{ik}	$[K]$	*temperature of hot stream i at hot end of stage k*
t_{jk}	$[K]$	*temperature of cold stream j at hot end of stage k*

Binary Variables

y_j	-	
$z_{i,j,k}$	-	*match between hot stream i, cold stream j, at*
z_{cui}	-	*match between hot stream i, and cold utility*
z_{huj}	-	*match between cold stream j, and hot utility*

3.2 Multiperiod Optimization Problem

In this work, the design stage is based on the stage-wise superstructure proposed by Yee and Grossmann (1991). The objective of the model is to find a network that minimizes the total annualized cost, i.e. the investment cost in units and the operating cost in terms of utility consumptions. The superstructure is depicted in Figure. 2, for the case with two hot streams and two cold streams.

Each hot stream is split into each potential match with all cold streams and vice versa. The outlet flows from the heat exchangers are mixed isothermically, which then defines the stream for the next stage. At the end, utility exchangers are allocated in order to ensure the specifications. The number of stages N_T, is normally set to $max\{N_H, N_C\}$, where N_H and N_C are the number of hot streams and the number of cold streams respectively. The main advantage of this model is that the feasible space of the problem is defined by a set of linear constraints. It generates a model robust to solve.

For the selected N periods the multiperiod optimization problem must be formulated. Different formulations are proposed in the literature. The extension of the Synheat Model for the multiperiod representation is very straightforward. The main issue is that the design variables are invariant over the periods.

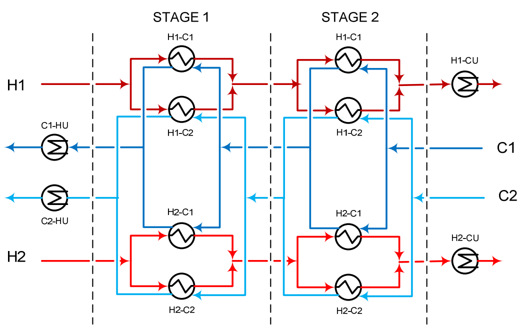

Figure 2. Superstructure for two hot and two cold streams.

The mathematical formulation considered here was presented by Verheyen and Zhang (2006). This multi-period MINLP model simultaneously minimizes the *TAC*. The costs included are capital costs for heat exchanger area and unit and the average operating costs for utility consumption. The optimization problem consist of:

$$\min_{x\in\Omega'}\left\{\begin{array}{c}\sum_{p\in PR}\frac{DOP(p)}{N_P}\left(\sum_{i\in HP}c_{cu}q_{cui}^p+\sum_{j\in CP}c_{hu}q_{huj}^p\right)+\\ \sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST}cf_{ijk}z_{ijk}+\sum_{i\in HP}cf_{cu}z_{cui}+\sum_{j\in CP}cf_{hu}z_{huj}+\\ \sum_{p\in PR}\frac{1}{N}\left(\sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST}c_{ij}\left(A_{ijk}\right)^{\beta}+\sum_{i\in HP}c_{cui}\left(A_{cui}\right)^{\beta}+\sum_{j\in CP}c_{huj}\left(A_{huj}\right)^{\beta}\right)\end{array}\right\}$$

and the feasible space is defined by the following set of constraints:

$$\Omega=\left\{\begin{array}{ll}
\left.\begin{array}{c}(T_i^{in,p}-T_i^{out})w_i^p=\sum_{\forall k\in ST}\sum_{\forall j\in CP}q_{ijk}^p+q_{cui}^p\\ (T_j^{out,p}-T_j^{in,p})w_j^p=\sum_{\forall k\in ST}\sum_{\forall i\in HP}q_{ijk}^p+q_{huj}^p\end{array}\right\} & \text{overall heat balance}\\
\left.\begin{array}{c}(t_{ik}^p-t_{i,k+1}^p)w_i^p=\sum_{\forall j\in CP}q_{ijk}^p\\ (t_{jk}^p-t_{j,k+1}^p)w_j^p=\sum_{\forall i\in HP}q_{ijk}^p\end{array}\right\} & \text{stagewise heat balances}\\
\left.t_{i1}^p=T_i^{in,p},\ t_{j,N_T+1}^p=T_j^{in,p}\right\} & \text{assignment of inlet temperature}\\
\left.\begin{array}{c}t_{ik}^p\geq t_{i,k+1}^p,\ t_{jk}^p\geq t_{j,k+1}^p\\ T_i^{out,p}\leq t_{i,N_T+1}^p,\ T_j^{out,p}\geq t_{j1}^p\end{array}\right\} & \text{feasibility of temperature}\\
\left.\begin{array}{c}\left(t_{i,N_T+1}^p-T_i^{out,p}\right)w_i^p=q_{cui}^p\\ (T_j^{out,p}-t_{j1}^p)w_j=q_{cui}^p\end{array}\right\} & \text{utility loads}\\
\left.\begin{array}{c}q_{ijk}^p-\Lambda_{ij}z_{ijk}\leq 0\\ q_{cui}^p-\Lambda_i z_{cui}\leq 0\\ q_{huj}^p-\Lambda_j z_{huj}\leq 0\end{array}\right\} & \text{logical constraints}\\
\left.\begin{array}{c}dt_{ijk}^p\leq t_{ik}^p-t_{jk}^p+\Gamma_{ij}\left(1-z_{ijk}\right)\\ dt_{ij,k+1}^p\leq t_{i,k+1}^p-t_{j,k+1}^p+\Gamma_{ij}\left(1-z_{ijk}\right)\\ dt_{cui}^p\leq t_{i,N_T+1}^p-T_{cu}^{out,p}+\Gamma_i(1-z_{cui})\\ dt_{cui}^p\leq T_{hu}^{out,p}-t_{j1}^p+\Gamma_j\left(1-z_{huj}\right)\end{array}\right\} & \text{approach temperatures}\\
dt_{ijk}^p,dt_{cui}^p,dt_{huj}^p\geq \Delta T_{min} & \\
z_{ijk},z_{cui},z_{huj}\in\{0,1\} & \\
q_{ijk}^p,q_{cui}^p,q_{huj}^p\geq 0 & \\
\forall i\in HP,j\in CP,k\in ST,p\in PR &
\end{array}\right\}$$

