Global Optimization In Design Under Uncertainty: Feasibility Test and Flexibility Index Problems

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Abstract

Design feasibility and flexibility are recognized as important operability characteristics of a chemical process. This is due to the variability of the parameters that appear in process operations, and the increasing market environment competition which requires reliability on meeting product demands and quality specifications. In this work, a novel approach is presented for the evaluation of design feasibility/flexibility based on the ideas of the deterministic global optimization algorithm $\boldsymbol{\alpha}\mathbf{BB}$[1,2,3,4], which in turn relies on a difference of convex functions transformation and a branch and bound framework. The proposed approach can address problems that are described through general nonconvex equality and inequality constraints. A number of examples illustrate the applicability and efficiency of the proposed global optimization framework, for both the feasibility test and flexibility index problems.

Keywords: Deterministic Global Optimization, Feasibility Test, Flexibility Index, Bilevel Programming

1 Introduction

In the last two decades the problem of developing quantitative techniques for planning the selection of new processes, the expansion of the existing ones and the plant production under

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changing conditions has received an increasing attention in the open literature[5;6;7;8;9;10;11;12;13;14]. To incorporate flexibility objectives in the design stage, the problems of evaluating the feasibility and flexibility for a given design first need to be addressed in a rigorous and efficient way. Different approaches that exist in the literature to quantify the feasibility and flexibility for a given design include the deterministic measures such as the Resilience Index, RI[15], the feasibility test and the flexibility index proposed by Grossmann and Floudas[5], Grossmann and Halemane[6], Grossmann et al.[16], Halemane and Grossmann[7], Swaney and Grossmann[13], Swaney and Grossmann[14], and the stochastic measures such as the design reliability[17], and the stochastic flexibility index[18;19].

In this work, a systematic and rigorous approach is proposed for the efficient solution of the feasibility test and flexibility index problems for a given design. The approach is based on the concept of feasible domain relaxation and the basic principles of the deterministic global optimization algorithm $\boldsymbol{\alpha}$**BB**[1;2;3;4]. The main feature of the presented approach is that it guarantees convergence to the global optimal solution for problems that are described by general nonconvex constraints. In section 2 the problems of feasibility test and flexibility index of a given design are discussed and the main difficulties of addressing both problems are highlighted. Section 3, presents the key ideas of the proposed approach. In sections 4 and 5, the new conceptual framework and the detailed steps of the proposed algorithmic procedures are outlined and their modifications for special cases are discussed in section 6. Subsequently, in section 7, a number of examples are presented to illustrate the theoretical and computational aspects of the proposed approach.

2 Problem Statement

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

$$h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0, \quad i \in I$$
$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0, \quad j \in J$$

where $\mathbf{d}$ corresponds to the vector of design variables, $\mathbf{z}$ is the vector of control variables, $\mathbf{x}$ is the vector of state variables and $\boldsymbol{\theta}$ is the vector of uncertain parameters. As it has been shown by Halemane and Grossmann[7], for a specific design $\mathbf{d}$ the design feasibility test problem can be formulated as the max-min-max problem:

$$\chi(\mathbf{d}) = \max_{\theta \in T} \min_{\mathbf{z}} \max_{j \in J, i \in I} \{h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0; g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0\}$$

where the function $\chi(\mathbf{d})$ represents a feasibility measure for design $\mathbf{d}$. If $\chi(\mathbf{d}) \leq 0$, the design $\mathbf{d}$ is feasible for all $\boldsymbol{\theta} \in T$, where $T = \{\boldsymbol{\theta} \mid \boldsymbol{\theta}^L \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^U\}$ is the uncertain parameter range.

If $\chi(\mathbf{d}) > 0$, the design cannot operate for at least some values of $\boldsymbol{\theta} \in T$. The above max-min-max problem defines a nondifferentiable global optimization problem which however can be reformulated, as has been shown by Swaney and Grossmann[13], to the following two-level optimization problem.

$$\chi(\mathbf{d}) = \max_{\theta \epsilon T} \ \psi(\mathbf{d},\boldsymbol{\theta})$$

$$\text{s.t.} \quad \psi(\mathbf{d},\boldsymbol{\theta}) \leq 0$$

$$\psi(\mathbf{d},\, \boldsymbol{\theta}) = \min_{\mathbf{z},u} \ u$$

$$\begin{aligned} \text{s.t.} \quad & h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\, \boldsymbol{\theta}) = 0 \ \ i \in I \\ & g_j(\mathbf{d}, \mathbf{z}, \mathbf{x},\, \boldsymbol{\theta}) \leq u \ \ j \in J \end{aligned}$$

where the function $\psi(\mathbf{d},\boldsymbol{\theta}) = 0$ defines the boundary of the feasible region in the space of the uncertain parameters $\boldsymbol{\theta}$.

Plant feasibility can be quantified and enhanced by determining the flexibility index of the design. Following the definition of the flexibility index as it is proposed by Swaney and Grossmann[13], this metric expresses the largest scaled deviation δ of any expected deviations $\Delta\boldsymbol{\theta}^+$, $\Delta\boldsymbol{\theta}^-$, that the design can handle. The mathematical formulation for the evaluation of the flexibility index problem becomes:

$$F = \max \delta$$

$$\text{s.t.} \quad \chi(\mathbf{d}) = \max_{\theta \epsilon T} \min_{\mathbf{z}} \max_{j \in J, i \in I} \{h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta}) = 0; g_j(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta}) \leq 0\} \leq 0$$

$$\begin{aligned} & T(\delta) = \{\boldsymbol{\theta} | \boldsymbol{\theta}^N - \delta\Delta\boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\Delta\boldsymbol{\theta}^+\} \\ & \delta \geq 0. \end{aligned}$$

Note that the above problem includes as a constraint the optimization problem of defining the feasibility measure, $\chi(\mathbf{d})$. Several approaches exist in the literature to address the feasibility test and flexibility index problems. These include the work of Halemane and Grossmann[7], for the case that the solution lies at one of the vertices of parameter set T, who proposed the evaluation of $\chi(\mathbf{d})$ at each vertex of T and the selection of the largest one; the work of Swaney and Grossmann[13], that proposed two algorithms, a vertex search and an implicit enumeration scheme that avoids the exhaustive enumeration of all vertices. Both algorithms however, rely on the assumption that the global solution lies at one of the vertices. Grossmann and Floudas [5] proposed an active set strategy that can identify non-vertex solutions and which decomposes the problem into NLP subproblems corresponding to different active sets. The approach guarantees global optimality to a restricted set of problems where $\chi(\mathbf{d})$ are quasi-concave in $\boldsymbol{\theta}$ and the constraint functions are jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$ and strictly quasi-convex in $\mathbf{z}$ for fixed $\boldsymbol{\theta}$. Ostrovsky et al.[10], proposed a branch and bound approach based on the evaluation of upper and lower bound of the feasibility measure $\chi(\mathbf{d})$. Although the suggested bounding problems are simpler than the original feasibility test problem, they correspond to bilevel optimization problems where global optimality cannot be guaranteed using local optimization methods.

The main theoretical contribution of this work is that it provides a rigorous approach for the feasibility test and flexibility index problems that guarantees global optimality for the general case of nonconvex equality and inequality constraints, that involve twice continuously differentiable functions. For the fundamentals in the theory, algorithms and applications of deterministic global optimization, the reader is directed to the book by Floudas[20].

3 New Conceptual Framework

The solution of the feasibility test and flexibility index problems is greatly complicated by the max-min-max problem, which corresponds to a nondifferentiable optimization problem[16]. To illustrate these difficulties, consider the following set of constraints:

$$\begin{aligned} g_1 = -z + \theta &\leq 0 \\ g_2 = z + 2\theta - d &\leq 0 \\ g_3 = -z + 6\theta - 9d &\leq 0 \\ 0 \leq \theta &\leq 4 \end{aligned}$$

that define the feasible region of the inner problem of both the feasibility test and the flexibility index problems, as illustrated in Figure 1(a) for $d = 1$. Note that the feasible region is convex. However, even for this simple example where all the constraints are linear, the optimal inner problem objective, $\psi(d, \theta)$, where

$$\begin{aligned} \psi(d,\theta) &= \min_{z,u} u \\ &\quad \text{s.t.} \quad g_j(d,z,x,\theta) \leq u, \; j = 1,..,4, \end{aligned}$$

is a nondifferentiable function as illustrated in Figure 1(b). Furthermore, when the constraint set involves nonlinear functions, the feasible region can be nonconvex, introducing additional difficulty to solving the problem to global optimality.