Since the area of the heat exchangers are design variables they must be invariant over the periods. In order to ensure feasible operation for the worst case the installed area used to compute the investment cost must be the maximum area. Verheyen and Zhang (2006) proposed to add nonlinear inequalities in order to ensure the variable A_{ijk} is the maximum area. Due to the direction of the objective function, the constraints (3) are forced to be active at least for the worst case, where the maximum area occurs.

$$\Omega'=\Omega\ \cup\ \left\{\begin{array}{c}A_{ijk}\geq\frac{q_{ijk}^p}{U_{ij}LMTD_{ijk}^p}\\ A_{cui}\geq\frac{q_{cui}^p}{U_{cui}LMTD_{cui}^p}\\ A_{huj}\geq\frac{q_{huj}^p}{U_{huj}LMTD_{huj}^p}\end{array}\right\} \qquad (3)$$

The resulting model is a MINLP where the nonlinearities are presented in the objective function and in the equations (3).

3.3 *Feasibility Test/ Flexibility Index*

The design problem can be described by a set of equality constraints I and inequality constraints J, representing the plant operation and design specifications:

$$h_i(d,z,x,\theta)=0, \quad i\in I \tag{4}$$

$$g_j(d,z,x,\theta)\le 0, \quad j\in J \tag{5}$$

As has been shown by Swaney and Grossmann (1985), for a specific design, d, given this set of constraints, the design feasibility test problem can be formulated as the max-min-max problem:

$$\chi(d)=\max_{\theta\in T} min_z\, max_{\substack{i\in I\\ j\in J}} \begin{Bmatrix} h_i(d,z,x,\theta)=0\\ g_j(d,z,x,\theta)\le 0\end{Bmatrix} \tag{6}$$

where the function $\chi(d)$ represents a feasibility measure for design d. If $\chi(d)\le 0$, design d is feasible for all $\theta\in T$, whereas if $\chi(d)>0$, the design cannot operate for at least some values of $\theta\in T$. The above max-min-max problem defines a nondifferentiable global optimization problem which however can be reformulated as the following two-level optimization problem:

$$\begin{cases} \chi(d)=\max\limits_{\theta\in T}\psi(d,\theta)\\ s.t. \quad \psi(d,\theta)\\ \qquad \psi(d,\theta)=\min\limits_{z} u\\ \qquad s.t.\ \ h_i(d,z,x,\theta)=0\\ \qquad\qquad g_j(d,z,x,\theta)\le u \end{cases} \tag{7}$$

where the function $\psi(d,\theta)$ defines the boundary of the feasible region in the space of the uncertain parameters θ.

The plant feasibility can be quantified by the determining the flexibility index of the design. Following the definition of the flexibility index proposed by Swaney and Grossmann (1985), this metric expresses the largest scaled deviation $\boldsymbol{\delta}$ of any expected deviation $\Delta\theta^+$, $\Delta\theta^-$, that the design can handle. The mathematical formulation for the evaluation of design's flexibility is the following:

$$\begin{cases} F=max\,\delta\\ s.t. \quad \chi(d)=\max\limits_{\theta\in T}\min\limits_{z}\max\limits_{\substack{i\in I\\ j\in J}}\begin{Bmatrix} h_i(d,z,x,\theta)=0\\ g_j(d,z,x,\theta)\le 0\end{Bmatrix}\le 0\\ \qquad T(\delta)=\{\theta|\theta^N-\delta\Delta\theta^-\le\theta\le\theta^N+\delta\Delta\theta^+\} \end{cases} \tag{8}$$

The design flexibility index problem can be reformulated to represent the determination of the largest hyperrectangle that can be inscribed within the feasible region. Following this idea the mathematical formulation of the flexibility problem has the following form:

$$\begin{cases} F=min\,\delta\\ s.t. \quad \psi(d,\theta)=0\\ \qquad \psi(d,\theta)=\min\limits_{z} u\\ \qquad s.t. \quad h_i(d,z,x,\theta)=0\\ \qquad\qquad g_j(d,z,x,\theta)\le u\\ \qquad T(\delta)=\{\theta|\theta^N-\delta\Delta\theta^-\le\theta\le\theta^N+\delta\Delta\theta^{\cdot} \end{cases} \tag{9}$$

3.3.1 *Vertex Enumeration Method*

For the case where the constraints are jointly 1-D quasi-convex in θ and quasi-convex in z it was proven (Swaney and Grossmann, 1985) that the point θ^c that defines the solution to (8) lies at one of the vertices of the parameter set T. Based on this assumption, the critical uncertain parameter points correspond to the vertices and the feasibility test problem is reformulated in the following manner:

$$\chi(d)=\max_{k\in V}\psi(d,\theta^k) \tag{10}$$

where $\psi(d,\theta^k)$ is the evaluation of the function $\psi(d,\theta)$ at the parameter vertex θ^k and V is the index set for the 2^{N_p} vertices for the N_p uncertain parameters θ. In similar fashion for the flexibility index, problem (9) is reformulated in the following way:

$$F=\min_{k\in V}\delta^k \tag{11}$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$, $k\in V$, and is determined by the following problem:

$$\begin{cases} \delta^k=\max\limits_{\delta,z}\delta\\ s.t. \quad h_i(d,z,x,\theta)=0\\ \qquad g_j(d,z,x,\theta)\le 0\\ \qquad \theta=\theta^N+\delta\Delta\theta^k\\ \qquad \delta\ge 0 \end{cases} \tag{12}$$

Based on the above formulations, a direct search method proposed (Halemane and Grossmann, 1983) that explicitly enumerate all the parameters set vertices. To avoid explicit vertex enumeration, two algorithms were proposed (Swaney and Grossmann, 1985) a heuristic vertex search and an implicit enumeration scheme.

3.3.1 *Active Set Strategy*

The algorithms presented in previous section rely on the assumption that the critical points correspond to the vertices of the parameter set T which is valid only for the type of constraints assumed above. To circumvent this limitation, a solution approach was proposed based on the following ideas:

(a) Replace the inner optimization problem

$$\begin{cases} \psi(d,\theta)=\min\limits_{z} u\\ s.t.\ \ h_i(d,z,x,\theta)=0\\ \qquad g_j(d,z,x,\theta)\le u \end{cases} \tag{13}$$

by the Karush-Kuhn-Tucker optimality conditions (KKT):

$$\begin{cases} \sum\limits_{j\in J}\lambda_j=1\\ \sum\limits_{j\in J}\lambda_j\dfrac{\partial g_j}{\partial z}+\sum\limits_{i\in I}\mu_i\dfrac{\partial h_i}{\partial z}=0\\ \sum\limits_{j\in J}\lambda_j\dfrac{\partial g_j}{\partial x}+\sum\limits_{i\in I}\mu_i\dfrac{\partial h_i}{\partial x}=0\\ \lambda_j s_j=0, \ \ j\in J\\ s_j=u-g_j(d,z,x,\theta), \ \ j\in J\\ \lambda_j,s_j\ge 0, \ \ j\in J \end{cases} \tag{14}$$

where s_j are slack variables of constraints j, λ_j, μ_i, are the Lagrange multipliers for inequality and equality constraints, respectively.

(b) For the inner problem the following property holds that if each square submatrix of dimension $(n_z \times n_z)$ where n_z is the number of control variables, of the partial derivatives of the constraints g_j, $\forall j \in J$ with respect to the control variables z is of full rank, then the number of the active constraints is equal to $n_z + 1$;

(c) Utilize the discrete nature of the selection of the active constraints by introducing a set of binary variables y_j to express if the constrain g_j is active. In particular:

$$\begin{cases} \lambda_j - y_j \leq 0, \ \ j \in J \\ s_j - U(1-y_j) \leq 0, \ \ j \in J \\ \sum_{j \in J} y_j = n_z + 1 \\ \delta \geq 0 \\ y_j = \{0,1\}, \ \ \lambda_j, s_j \geq 0, \ \ j \in J \end{cases} \tag{15}$$

Where U represents an upper bound to the slack variables s_j. It should be noted that:

For active constraints:

$$y_j = 1 \xrightarrow{yields} \lambda_j \geq 0, \ \ s_j = 0 \tag{16}$$

For inactive constraints:

$$y_j = 0 \xrightarrow{yields} \lambda_j = 0, \ \ 0 \leq s_j \leq U \tag{17}$$

Based on these ideas, the feasibility test and the flexibility test problem can be reformulated in the following way:

$\underline{Flexibility\ Index\ Problem\ (P_2)}$:

$$\begin{aligned} & F = min\, \delta \\ & s.t. \ \ h_i(d,z,x,\theta) = 0 \\ & \qquad g_j(d,z,x,\theta) + s_j - u = 0 \\ & \qquad u = 0 \\ & \qquad \sum_{j \in J} \lambda_j = 1 \\ & \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ & \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ & \qquad \lambda_j - y_j \leq 0, \ \ j \in J \\ & \qquad s_j - U(1-y_j) \leq 0, \ \ j \in J \\ & \qquad \sum_{j \in J} y_j = n_z + 1 \\ & \qquad \theta^L \leq \theta \leq \theta^U \\ & \qquad \delta \geq 0 \\ & \qquad y_j = \{0,1\}, \ \ \lambda_j, s_j \geq 0, \ \ j \in J \end{aligned}$$

Which corresponds to a mixed integer optimization problem either linear or nonlinear depending on the nature of the constraints.

The formulation described above can be used for flexibility index evaluation of any design. For the specific case of Heat Exchangers Networks based on the Synheat Model (Yee and Grossmann, 1991) the following formulation was proposed in this work. In order to carry out the flexibility analysis of HENs, all relevant equality and inequality for the HEN model, can be reorganized as described below. The equality constraints $h(d,z,x,\theta)$ are:

$$\begin{Bmatrix} \sum_{\forall j \in CP} q_{ijk} - (t_{ik} - t_{i,k+1}) w_i \\ \sum_{\forall i \in HP} q_{ijk} - (t_{jk} - t_{jk+1}) w_j \\ q_{cui} - (t_{i,N_T+1} - T_i^{out}) w_i \\ q_{huj} - (T_j^{out} - t_{j1}) w_j \\ T_i^{in} - t_{i1} \\ T_j^{in} - t_{j,N_T+1} \end{Bmatrix} = 0 \tag{18}$$

and the specifications $g(d,z,x,\theta)$:

$$\begin{Bmatrix} t_{i,k+1} - t_{ik}, & \sum_{j \in CP} z_{ijk} \geq 1 \\ t_{j,k+1} - t_{jk}, & \sum_{i \in HP} z_{ijk} \geq 1 \\ T_i^{out} - t_{i,N_T+1}, & z_{cui} = 1 \\ t_{j1} - T_j^{out}, & z_{huj} = 1 \\ \Delta T_{\min} + t_{jk} - t_{ik}, & z_{ijk} = 1 \\ \Delta T_{\min} + t_{j,k+1} - t_{i,k+1}, & z_{ijk} = 1 \\ \Delta T_{\min} + T_{cu}^{out} - t_{i,N_T+1}, & z_{cui} = 1 \\ \Delta T_{\min} + t_{j1} - T_{hu}^{out}, & z_{huj} = 1 \end{Bmatrix} \leq 0 \tag{19}$$

where $i \in HP$, $j \in CP$, and $k \in ST$. Substituting the equations (18) and (19) in the formulation described in this section, e.g. problem P_2 it is possible to solve the feasibility and flexibility test. These equations are based on the constraints of Synheat Model, and the overall heat balances are not included because they can be obtained by combining other independent equalities. It ensures the full rank of the partial derivatives of the constraints with respect to the control variables z, which is a premise of the active set strategy. The control variables are chosen as the degrees of freedom during operation, determined by the number of equations minus the number of unknown variables, and they are preferable the utility loads.

4. Numerical Examples

4.1 Numerical Example 01

The problem data and the uncertainty description for this numerical example are presented in Table 1. It was assumed only inlet temperatures as uncertain parameters. For this particular case the set of equations (18) and (19) are linear. Therefore the critical operation conditions are explored on the basis of the vertices of the polyhedral region of uncertainty trough a scalar δ_T (flexibility target). Considering N uncertain parameters, the total number of vertex directions is 2^N, i. e. combinations of the $\pm$ directed deviations from the nominal values of the uncertain parameters. Considering the inlet temperatures as uncertain parameters, the total number of vertices V is equal to $2^{(NH+NC)} = 16$.

Table 1. Problem data for Ex.1 (Floudas and Grossmann, 1987).