The basic idea of the proposed framework that leads to the determination of the global optimal solution for both the feasibility test and the flexibility index problem will be illustrated

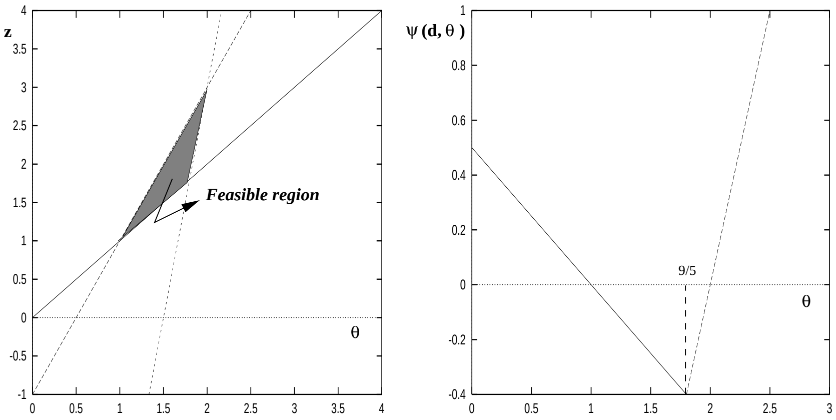

Figure 1: (a) Feasible region. (b) $\psi(d, \theta)$ function.

first via the following motivating example taken from McCormick[22]. It consists of a single nonlinear constraint in two variables and simple bounding constraints:

$$
\begin{aligned}
&(\exp(x_1) - x_2^2)x_1x_2 \leq 0.0, \\
&-1 \leq x_1 \leq 3, \\
&-2 \leq x_2 \leq 3.
\end{aligned}
$$

For this problem, the feasible region consists of the lighter shaded part of the area shown in Figure 2 which is a nonconvex discontinuous region.

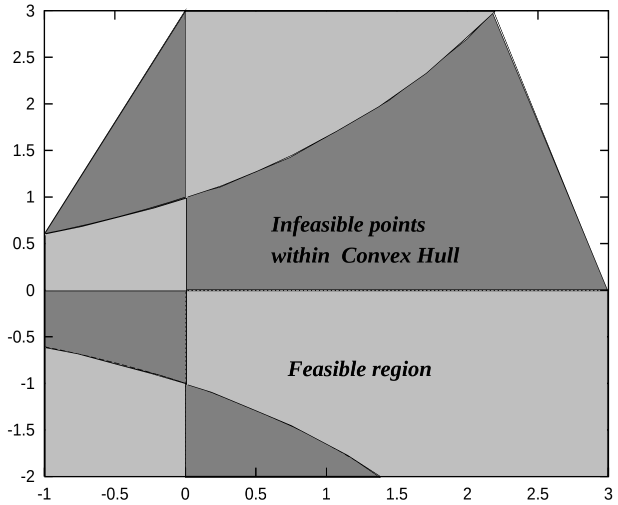

Figure 2: Feasible region and Convex Hull

The feasible region can be enlarged in such a way that the infeasible points within the convex hull, which correspond to the darker shaded areas of Figure 2 are also included into the feasible set. This can be done by a convexification/underestimation method, that underestimates the nonlinear functions over the variable domain. Due to this underestimation, the resulting convex feasibility test, and convex flexibility index problems will provide a lower bound on the original nonconvex problem. The lower bound can be refined by successive branching and bounding of the variable space. Thus, the underestimation idea can be used for obtaining the global minimum feasibility test and flexibility index problems. The basic ideas of this novel tecnique, involve the following key steps:

(a) If any of the inequality constraints $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ are nonconvex and/or the equality constraints $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ are nonlinear, the inner level of the feasibility test and the flexibility index problems is nonconvex. Therefore, the *Karush-Kuhn-Tucker*, KKT, optimality conditions are necessary but not sufficient to guarantee the global optimum of the $\psi(\mathbf{d},\boldsymbol{\theta})$ function. Local, or even suboptimal solutions may be obtained. Hence, the first step of the proposed framework involves the convexification of the feasible region defined by the constraints $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ and $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ of the original problem. Note that all $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ constraints must be linear in $\mathbf{x}$ and $\mathbf{z}$ for the KKT conditions to hold. The nonlinear $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta})$ are eliminated easily by rewriting as two inequality constraints:

$$h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta}) \leq 0,$$
$$-h_i(\mathbf{d}, \mathbf{z}, \mathbf{x},\boldsymbol{\theta}) \leq 0.$$

and are added to the set of inequality constraints. The basic underestimation principles of the $\boldsymbol{\alpha}$**BB**[1;2;3;4] global optimization approach are utilized to underestimate the inequality constraints nonconvex in $\mathbf{x}$ and $\mathbf{z}$. This results in a relaxation of the original feasible space as illustrated in the aforementioned example. For the convexified problem the KKT optimality conditions are necessary and sufficient[23;5], assuming that the linear independence constraint qualification is satisfied. Under these conditions, the convexified inner level optimization problem is equivalent to its KKT optimality conditions.

(b) The convexified inner level optimization problem is replaced with its equivalent set of equations that are defined by the KKT optimality conditions. This transforms the bilevel problem into a single level optimization problem. Note that this problem is, in general, a nonconvex optimization problem due to the complementarity conditions. As a result, further convex underestimation may be needed which takes place according to the $\boldsymbol{\alpha}$**BB** [1;2;3;4] principles. The solution of the convexified single stage problem provides a *lower bound* of the design flexibility function $\chi(\mathbf{d})$ and the flexibility index of the design, F.

(c) An upper bound to the design flexibility function $\chi(\mathbf{d})$ and flexibility index F is determined through a feasible solution of the original Mixed Integer Nonlinear Programming, MINLP, formulation obtained by substituting the inner problem by the KKT optimality conditions (which are only necessary), as proposed by Grossmann and Floudas[5].

(d) The next step after establishing an upper and a lower bound on the global solution, is to refine them. This is accomplished by successfully partitioning the initial region of the variables into smaller ones. The partitioning strategy involves the successive subdivision of a hyperectangle into two sub-rectangles by halving on the middle point of the longest side of the initial rectangle (bisection). In each iteration the lower bound of the feasibility test and the flexibility index problem is the minimum overall the minima found in every subrectangle composing the initial rectangle. Consequently, a non-decreasing sequence of lower bounds is generated by halving the sub-rectangle that is responsible for the infimum over the minima obtained at each iteration. A non-increasing sequence of upper bounds is derived by solving the nonconvex MINLP single optimization problem obtained after the substitution of the inner problem by the KKT optimality conditions, and selecting as an upper bound the minimum over all previously determined upper bounds. If at any iteration the solution of the convexified MINLP in any sub-rectangle is found to be greater than the upper bound, this sub-rectangle is fathomed since the global solution cannot be found inside it.

Note that in order to replace the convexified inner problem with its equivalent KKT optimality conditions, the linear independence condition must be satisfied. Otherwise, the transformed single level problem may be infeasible or it can not be guaranteed that it is a lower bound. A simple linear independence check can be made by testing whether the best $(\mathbf{z}^*,\boldsymbol{\theta}^*, u^*)$ values obtained from the solution of the original nonconvex upper bounding problem result in linearly independent active constraints in the convexified problem.

The steps of the proposed framework for the design feasibility test and the flexibility index problems are presented in the next two sections.

4 Framework for the Feasibility Test

As illustrated in Figure 3, the proposed procedure for the design feasibility problem involves the following steps:

Step 1: Consider the whole uncertainty space. Set the lower bound, LB, = - ∞, K=1 and select a tolerance ϵ.

Step 2: Substitute the inner optimization problem of the original problem (i.e., without convexifying the constraints)

$$\psi(\mathbf{d},\boldsymbol{\theta}) = \min_{\mathbf{z},u} u$$

$$\text{s.t.} \quad h_i(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) = 0 \;\; i \in I$$

$$g_j(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) \leq u \;\; j \in J$$

by the KKT optimality conditions:

$$\sum_{j=1}^{J} \lambda_j = 1$$
$$\sum_{j=1}^{J} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} + \sum_{i=1}^{I} \mu_i \frac{\partial h_i}{\partial \mathbf{z}} = 0$$
$$\sum_{j=1}^{J} \lambda_j \frac{\partial g_j}{\partial \mathbf{x}} + \sum_{i=1}^{I} \mu_i \frac{\partial h_i}{\partial \mathbf{x}} = 0$$
$$\lambda_j s_j \leq 0, \;\; j \in J$$
$$s_j = u - g_j(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}), \;\; j \in J$$
$$\lambda_j, \;\; s_j \geq 0, \;\; j \in J.$$

Then, based on the Property *1*[5] of the inner optimization problem $\psi(\mathbf{d},\boldsymbol{\theta})$, which states that n_z+1 constraints become active at the solution of the problem 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 $\mathbf{z}$ is of full rank. Introducing binary variables y_j to represent the active constraints, the feasibility test problem takes the following form:

Problem (P1)

$$\chi(d) = \max u$$

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

where s_j are the slack variables of design inequalities, λ_j are the associated Lagrange multipliers; y_j are the binary variables (y_j=1 if constraint j is active; 0 otherwise).