Stream	T_{in} (K)	T_{out} (K)	w (kWK^{-1})	h (kW m^2 K^{-1})
$H1$	583±10	323	1.4	0.16
$H2$	723±10	553	2.0	0.16
$C1$	313±10	393	3.0	0.16
$C2$	388±10	553	2.0	0.16
CU	303	323		0.16
HU	573	573		0.16
Cost of Heat Exchangers (\$y^{-1}) = 5500+4333[Area (m^2)]$^{0.60}$				
Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})				
Cost of Heating Utility = 172.428 (\$kW^{-1}y^{-1})				

For the nominal conditions presented in Table 1 using the Synheat Model it was generated the Heat Exchanger Network depicted in Figure 4. The MINLP model was solved using the solver DICOPT with a CPU time of 0.184 seconds. The resulting configuration has a Total Annual Cost (TAC) of 92.210,14 \$/year and the utility consumption as the minimum possible.

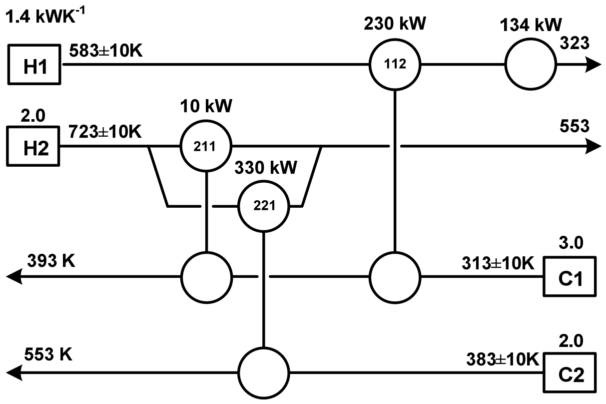

Figure 3. Heat Exchanger Network for Example 1.

The inlet temperatures, for each vertex k, and for target flexibility $(\delta_T = 10K)$ are assigned to the inlet temperatures of the HEN configuration through the equations (20) and (21) as dependent on the vertices of the polyhedral uncertainty region, the size of the size of which is defined by the scalar target flexibility, δ, that acts as a scale factor. The parameters $r_{i,k}, r_{j,k}$ are the vertex identifier and take the values of V combinations of the ± directed deviations from the nominal values of the uncertain parameters according illustrated in Table 2.

$$T_{i,k}^{in} = T_{i,k}^{in,0} + \delta \Delta T_{i,k}^{in} \quad i \in HP, k = 1, \dots, V \qquad (20)$$

$$T_{j,k}^{in} = T_{j,k}^{in,0} + \delta \Delta T_{j,k}^{in} \quad j \in CP, k = 1, \dots, V \qquad (21)$$

where

$$\Delta T_{i,k}^{in} = r_{i,k} \delta_T \quad i \in HP, k = 1, \dots, V \qquad (22)$$

$$\Delta T_{j,k}^{in} = r_{j,k} \delta_T \quad j \in CP, k = 1, \dots, V \qquad (23)$$

It was solved 16 LPs subproblems by using CPLEX in order to evaluate the flexibility along each vertex direction. The general results are presented in Table 2. The minimum value was identified in the vertices 6, 8, 14, and 16 with the correspondent value of 0.250, which represents the Flexibility Index of the configuration. In other words, for the given design, the configuration can remain feasible only for 25 % of the desired target of 10 K. The total CPU time spent was 0.221 seconds.

Table 2. Flexibility Evaluation for each vertex k for Example 1.

Vertex k	*Vertex Direction* $r_{i=1,k}$	$r_{i=2,k}$	$r_{j=1,k}$	$r_{j=2,k}$	*Flexibility Index Candidate* δ^k	$CPU(s)$
1	+	+	+	+	3.286	0.013
2	+	+	+	−	7.667	0.011
3	+	+	−	+	15.500	0.012
4	+	−	+	+	7.667	0.012
5	+	+	−	−	7.762	0.012
6	+	−	+	−	**0.250**	0.013
7	+	−	−	+	7.762	0.012
8	+	−	−	−	**0.250**	0.013
9	−	+	+	+	3.286	0.012
10	−	+	+	−	7.667	0.012
11	−	+	−	+	15.500	0.013
12	−	+	−	−	2.823	0.013
13	−	−	+	+	7.667	0.023
14	−	−	+	−	**0.250**	0.011
15	−	−	−	+	2.823	0.027
16	−	−	−	−	**0.250**	0.011

For the structure presented in Figure 3 the number of control variables (degrees of freedom) is equal to 0, and hence only one of the 13 constraints described by the equation (20) will be active. It was solved 13 LPs subproblems by using the solver CPLEX in order to evaluate the flexibility considering each inequality as active. The total CPU time was 0.20 seconds, and as expected the same solution was found.

Instead of explicit enumeration of the active set, it is possible to use binary variables to perform this discrete decision. The resulting problem can be solved using one MILP instead of 13 LPs in order to obtain the same result. The general comparison for the Flexibility Index evaluation by these different methods is presented in Table 3. It is clear that the MILP formulation for the active set strategy had the best computational performance.

Table 3. General comparison for Flexibility Evaluation by different methods for Example 1.