Solve the resulting problem using a local MINLP optimizer (e.g., DICOPT[24], MINOPT[25]). Set the upper bound, UB, equal to the best obtained solution.

Step 3: Rewrite the nonlinear equality constraints as a set of two inequalities, that is, $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0$, $-h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0$ and add them to the set of inequality constraints, $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$. The remaining equality constraints are linear, and denoted as $h_i^l(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$. Then, evaluate the valid underestimators for the terms nonlinear in $\mathbf{x}$ and $\mathbf{z}$ for the $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$ constraints, utilizing the basic principles of the deterministic global optimization algorithm $\boldsymbol{\alpha}$**BB**[1;2;3;4]. These are denoted as $g_j^c(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$. Note that these constraints are convex in $\mathbf{z}$ and $\mathbf{x}$ for every fixed $\mathbf{d}$ and $\boldsymbol{\theta}$.

Step4: Develop the underestimators for the equality and inequality constraints and calculate tight upper and lower bounds on variables that participate in nonconvex terms that will be underestimated, by solving:

$$\mathbf{x}^L / \ \mathbf{z}^L / \ \boldsymbol{\theta}^L = \min \mathbf{x} / \ \mathbf{z} / \ \boldsymbol{\theta}$$
$$\text{s.t.}$$
$$h_i^l(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0$$
$$g_j^c(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0$$

and

$$\mathbf{x}^U / \ \mathbf{z}^U / \ \boldsymbol{\theta}^U = \max \mathbf{x} / \ \mathbf{z} / \ \boldsymbol{\theta}$$
$$\text{s.t.}$$
$$h_i^l(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0$$
$$g_j^c(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0$$

and add the simple bounds thus obtained to the set of constraints.

Step 5: Considering the convexified constraints substitute the inner optimization problem with the necessary and sufficient KKT optimality conditions and construct the following single stage MI(N)LP optimization problem[5]:

Problem (P1C)

$$\chi(\mathbf{d}) = \max u$$

$$\begin{aligned}
\text{s.t.} \quad & s_j^c + g_j^c(\mathbf{d}, \mathbf{z}, \mathbf{x}, \ \boldsymbol{\theta}) - u = 0 \quad j = 1, \ldots J \\
& h_i^l(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0 \quad i = 1, \ldots I \\
& \sum_{j=1}^{J} \lambda_j^c = 1 \\
& \sum_{j=1}^{J} \lambda_j^c \frac{\partial g_j^c}{\partial \mathbf{z}} + \sum_{i=1}^{I} \mu_i^c \frac{\partial h_i^l}{\partial \mathbf{z}} = 0 \\
& \sum_{j=1}^{J} \lambda_j^c \frac{\partial g_j^c}{\partial \mathbf{x}} + \sum_{i=1}^{I} \mu_i^c \frac{\partial h_i^l}{\partial \mathbf{x}} = 0 \\
& \lambda_j^c - y_j^c \leq 0 \\
& s_j^c - U(1 - y_j^c) \leq 0 \\
& \sum_{j=1}^{J} y_j^c \leq n_z' + 1 \\
& \boldsymbol{\theta}^L \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^U \\
& \delta \geq 0, \ \ y_j^c = 0, 1, \ \ \lambda_j^c \geq 0, \ \ s_j^c \geq 0
\end{aligned}$$

where s_j^c are the slack variables of design convexified inequalities, λ_j^c are the associated Lagrange multipliers; y_j^c are the binary variables involved in the active set strategy[5] (y_j^c=1 if constraint j is active;0 otherwise) and n_z' is the number of control variables in the convexified inner problem.

Note that with the introduction of the slack variables as part of the active set procedure, all the convexified inner problem inequality constraints become equality constraints on the resulting problem. If the original inequality constraints become linear when underestimated, leave them as equality constraints. Otherwise, they need to be written as two inequalities, along with the nonlinear equality constraints that may arise from the KKT stationarity conditions. Recall that the underestimation of a univariate concave term is linear, and its negation is convex. Thus, if the resulting equality constraint is nonlinear, and needs to be written as two inequality constraints, the underestimation of univariate concave terms define an overestimation of the convex term in the negated inequality constraint. To prevent this overestimation, rewrite the negated inequality constraint in its original form, which is convex. Write other terms that are overestimated in negated form in a similar manner.

Check if the linear independence condition is satisfied at the best upper bound value obtained.

Step 6: Solve the resulting MINLP formulation to global optimality using the deterministic global optimization algorithm **SMIN-$\boldsymbol{\alpha}$BB**,[26;27] or **GMIN-$\boldsymbol{\alpha}$BB** [26;27]. Note that for cases where the resulting single level problem is an MILP, then using a local mixed integer optimization method will suffice to locate the minimum. If the obtained solution is greater than the current lower bound, LB, then update the bound LB.

Step 7: Check for convergence. If $UB - LB \leq \epsilon$, STOP, otherwise go to step 8.

Step 8: Branch on a selected control or uncertain parameter to partition the initial domain into two subdomains to be considered at the next iteration. The selection of a branching variable can be made following different branching rules. Since the aim of the branching step is the generation of problems with tighter lower bounds, the control variables, $\mathbf{z}$, that participate in nonconvex terms and the uncertain parameters, $\boldsymbol{\theta}$, are involved in the set of candidate branching variables. Alternative branching strategies can be applied to the problem, since branching strategies have a significant effect on the performance of the algorithm. Note that there are seven alternative branching strategies implemented within the **$\boldsymbol{\alpha}$BB** global optimization algorithm, as described by **?**[1;3]. Once the branching variable is selected the subdivision is performed by halving on the middle point of the longest side of the initial rectangle (bisection).

Remark: Note that since a positive value for the plant feasibility measure $\chi(\mathbf{d})$ illustrates plant infeasibility the above iterative procedure terminates if the lower bound is positive resulting in an infeasible design. Also note that negative upper bound values illustrate a feasible design within the region T and no further steps are required. The application of the above algorithmic procedure is illustrated through Example 1 in section 7.

5 Framework for the Flexibility Index

The design flexibility index problem can be reformulated to represent the determination of the largest hyperectangle that can be inscribed within the feasible region of the design[13]. Following this idea, the mathematical formulation of the flexibility index problem becomes:

$$
\begin{aligned}
& F = \min \delta \\
& \quad \text{s.t. } \psi(\mathbf{d},\boldsymbol{\theta}) = 0 \\
& \qquad \psi(\mathbf{d},\boldsymbol{\theta}) = \min_{\mathbf{z}} u \\
& \qquad h_i(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) = 0, \quad i \in I \\
& \qquad g_j(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) \leq u, \quad j \in J \\
& \qquad T(\delta) = \{\boldsymbol{\theta} | \boldsymbol{\theta}^N - \delta\Delta\boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\Delta\boldsymbol{\theta}^+\} \\
& \qquad \delta \geq 0
\end{aligned}
$$

Note that the solution of the flexibility index problem involves the evaluation of feasibility function the $\psi(\mathbf{d},\boldsymbol{\theta})$ which describes the boundary of the feasible region. The basic idea of the proposed approach for the global solution of the flexibility index problem is similar to the idea used for the solution of the feasibility test problem in section 4, that is we relax the inner feasibility function subproblem by providing valid underestimating functions of the original constraints. The resulting formulation is then solved by applying the necessary and sufficient KKT optimality conditions that transform the flexibility index problem into a single optimization problem. Upon further convexification of this problem, we generate a model that will provide a valid lower bound to the original flexibility index problem since it corresponds to the relaxation of the original minimization problem. A valid upper bound is determined through the solution of the original flexibility problem that can be obtained from the solution of the one-stage nonconvex MINLP optimization problem or by applying the active set strategy procedure[5]. The proposed approach for the flexibility index problem involves the following steps as illustrated in Figure 3.

Step 1: Consider the whole uncertainty space. Set the lower bound LB = - ∞, K=1 and select a tolerance ϵ.