Method	*Subproblems*	*Flexibility Index (FI)*	$CPU(s)$
VEM	16 LPs	0.25	0.221
ASS	13 LPs	0.25	0.200
ASS	1 MILP	0.25	0.054

Once the Flexibility Index is lower than 1, the critical point identified is identified and the current set (only the nominal conditions) is updated with this new point and a second iteration is performed. The new multiperiod is solved and the configuration depicted in Figure 4 is found.

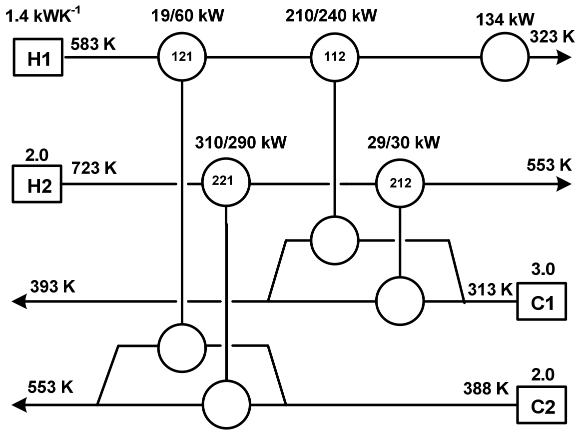

Figure 4. Heat Exchanger Network for Example 1 at iteration 2.

The evaluation of the Flexibility Index for the configuration obtained was again solved using the Vertex Enumeration Method (VEM). It was solved 16 LPs subproblems by using CPLEX in order to evaluate the flexibility along each vertex direction. The minimum value was identified in the vertex 16, with the correspondent value of 1.479, which represents the Flexibility Index of the configuration. In Table 4 is presented the general comparison for the flexibility index evaluation using active set strategy, where 1 MILP was solved with better computational performance.

Table 4. General comparison for Flexibility Evaluation by different methods for Example 1.

$Method$	$Subproblems$	$Flexibility$ $Index\ (FI)$	$CPU(s)$
VEM	16 LPs	1.479	0.211
ASS	1 MILP	1.479	0.071

The general results are presented in Table 5 and the cumulative critical points considered at iteration k is presented in Table 6.

Table 5. General Results for TSS applied to Example 01.

$Iter.$	$Operating$ $Cost$ $(\$/y)$	$Investment$ $Cost(\$/y)$	$Total\ Annual$ $Cost\ (\$/y)$	$Flexibility$ $Index$
1	8117	84093	92210	0.250
2	5573	124901	130474	1.429

Once the Flexibility Index is greater than one, the design is sufficient flexible according to the flexibility target, i.e. this configuration is capable to operate feasibly under the expected uncertainty region.

Table 6. Points considered for the TSS for Example 01.

$Iter.$	$T_{in}^{H1}(K)$	$T_{in}^{H2}(K)$	$T_{in}^{C1}(K)$	$T_{in}^{C2}(K)$
1	583	723	313	388
2	573	713	303	378

It should be noted that the final configuration supports variations in the inlet tempartures of 14.79 K. The total CPU time for the generation of this flexible design was 0.553 seconds.

4.2 Numerical Example 02

For the second numerical example it was considered the same nominal conditions as in the example 01. However, three different cases with different uncertainty description were created. The general data for the cases (A,B, and C) are showed in Table 7.

Table 7. Problem data for Ex.2 (Floudas and Grossmann, 1987).

Case	*Stream*	T_{in} (K)	T_{out} (K)	w (kWK^{-1})	h (kW m^2 K^{-1})
A	$H1$	583±10	323	1.4±5%	0.16
	$H2$	723±10	553	2.0±5%	0.16
	$C1$	313±10	393	3.0±5%	0.16
	$C2$	388±10	553	2.0±5%	0.16
	CU	320	323		0.16
	HU	573	573		0.16
B	$H1$	583±10	323	1.4±0.4	0.16
	$H2$	723	553	2.0	0.16
	$C1$	313	393	3.0	0.16
	$C2$	388±5	553	2.0±0.4	0.16
	CU	320	323		0.16
	HU	573	573		0.16
C	HU	573	573		0.16
	$H1$	583	323	1.4±10%	0.16
	$H2$	723	553	2.0±10%	0.16
	$C1$	313	393	3.0±10%	0.16
	$C2$	388	553	2.0±10%	0.16
	CU	320	323		0.16
	HU	573	573		0.16

Cost of Heat Exchangers (\$y^{-1}) = 5500+4333[Area (m^2)]$^{0.60}$
Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 172.428 (\$kW^{-1}y^{-1})

For these cases, the uncertainties are presented at also in the heat capacity flowrates. The vertex search method cannot be used, since there is no guarantee that the critical point rely on a vertex. The equations (18) are nonlinear due to the product of temperatures and flowrates generating a set of bilinear constraints that are nonconvex. Using the implicit active set strategy requires the solution of a nonconvex MINLP. Once an important decision is made based on this value, it is very important that this problem be solved to global optimality.

The bilinear terms can be replaced by a convex relaxation, e.g. McCormick's envelopes and and a spatial branch and bound algorithm can be used to solve this problem.

Furthermore, for process synthesis applications, where approximate solutions would be suitable for screening purposes, a quicker way to solve the nonlinear versions of the flexibility index by active set strategy is to linearize the constraint functions around nominal conditions. For example:

$$h(d,z,x,\theta) \cong \quad h(d,z^N,z^N,\theta^N) + \left(\frac{\partial h_i}{\partial \theta}\right)^T (\theta - \theta^N) + \left(\frac{\partial h_i}{\partial z}\right)^T (z - z^N) + + \left(\frac{\partial h_i}{\partial x}\right)^T (x - x^N) \tag{24}$$

where (x^N, z^N, θ^N) corresponds to the nominal point. In this way the problem is reduced to a MILP. As discussed by Grossmann and Floudas (1987), these linearizations often yield good approximations.

The heat exchanger network for the nominal conditions has already been generated in the previous numerical example and the network obtained can be seen in Figure 3. Based on this configuaration the flexibility index was evaluated for the three cases using active set strategy. The resulting problem was solved with global optimization (BARON) and by convexification through linearization. The general results are presented in Table 8.

Table 8. General Comparison for Flexibility Evaluation by different methods for Example 2.

Case	*Method*	*Subproblems*	*Flexibility Index (FI)*	*CPU(s)*
A	*ASS Linearized*	1 MILP	0.134	0.071
	ASS Global Optimization	1 MNILP	0.136	0.367
B	*ASS Linearized*	1 MILP	0.132	0.069
	ASS Global Optimization	1 MNILP	0.131	0.390
C	*ASS Linearized*	1 MILP	0.149	0.078
	ASS Global Optimization	1 MNILP	0.149	0.410

It is clear that the linearized version equation provides a quite good approximation for the nonlinear model. An important evidence is that the approximate solutions were obtained with much less computational effort.

The two stage strategy was applied for the Case B and the results are summarized in Table 9. The procedure converged after 4 iterations for a design with a TAC of 148515 $/ year and a flexibility Index of 1.71.

Table 9. Results for TSS applied to Example 02 Case B.

It.	*Operating Cost ($/y)*	*Investment Cost ($/y)*	*Total Annual Cost ($/y)*	*Flexibility Index*	*Flexibility Index (lin.)*
1	24758	67452	92210	0.1311	0.1316
2	28823	96083	124905	0.1847	0.2190
3	39540	92563	132194	0.6358	0.6060
4	41749	106765	148515	1.7134	1.9800

This example showed that despite the linearization around nominal conditions generate a problem that can be solved with much less computational effort, it must be applied carefully. For some iterations the linearization provided an error about 20 %. The final configuration obtained is depicted in Figure 5.

The total CPU time for the whole procedure was 11.468 seconds for the global optimization and 1.744 for the linearized version. Only a total one second was spent at the design phase (multiperiod problem). In order to speed up the algorithm a good heuristic would be use the linear version and after convergence check using a global optimization technique.

Table 10. Results for TSS applied to Example 02 Case B.

$Iter.$	T_{in}^{H1} (K)	f_{H1} (kW/K)	T_{in}^{C2} (K)	f_{C2} (kW/K)
1	583	1.4	388	2.0
2	593	1.8	383	2.4
3	593	1.8	393	1.6
4	573	1.0	383	2.4

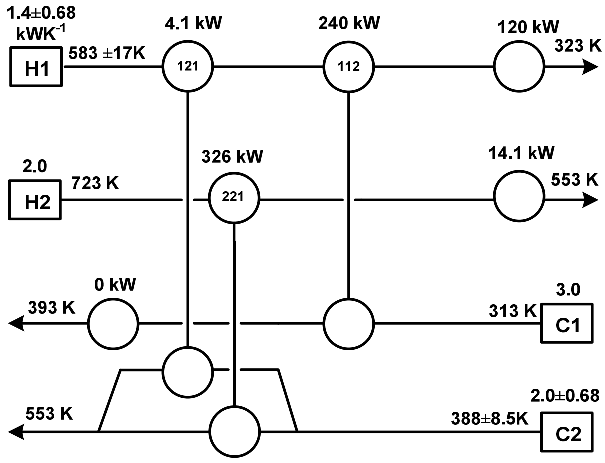

Figure 5. Final Configuration for Example 2.