Step 2: Based on the same ideas as for the feasibility test problem, Grossmann and Floudas[5], presented the following single stage MINLP optimization problem for the flexibility index problem:

Problem (P2)

$$\mathrm{F}(d) = \min \delta$$

$$\begin{aligned}
\text{s.t. } & g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) + s_j = 0 \quad j = 1, ..., J \\
& h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0 \quad i = 1, ..., I \\
& \sum_{j=1}^{J} \lambda_j = 1 \\
& \sum_{j=1}^{J} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} + \sum_{i=1}^{I} \mu_i \frac{\partial h_i}{\partial \mathbf{z}} = 0 \\
& \sum_{j=1}^{J} \lambda_j \frac{\partial g_j}{\partial \mathbf{x}} + \sum_{i=1}^{I} \mu_i \frac{\partial h_i}{\partial \mathbf{x}} = 0 \\
& \lambda_j - y_j \leq 0 \\
& s_j - U(1 - y_j) \leq 0 \\
& \sum_{j=1}^{J} y_j \leq n_z + 1 \\
& \boldsymbol{\theta}^N - \delta \Delta \boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta \Delta \boldsymbol{\theta}^+ \\
& \delta \geq 0, \quad y_j = 0, 1, \quad \lambda_j, \quad s_j \geq 0
\end{aligned}$$

where s_j are the slack variables of design inequalities, λ_j are the associated Lagrange multipliers; y_j are 0,1 variables (y_j=1 if constraint j is active; 0 otherwise).

Solve the resulting problem using a local MINLP optimizer (e.g., DICOPT[24], MINOPT[25]). Set the upper bound UB equal to the best obtained solution.

Step 3: Rewrite the nonlinear $h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$ constraints as two inequality constraints and add them to the set of $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$. Denote the remaining linear ones as $h_i^l(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$. Determine the valid underestimators of the constraints $g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$ for terms nonlinear in $\mathbf{x}$ and $\mathbf{z}$, utilizing the basic principles of the deterministic global optimization algorithm $\boldsymbol{\alpha}$**BB**[1;2;3;4] and denote as $g_j^c(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta})$.

Step 4: Establish tight upper and lower bounds on variables that participate in nonconvex terms as described in Step 4 of feasibility test algorithm.

Step 5: Based on the convexified constraints substitute the inner optimization problem by the necessary and sufficient KKT optimality conditions. This results in:

Problem (P2C)

$$
\begin{aligned}
&\mathrm{F}(d) = \min \delta \\
&\quad s.t.\ \ g_j^c(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) + s_j = 0 \ \ j = 1,...,J \\
&\qquad h_i^l(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) = 0 \ \ i = 1,...,I \\
&\qquad \sum_{j=1}^{J} \lambda_j^c = 1 \\
&\qquad \sum_{j=1}^{J} \lambda_j^c \frac{\partial g_j^c}{\partial \mathbf{z}} + \sum_{i=1}^{I} \mu_i^c \frac{\partial h_i^l}{\partial \mathbf{z}} = 0 \\
&\qquad \sum_{j=1}^{J} \lambda_j^c \frac{\partial g_j^c}{\partial \mathbf{x}} + \sum_{i=1}^{I} \mu_i \frac{\partial h_i^l}{\partial \mathbf{x}} = 0 \\
&\qquad \lambda_j^c - y_j^c \leq 0 \\
&\qquad s_j^c - U(1 - y_j^c) \leq 0 \\
&\qquad \sum_{j=1}^{J} y_j^c \leq n_z' + 1 \\
&\qquad \boldsymbol{\theta}^N - \delta\Delta\ \boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\Delta\boldsymbol{\theta}^+ \\
&\qquad \delta \geq 0,\ \ y_j^c = 0,1,\ \ \lambda_j^c,\ \ s_j^c \geq 0
\end{aligned}
$$

where s_j^c are the slack variables of the convexified design inequalities, λ_j^c are the associated Lagrange multipliers; y_j^c are the binary variables (y_j^c=1 if constraint j is active; 0 otherwise); n_z' is the number of control variables in the convexified inner problem. Rewrite the nonlinear equality constraints as in Step 5, Section 4. Check if the linear independence condition is satisfied at the best upper bound value obtained.

Step 6: Solve the resulting MINLP formulation to global optimality using the deterministic global optimization algorithm **SMIN-αBB**[26;27] , or **GMIN-αBB** [26;27]. If the obtained solution is greater than the current LB, update the LB.

Step 7: Check for convergence. If $UB - LB \leq \epsilon$, STOP, otherwise go to step 8.

Step 8: Apply one of the branching criteria to partition the initial domain into two subrectangles to be considered at the next iteration (see also Step 8 of Section 4).

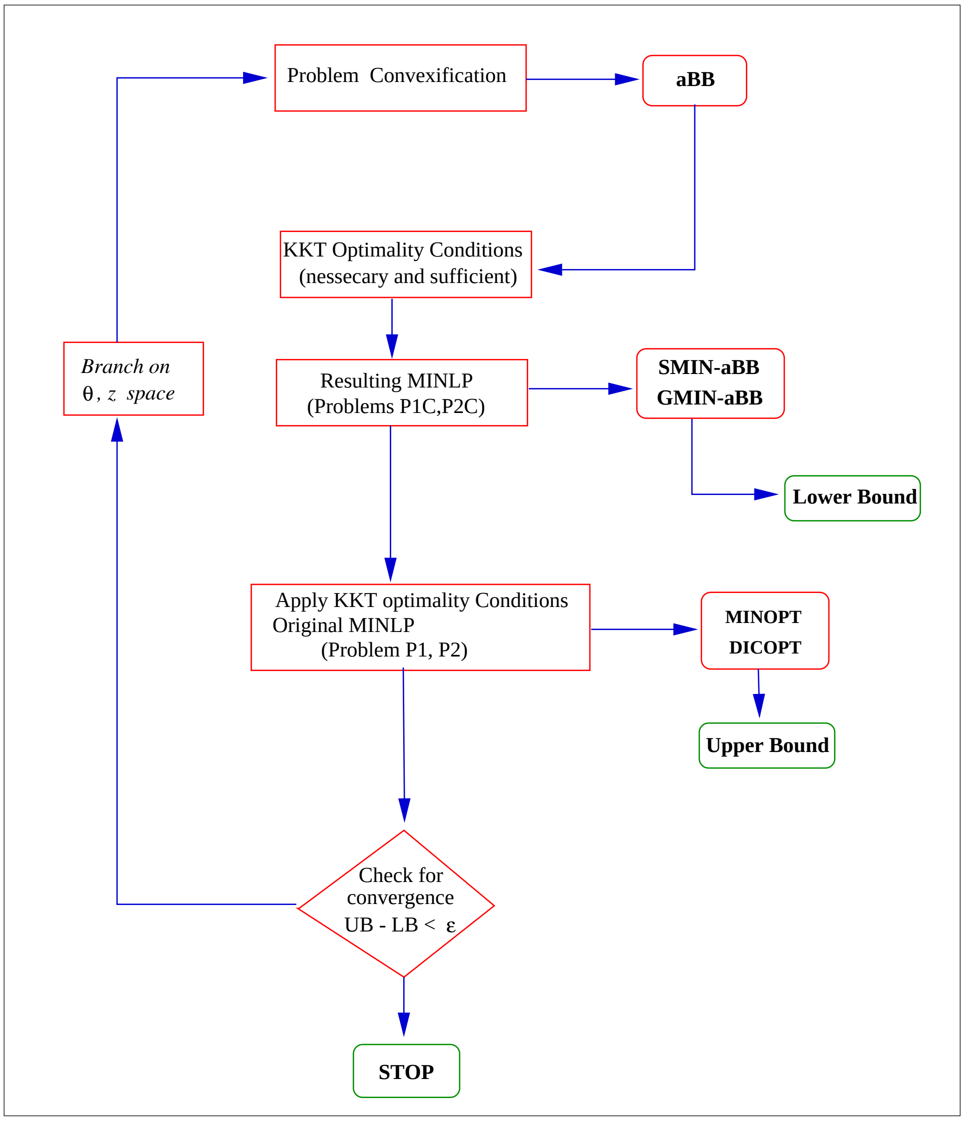

Figure 3: Framework for the Feasibility Test and Flexibility Index Problem

6 Modified Algorithm for Monotonic Functions in z

For problems where we eliminate the variables $\mathbf{x}$ using the equality constraints, and the constraint functions $g_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}), j \in J$ are monotonic in the control variables $\mathbf{z}$, $\forall\ \theta$, it is very convenient to decompose the MINLP problem of section 4 into a set of NLP subproblems by applying a modified version of the active set strategy of Grossmann and Floudas[5]. The strategy is based on determining the potential sets of active constraints from the stationarity conditions, by using the Property *1*[5] and the complementarity conditions. Property *1*[5],

$$\sum_{j \in J} y_j \leq n_z + 1,$$

enforces that the potential sets of active constraints are of rank $n_z + 1$, provided that the constraints are independent, or strictly less, if the linear independence condition is not satisfied. On the other hand the complementarity constraint,

$$\lambda_j - y_j \leq 0$$

enforces that the constraint j is active, if $\lambda_j > 0$. Thus, the potential sets of different $n_z + 1$ active constraints are the ones that satisfy the stationarity conditions:

$$\sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} = 0,$$

where $\partial g_j / \partial \mathbf{z}$ are all one-signed for monotonic g_j, and $\lambda_j \geq 0$, $\forall j \in J$ by definition and the state variables are eliminated.

After the active sets are identified, two different approaches can be taken to solve the resulting NLPs: (1) Each nonconvex NLP corresponding to different active sets can be solved to global optimality by using the $\boldsymbol{\alpha}$**BB**[1;2;3;4] global optimization procedure. The global minimum is smallest value that is obtained from the solution of different active sets; (2) The framework for the feasibility test and flexibility index problems can be applied for the resulting set of NLP subproblems in a modified form. For the feasibility test problem, the framework steps are modified as follows: In Step 2, each NLP subproblem is solved to local optimality by using a local optimizer (e.g., MINOS, NPSOL). The solution of the NLP subproblem with the lowest objective value is taken as the upper bound on the feasibility problem. In Step 5, each convexified NLP subproblem is solved by using a local optimizer (e.g., MINOS, NPSOL). The convexified NLP active set combination with the smallest objective function value yields the lower bound. The branching and bounding steps remain the same. By successive underestimation and branching, the ϵ-global optimum is obtained. The framework for the flexibility index problem is modified in a similar manner.

7 Computational Studies

In this section, five examples are considered to illustrate the applicability of the proposed approach for the determination of the global optimum for both the feasibility test and flexibility index optimization problems involving nonconvex constraints. Example 1 considers a heat exchanger network and is used to illustrate the steps of the proposed approaches for the feasibility test and the flexibility index problems. Example 2, involves a pump network as described by Swaney and Grossmann [13] and considers two uncertain parameters. Design flexibility is determined for the existing design and feasibility test is performed for an alternative design in order to illustrate the capability and effectiveness of the proposed approach. Example 3, features the same pump network as example 2 but considers five uncertain parameters which results in a more complicated form of the nonconvex constraints. Plant flexibility is also evaluated for this case. Example 4, considers the reactor-heat exchanger network used by Pistikopoulos and Grossmann [28] in order to illustrate the capability of the proposed approach to handle general nonconvex constraints. Finally, example 5 examines the design feasibility and determines the design flexibility for the chemical process flowsheet described by Ostrovsky et al. [10], using the modified active set strategy.

7.1 Example 1

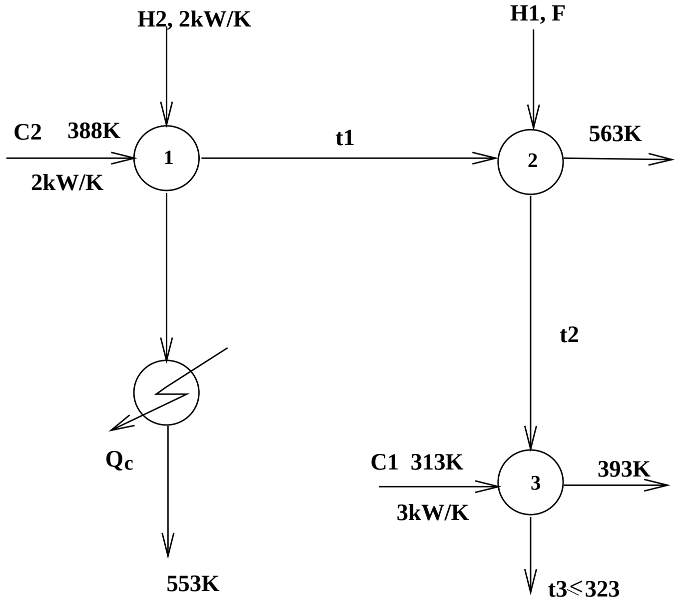

Figure 4: Heat Exchanger network for Example 1

The heat exchanger network given in Grossmann and Floudas [5] is considered here as shown in Figure 4. The uncertain parameter is the heat flowrate of stream H1 which has a nominal value of 1 kW/K and an expected deviation of +0.8 kW/K. The following inequalities determine the feasible operation of this network as they are formulated after the elimination of the state variables. The feasible region of the network is illustrated in Figure 5. Note that the feasible region consists of the two disconnected domains which are highlighted in black.

$$g_1 = -25F_{H1} + Q_c - 0.5Q_cF_{H1} + 10 \leq 0$$
$$g_2 = -190F_{H1} + Q_c + 10 \leq 0$$
$$g_3 = -270F_{H1} + Q_c + 250 \leq 0$$
$$g_4 = 260F_{H1} - Q_c - 250 \leq 0$$

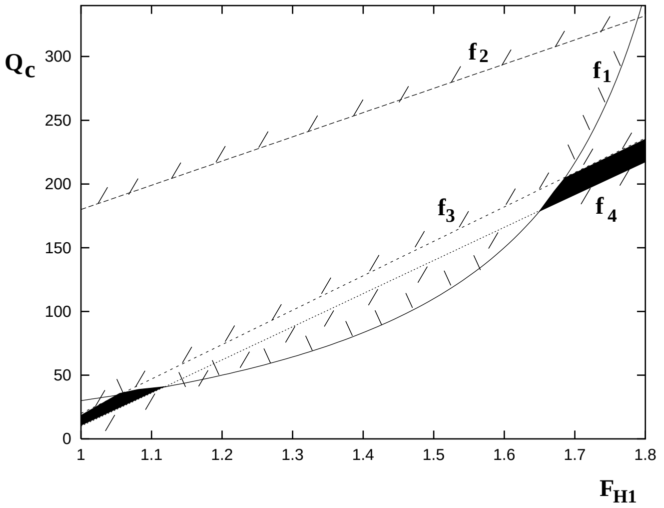

Figure 5: Feasible region Example 1

First the feasibility test problem is solved following the approach proposed in section 4. Considering this set of linear constraints in the whole uncertainty space, first $LB = -\infty$, $K = 1$ are set. However, the inner problem defined by the constraints $g_1 - g_4$ is linear at fixed outer parameter value F_{H1}. Thus, no underestimation is required, and the inner problem is equivalent to its KKT optimality conditions. Then, in Step 2, the inner optimization problem of the original feasibility test problem is substituted by the necessary and sufficient KKT optimality conditions, and is formulated as in (P1). The resulting single level optimization problem becomes:

$$
\begin{aligned}
&\chi(d) = \max u \\
&\qquad g_1 : -25F_{H1} + Q_c - 0.5Q_cF_{H1} + 10 + s_1 - u = 0 \\
&\qquad g_2 : -190F_{H1} + Q_c + 10 + s_2 - u = 0 \\
&\qquad g_3 : -270F_{H1} + Q_c + 250 + s_3 - u = 0 \\
&\qquad g_4 : 260F_{H1} - Q_c - 250 + s_4 - u = 0 \\
&\qquad \sum_{j=1}^{4} \lambda_j = 1 \\
&\qquad \lambda_1 - 0.5F_{H1}\lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 = 0 \\
&\qquad \lambda_j - y_j \leq 0 \;\; j = 1, ..., 4 \\
&\qquad s_j - U(1 - y_j) \leq 0 \;\; j = 1, ..., 4 \\
&\qquad \sum_{j=1}^{4} y_j \leq 2 \\
&\qquad F_{H1}^N - \delta\Delta F_{H1}^- \leq F_{H1} \leq F_{H1}^N + \delta\Delta F_{H1}^+ \\
&\qquad \delta \geq 0, \;\; y_j = 0, 1, \;\; \lambda_j, \;\; s_j \geq 0, \; j = 1, ..., 4
\end{aligned}
$$

which is nonlinear and nonconvex due to the bilinear term Q_cF_{H1} in constraint g_1 and the bilinear term $F_{H1}\lambda_1$ in the gradient KKT constraint. The nonconvex MINLP is solved using the deterministic global optimization procedure, **SMIN-$\boldsymbol{\alpha}$BB**[26;27], resulting in 7.07724, in 21 iterations and 8.570 CPUs. This result suggests that the network is not feasible within the whole range of uncertainty, $F_{H1} \in (1, 1.8)$, and no further steps are required. Note that the **SMIN-$\boldsymbol{\alpha}$BB**[26;27] algorithm does not have to be solved to completion for the solution of this problem, as the iteration can be terminated when the lower bound on the objective function value corresponds to the lower bound of network feasibility $\chi(\mathbf{d})$, 0, as shown in section 4.