5. Conclusions and Final Remarks

It has been developed a computational framework for synthesis of flexible and controllable Heat Exchanger Networks; The framework is based on the Two Stage Strategy proposed by Halemane and Grossmann (1983) for design process under uncertainty and oriented to the Synheat Model (Yee and Grossmann, 1991) using Multiperiod Formulations in order to approximate; For the design stage a multiperiod formulation proposed by Verheyen and Zhang (2006); while The Flexibility Analysis is performed using the Active Set Strategy (Grossmann and Floudas, 1987) for the general case.

When the uncertain parameters are only in the inlet temperatures the assumption of the critical point relying on a vertex of the uncertainty region is appropriate. We can also use the Active Set Strategy in order to solve for the general case (nonvertex critical point). In that case the problem is nonlinear and a global optimization technique must be used. It is also possible to obtain a good approximation linearizing the problem around the nominal conditions.

In this particular work the main contribution was the integration of different models available in the literature in order to generate an automatic procedure for designing flexible heat exchanger networks.

The framework was implemented in GAMS 23.3. Some tricky points during the implementation were overcome, such as, the automatic calculation of the number of degrees of freedom after each design stage and the automatic derivation of the KKT conditions. Despite the numerical examples presented here were in fact small scale problems, the whole procedure was implemented in such way that it can be directly applied for large scale problems. The main limitation would be the dimension of the multiperiod problem. To circumvent this problem, we propose an algorithm based on Lagrangean Decomposition coupled with a heuristic technique in order to generate a sequence of upper and lower bounds. A brief idea is presented in Appendix A.

The application of the proposed HEN synthesis strategy and its computational efficiency were illustrated with two numerical examples. This computational framework yields a HEN design which is guaranteed to operate under varying conditions ensuring stream temperature targets and optimal energy integration.

6. References

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Appendix A: Decomposition Technique[2]

The multiperiod models such as (*P'*) grow quickly in size with the number of periods, making it very difficult to solve them to global optimality without the help of specialized techniques. However, Multiperiod design problems present an interesting structure that can be exploited. Generally, a subset of constraints holds for each period and a subset of constraints links all periods. Regarding this linking constraints as complicating constraints in the sense that removing these constraints from the feasible space though Lagrangean Relaxation allows a straightforward decomposition into periods. The subproblems for each period can be solved independently and the solutions combined to generate a lower bound for the minimization problem. From the subproblems a feasible solution is postulated for the original problem and an upper bound is generated. The Lagrangean multipliers are updated using the subgradient method. The procedure terminates when the upper and lower bounds converges to the same value within a specified tolerance. A general overview can be seen in Figure 6. The proposed algorithm has performed well for large scale problems.

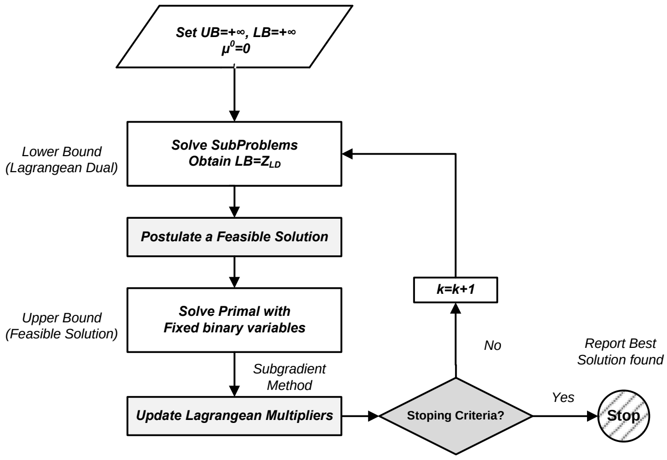

Figure 6. Lagrangean Heuristic Approach for solving Multiperiod Synheat model.

Appendix B: SynFlex Toolbox

A concern during the implementation was the automatization of the whole procedure. This computational framework. The problems are solved using GAMS but the procedure is managed by Matlab. In Figure 7 is depicted the initial interface of the SynFlex toolbox that has been developed.

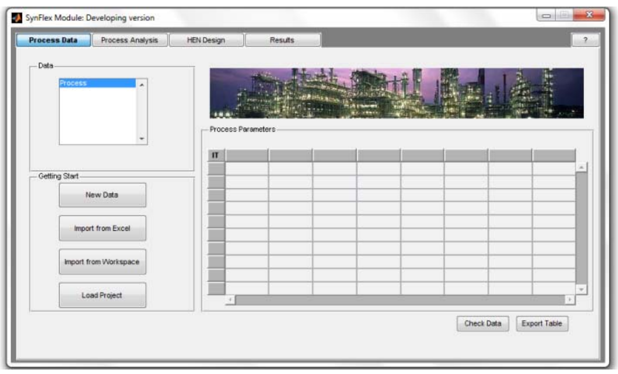

Figure 7. SynFlex Toolbox Interface.

[2] This proposed approach was presented in CAPD Annual Meeting 2010 in Carnegie Mellon University, USA.