The plant flexibility is then determined using the approach proposed in section 5. After setting the LB and optimality tolerance, the inner feasibility problem is substituted by the necessary and sufficient KKT optimality conditions.

$$
\begin{aligned}
F = \min \delta & \\
s.t. \quad & g_1 : -25F_{H1} + Q_c + 10 - 0.5Q_cF_{H1} + s_1 = 0 \\
& g_2 : -190F_{H1} + 10 + Q_c + s_2 = 0 \\
& g_3 : -270F_{H1} + 250 + Q_c + s_3 = 0 \\
& g_4 : 260F_{H1} - 250 - Q_c + s_4 = 0 \\
& \sum_{j=1}^{4} \lambda_j = 1 \\
& -0.5F_{H1}\lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 = 0 \\
& \lambda_j - y_j \leq 0 \;\; j = 1, ..., 4 \\
& s_j - U(1 - y_j) \leq 0 \;\; j = 1, ..., 4 \\
& \sum_{j=1}^{4} y_j \leq 2 \\
& F_{H1}^N - \delta \Delta F_{H1}^- \leq F_{H1} \leq F_{H1}^N + \delta \Delta F_{H1}^+ \\
& \delta \geq 0, \;\; y_j = 0, 1, \;\; \lambda_j, \;\; s_j \geq 0, \; j = 1, ..., 4
\end{aligned}
$$

Note that this formulation corresponds to a nonlinear nonconvex MINLP, as described in the solution of the feasibility problem. The resulting nonconvex MINLP problem is solved using the deterministic global optimization procedure **SMIN-αBB**[26;27]. The solution provides the heat exchanger network flexibility index of 0.148, in 1 **SMIN-αBB** iteration and 1.080 CPUs.

7.2 Example 2

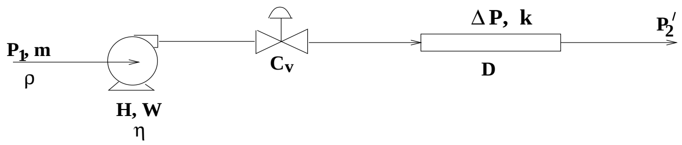

Figure 6: Pump and pipe run of Example 2

The example problem studied by Swaney and Grossmann[13], is considered. It involves a centrifugal pump as shown in Figure 6 which transports liquid at a flowrate m from its source at $100kPa$ pressure P_1 through a pipe to its destination at pressure P_2'. The design variables are the pipe diameter D, the pump head H, the driver power W and the control valve size C_v^{max}. The existing design corresponds to the values shown in Table I.

Design	$D(m)$	$H(kj/kg)$	$W(KW)$	C_v^{max}
d_{ex}	0.0762	1.3	31.2	0.0577
d_1	0.07643	1.405	33.74	0.0934

Table I: Design Variables

The control variable is the valve coefficient C_v. In this example, the flowrate m and the pressure P_2' are considered as uncertain parameters with nominal values of 10 kg/s and 800 KPa, respectively, and positive and negative deviations of +200, -550 KPa and +2, -5 kg/s, respectively. After the elimination of the state variables, the pump operation is described by the following set of inequality constraints:

$$
\begin{aligned}
g_1 = P_1 + \rho H - \epsilon - \frac{m^2}{\rho C_v^2} - km^{1.84} D^{-5.16} - P_2 &\leq 0 \\
g_2 = -P_1 - \rho H - \epsilon + \frac{m^2}{\rho C_v^2} + km^{1.84} D^{-5.16} + P_2 &\leq 0 \\
g_3 = mH - \eta W &\leq 0 \\
g_4 = C_v - C_v^{max} &\leq 0 \\
g_5 = -C_v + rC_v^{max} &\leq 0
\end{aligned}
$$

where $r = 0.05$ is the control valve range and $\epsilon = 20KPa$ is a tolerance for the delivery pressure. Also, $\eta = 0.5, \rho = 1000kg/s$ and $k = 9.101\text{x}10^{-6} kPa(kg/s)^{-1.84} m^{5.16}$. The approach proposed in section 5 is applied here for the evaluation of the global solution of the flexibility index problem for the existing design. Moreover, considering an additional alternative flexible design, the feasibility test was also performed.

First, the following single stage MINLP problem that corresponds to the substitution of the inner level KKT optimality conditions is formulated.

$$
F = \min \delta
$$

$$
\begin{aligned}
s.t. \quad & g_1 = P_1 + \rho H - \epsilon - \frac{w^2}{\rho} - km^{1.84} D^{-5.16} - P_2 + s1 = 0 \\
& g_2 : -P_1 - \rho H - \epsilon + \frac{w^2}{\rho} + km^{1.84} D^{-5.16} + P_2 + s2 = 0 \\
& g_3 : mH - \eta W + s3 = 0 \\
& g_4 : C_v - C_v^{max} + s4 = 0 \\
& g_5 : -C_v + rC_v^{max} + s5 = 0
\end{aligned}
$$

$$h_1 = m - wC_v = 0$$
$$\sum_{j=1}^{5} \lambda_j = 1$$
$$\lambda_4 - \lambda_5 - w\mu = 0$$
$$-\frac{2}{\rho} w\lambda_1 + \frac{2}{\rho} w\lambda_2 - C_v\mu = 0$$
$$\lambda_j - y_j \leq 0 \quad j = 1, ..., 5$$
$$s_j - U(1 - y_j) \leq 0 \quad j = 1, ..., 5$$
$$\sum_{j=1}^{5} y_j \leq 2$$
$$m^N - \delta\Delta m^- \leq m \leq m^N + \delta\Delta m^+$$
$$P_2^N - \delta\Delta P_2^- \leq P_2 \leq P_2^N + \delta\Delta P_2^+$$
$$\delta \geq 0, \quad y_j = 0, 1, \quad \lambda_j, \quad s_j \geq 0, \ j = 1, ..., 5$$

where $w = \frac{m}{C_v}$ artificially introduced variable to simplify the model representation. This MINLP problem is nonconvex due to the nonlinear equality constraints and the bilinear term in the KKT gradient conditions. The solution of this problem using MINOPT[25] provides an upper bound of 0.618 to the flexibility index problem, in 0.1 CPUs.

In step 3, the principles of the $\boldsymbol{\alpha}$**BB** global optimization algorithm are used to formulate the convexified form of the original problem. Note, that in the original formulation constraint g_1 involves a sum of two univariate concave terms:

$$-w^2$$
$$-D^{-5.16} * 9.101 * 10^{-3} * m^{1.84}$$

and has the following linear underestimating function:

$$-1.18564 * w - 59.1618 * m - 350.32 \tag{1}$$

within the bounds of the variables w, m:

$$5/C_v^{max} \leq w \leq 12/(0.05 * C_v^{max})$$
$$5 \leq m \leq 12.$$

Also constraint g_6 is nonconvex due to its bilinear terms $w * C_v$ that can be underestimated using the[22] linear cuts. Considering the KKT optimality conditions for the convexified problem in step 5 the following MINLP problem is formulated.

$$
\begin{aligned}
&F = \min \delta \\
&\quad s.t. \quad g_1^c : -P_2 - 1.18564w - 59.1618m + 1730.32 + s_1 = 0 \\
&\qquad\qquad g_2 : P_2 + 0.001w^2 + 5.348m^{1.84} - 1420 + s_2 = 0 \\
&\qquad\qquad g_3 : 1.3m - 15.6 + s_3 = 0 \\
&\qquad\qquad g_4 : C_v - 0.0577 + s_4 = 0 \\
&\qquad\qquad g_5 : -C_v + 0.002885 + s_5 = 0 \\
&\qquad\qquad h_1 = m - xx4 = 0 \\
&\qquad\qquad g_6 : 152.849C_v + 0.00484126w - xx4 - 0.739981 + s_6 = 0 \\
&\qquad\qquad g_7 : 1032.79C_v + 0.0577w - xx4 - 59.5919 + s_7 = 0 \\
&\qquad\qquad g_8 : -152.849C_v - 0.0577w + xx4 + 8.81937 + s_8 = 0 \\
&\qquad\qquad g_9 : -1032.79C_v - 0.00484126w + xx4 + 5 + s_9 = 0 \\
&\qquad\qquad \sum_{j=1}^{9} \lambda_j = 1 \\
&\qquad\qquad \lambda_4 - \lambda_5 + 152.849\lambda_6 + 1032.79\lambda_7 - 152.849\lambda_8 - 1032.79\lambda_9 = 0 \\
&\qquad\qquad -1.18564\lambda_1 + 0.00484126\lambda_6 + 0.0577\lambda_7 - 0.0577\lambda_8 - 0.00484126\lambda_9 \\
&\qquad\qquad +0.002w\lambda_2 = 0 \\
&\qquad\qquad \mu - \lambda_6 - \lambda_7 + \lambda_8 + \lambda_9 = 0 \\
&\qquad\qquad \lambda_j - y_j \le 0 \;\; j = 1, ..., 9 \\
&\qquad\qquad s_j - U(1 - y_j) \le 0 \;\; j = 1, ..., 9 \\
&\qquad\qquad \sum_{j=1}^{9} y_j \le 3 \\
&\qquad\qquad m^N - \delta\Delta m^- \le m \le m^N + \delta\Delta m^+ \\
&\qquad\qquad P_2^N - \delta\Delta P_2^- \le P_2 \le P_2^N + \delta\Delta P_2^+ \\
&\qquad\qquad \delta \ge 0, \;\; y_j = 0, 1, \;\; \lambda_j, \;\; s_j \ge 0, \; j = 1, ..., 9
\end{aligned}
$$

Note that the above formulation corresponds to a nonconvex MINLP problem since it involves equalities with bilinear terms generated by the substitution of the inner feasibility function problem by the corresponding KKT gradient optimality conditions. The **SMIN-$\boldsymbol{\alpha}$BB**[26;27] is used for the solution of this problem resulting in a lower bound of 0.618 obtained in only one iteration, that is equal to the upper bound, in 6.84 CPUs.

An alternative design d_1 with the values of the design variables shown in Table I, is also tested for feasibility utilizing the approach proposed in section 4. First the MINLP problem (P1) is formulated by considering the KKT optimality conditions of the inner feasibility function problem.

$$
\begin{aligned}
\chi(d) = \max u & \\
s.t. \quad & g_1 : P_1 + \rho H - \epsilon - \frac{w^2}{\rho} - k m^{1.84} D^{-5.16} - P_2 + s1 - u = 0 \\
& g_2 : -P_1 - \rho H - \epsilon + \frac{w^2}{\rho} + k m^{1.84} D^{-5.16} + P_2 + s2 - u = 0 \\
& g_3 : mH - \eta W + s3 - u = 0 \\
& g_4 : C_v - C_v^{max} + s4 - u = 0 \\
& g_5 : -C_v + r C_v^{max} + s5 - u = 0 \\
& h_1 = m - w C_v = 0 \\
& \sum_{j=1}^{5} \lambda_j = 1 \\
& \lambda_4 - \lambda_5 - w\mu = 0 \\
& -\frac{1}{\rho} w \lambda_1 + \frac{1}{\rho} w \lambda_2 - C_v \mu = 0 \\
& \lambda_j - y_j \leq 0 \;\; j = 1, ..., 5 \\
& s_j - U(1 - y_j) \leq 0 \;\; j = 1, ..., 5 \\
& \sum_{j=1}^{5} y_j \leq 2 \\
& m^L \leq m \leq m^U \\
& P_2^L \leq P_2 \leq P_2^U \\
& y_j = 0, 1, \;\; \lambda_j, \;\; s_j \geq 0, \; j = 1, ..., 5
\end{aligned}
$$

The resulting nonconvex MINLP problem is solved using the MINOPT[25] local MINLP solver that results in $\chi(\mathbf{d}) = 0.0$, in 0.11 CPUs that corresponds to an upper bound to the original feasibility test problem. This result suggests that no further steps are required in order to test design feasibility since $\chi(\mathbf{d})$ should be less than 0.0 which means that this design is feasible in the region under consideration, $5 \leq m \leq 12$, $250 \leq P_2' \leq 1000$.

7.3 Example 3

In this example the same pump and pipe network is considered assuming that all the parameters m, P_2, η, k, ρ, are uncertain with the expected deviations as shown in Table II, and

Parameter	$P_2(kPa)$	$m(kg/s)$	η	$k(kPa)((kg/s)^{-1.84})(m^{5.16})$	$\rho(kg/m^3)$
Nominal Value	800	10	0.5	9.101×10^{-6}	1000
Positive Deviation	200	2	0.05	0.45505×10^{-6}	50
Negative Deviation	500	5	0.05	0.45505×10^{-6}	50

Table II: Uncertain Parameters - Example 3

the known parameters are as follows: $\epsilon = 20kPa, r = 0.05, W = 31.2kW, H = 1.3kJ/kg, D = 0.0762m, cv^{max} = 0.039673$.

Note that the introduction of additional uncertain parameters results in increasing complexity since k, m and ρ become variables. In order to exploit further the mathematical structure of this problem, the following exponential transformation is adopted.

$$m = \exp(m'), \rho = \exp(\rho'), C_v = \exp(C_v'), k = \exp(k')$$

where m', ρ', C_v', k' are the new transformed variables.

Following this transformation the mathematical description of the problem has the following form:

$$\begin{aligned} g_1 = 1.3\exp(\rho') - \exp(2m' - \rho' - 2C_v') - 0.587641\exp(k' + 1.84m') - P_2 \leq -80 \\ g_2 = -1.3\exp(\rho') + \exp(2m' - \rho' - 2C_v') + 0.587641\exp(k' + 1.84m') + P_2 \leq 120 \\ g_3 = 1.3\exp(m') - 31.2\eta \leq 0 \\ g_4 = \exp(C_v') - 0.039673 \leq 0 \\ g_5 = -\exp(C_v') + (0.05 * 0.039673) \leq 0 \end{aligned}$$

Note that by employing the above exponential transformation the resulting mathematical model involves convex and univariate concave terms, for which linear underestimators exist. Further, the constraints g_4 and g_5 basically define the bounds on cv' and can be simply rewritten as:

$$\begin{aligned} g_4 = Cv' - \ln(0.039673) \leq 0 \\ g_5 = -Cv' + \ln(0.05 * 0.039673) \leq 0 \end{aligned}$$

reducing the number of nonlinear constraints. First, the original nonconvex inner feasibility function problem is substituted by the corresponding KKT optimality conditions leading to the following single nonconvex MINLP optimization problem.

$$
\begin{aligned}
F = \min \delta & \\
s.t. \quad & g_1 : 1.3 \exp(\rho') - P_2 - \exp(2m' - \rho' - 2C_v') \\
& \qquad -0.587641 \exp(k' + 1.84m') + 80 + s_1 = 0 \\
& g_2 : -1.3 \exp(\rho') + P_2 + \exp(2m' - \rho' - 2C_v') \\
& \qquad +0.587641 \exp(k' + 1.84m') - 120 + s_2 = 0 \\
& g_3 : 1.3 \exp(m') - 31.2\eta \leq 0 \\
& g_4 : C_v' - \ln(0.039673) + s_3 = 0 \\
& g_5 : -C_v' + \ln(0.05 * 0.039673) + s_4 = 0 \\
& \sum_{j=1}^{4} \lambda_j = 1 \\
& 2 \exp(2m' - \rho' - 2C_v')\lambda_1 - 2 \exp(2m' - \rho' - 2C_v')\lambda_2 \\
& \qquad +\lambda_3 - \lambda_4 = 0 \\
& \sum_{j=1}^{4} y_j \leq 2
\end{aligned}
$$

$$
\begin{array}{lclcl}
\lambda_j - y_j & \leq & 0, & & j = 1, ..., 4 \\
s_j - U(1 - y_j) & \leq & 0, & & j = 1, ..., 4 \\
{m'}^N - \delta \Delta {m'}^- & \leq & \exp(m') & \leq & {m'}^N + \delta \Delta {m'}^+ \\
P_2^N - \delta \Delta P_2^- & \leq & P_2 & \leq & P_2^N + \delta \Delta P_2^+ \\
{k'}^N - \delta \Delta {k'}^- & \leq & \exp(k') & \leq & {k'}^N + \delta \Delta {k'}^+ \\
{\rho'}^N - \delta \Delta {\rho'}^- & \leq & \exp(\rho') & \leq & {\rho'}^N + \delta \Delta {\rho'}^+ \\
\eta^N - \delta \Delta \eta^- & \leq & \eta & \leq & \eta^N + \delta \Delta \eta^+
\end{array}
$$

$$
\delta \geq 0, \quad y_j = \{0, 1\}, \quad \lambda_j, \quad s_j \geq 0, \; j = 1, ..., 4
$$

Note that the constraint g_4 is only a function of the uncertain parameters, thus does not participate in the KKT transformation. The solution of the above nonconvex MINLP problem using the MINOPT[25] local MINLP minimizer is found to be 0.407, in 0.52 CPUs, which corresponds to an upper bound of the design flexibility index. Then the problem is convexified using the basic principles of the $\boldsymbol{\alpha}$**BB**[1;2;3;4], global optimization algorithm. First the following transformation is performed:

$x = 2m' - \rho' - 2C_v'$, $y = k' + 1.84m'$.

This results in the constraints g_1 and g_2 having the form:

$$g_1 = 1.3\exp(\rho') - P_2 - \exp(x) - 0.587641\exp(y) + 80 \leq 0$$
$$g_2 = -1.3\exp(\rho') + P_2 + \exp(x) + 0.587641\exp(y) - 120 \leq 0$$

which involve the univariate concave terms $-\exp(x)$, $-0.587641\exp(y)$ and $-1.3\exp(\rho')$. Notice that the latter two terms only involve outer problem variables and therefore do not have to be underestimated for the KKT conditions to be both necessary and sufficient. However, the first term involves an inner problem variable, and has to be underestimated through a linear function. Considering the KKT conditions of the inner convexified problem results in the following MINLP which involves nonconvexities only due to KKT optimality conditions.

$$
\begin{aligned}
F = \min \delta & \\
\text{s.t.} \quad & g_1 : 1.3\exp(\rho') - P_2 + \frac{(-\exp(x^U) + \exp(x^L))}{(x^U - x^L)}(x - x^L) \\
& \quad - \exp(x_L) - 0.587641\exp(y) + 80 + s_1 \leq 0 \\
& -g_1 : -1.3\exp(\rho') + P_2 + \exp(x) + 0.587641 * \exp(y) - 80 - s_1 \leq 0 \\
& g_2 : \exp(x) + 0.587641\exp(y) - 1.3 * \exp(\rho) + P_2 - 120 + s_2 \leq 0 \\
& -g_2 : -exp(x) - 0.587641\exp(y) + 1.3 * \exp(\rho) - P_2 + 120 - s_2 \leq 0 \\
& g_3 : 1.3\exp(m') - 31.2\eta \leq 0 \\
& g_4 : C'_v - ln(0.039673) + s_3 = 0 \\
& g_5 : -C'_v - ln(0.05 * 0.039673) + s_4 = 0 \\
& h_1 : -x + 2m' - \rho' - 2C'_v = 0 \\
& h_2 : -y + k' + 1.84m' = 0 \\
& \sum_{j=1}^{4} \lambda_j = 1 \\
& \lambda_3 - \lambda_4 - 2\mu_1 = 0 \\
& \frac{(-\exp(x^U) + \exp(x^L))}{(x^U - x^L)}\lambda_1 - (\exp(x))\lambda_2 - \mu_1 = 0 \\
& \sum_{j=1}^{4} y_j \leq 2
\end{aligned}
$$

$$\begin{array}{lllll}
\lambda_j - y_j & \leq & 0, & & j = 1, ..., 4 \\
s_j - U(1-y_j) & \leq & 0, & & j = 1, ..., 4 \\
m^N - \delta\Delta m^- & \leq & \exp(m') & \leq & m^N + \delta\Delta m^+ \\
P_2^N - \delta\Delta P_2^- & \leq & P_2 & \leq & P_2^N + \delta\Delta P_2^+ \\
k^N - \delta\Delta k^- & \leq & \exp(k') & \leq & k^N + \delta\Delta k^+ \\
\rho^N - \delta\Delta\rho^- & \leq & \exp(\rho') & \leq & \rho^N + \delta\Delta\rho^+ \\
\eta^N - \delta\Delta\eta^- & \leq & \eta & \leq & \eta^N + \delta\Delta\eta^+
\end{array}$$

$$\delta \geq 0, \quad y_j = 0, 1, \quad \lambda_j, \quad s_j \geq 0, \ j = 1, .., 4$$

where as defined by constraints h_1, h_2, $x = 2m' - \rho' - 2C_v'$, $y = k' + 1.84m'$. Note that the above formulation involves convex, univariate concave and nonconvex terms of the form $x\exp(y)$. For these terms exact values of $\boldsymbol{\alpha}$ can be calculated exactly[29] and incorporated in the $\boldsymbol{\alpha}$**BB** global optimization algorithmic procedure in order to construct tight underestimating functions. The solution of the above nonconvex MINLP using the **SMIN-**$\boldsymbol{\alpha}$**BB** global optimization algorithm [26;27], results in a lower bound of 0.407, in 82.61 CPUs. Consequently, after the first iteration the approach converges to the global optimal solution of 0.407 for the network flexibility.

7.4 Example 4

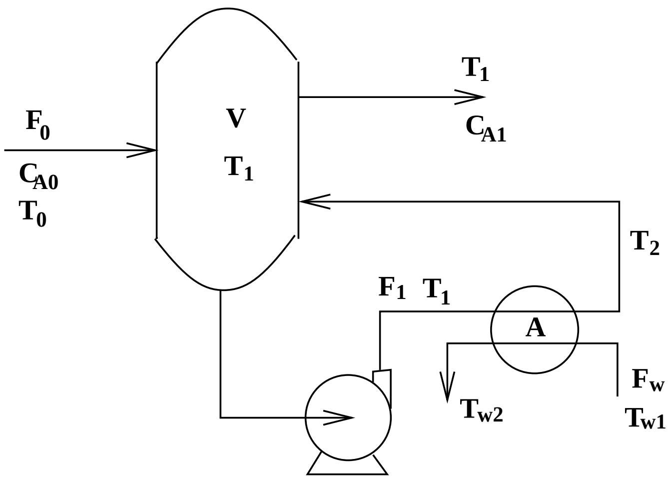

Figure 7: Reactor-Cooler system of Example 4

This example represents the flowsheet shown in Figure 7 which involves a reactor and a heat exchanger[6]. The reaction is a first-order exothermic reaction A→B. The existing design has a reactor of volume $V = 4.6m^3$ and a heat exchanger with an area of $A = 12m^2$. Two

Parameter	$F_0 (kmolh^{-1})$	$k_0(h^{-1})$
Nominal Value	45.36	12
Positive Deviation	22.68	1.2
Negative Deviation	22.68	1.2

Table III: Uncertain Parameters - Example 4

uncertain parameters are considered, the feed flowrate F_0 and the reaction rate constant k_0. The statistical data for these uncertain parameters are given in Table III.

The mathematical model of this process is[7]:

$$
\begin{aligned}
F_0(c_{A0} - c_{A1})/c_{A0} &= V k_0 \exp{(-E/RT)} c_{A1} \\
(-\Delta H) F_0 (c_{A0} - c_{A1})/c_{A0} &= F_0 c_p (T_1 - T_0) + Q_{HE} \\
Q_{HE} &= F_1 c_p (T_1 - T_2) \\
Q_{HE} &= F_w c_{pw} (T_{w2} - T_{w1}) \\
Q_{HE} &= AU \Delta T_{ln} \\
\Delta T_{ln} &= \frac{(T_1 - T_{w2}) - (T_2 - T_{w1})}{\ln{(T_1 - T_{w2})/(T_2 - T_{w1})}} \\
V^d &\geq V \\
(c_{A0} - c_{A1})/c_{A0} &\geq 0.9 \\
311 \leq T_1 &\leq 389 \\
T_1 - T_2 &\geq 0.0 \\
T_{w2} - T_{w1} &\geq 0.0 \\
T_1 - T_{w2} &\geq 11.1 \\
T_2 - T_{w1} &\geq 11.1 \\
T_0 = 333K, T_{w1} = 300K, U &= 1635 kj/(m^2 hK), \\
c_p = 167.4 kj/kmol, c_{A0} = 32.04 kmol/m^3, -\Delta H &= 23260 kJ/kmol
\end{aligned}
$$

The control variables of the system are the reactor temperature T_1, the temperature of the outlet stream after the cooler, T_2, and the outlet temperature of the cooling water, T_{w2}. Elimination of the state variables leads to the following set of inequality constraints.

$$g_1 = \frac{F_0 c_p (T_1 - T_0) + AU\Delta T_{ln}}{(-\Delta H)F_0 - F_0 c_p (T_1 - T_0) - AU\Delta T_{ln}} - \frac{c_{A0} k_0}{F_0} \exp{(-E/RT)} V^d \leq 0.0$$
$$g_2 = 0.9(-\Delta H)F_0 - F_0 c_p (T_1 - T_0) - AU\Delta T_{ln} \leq 0.0$$
$$g_3 = T_1 \leq 389$$
$$g_4 = -T_1 \leq -311$$
$$g_5 = -T_1 + T_2 \leq 0.0$$
$$g_6 = -T_{w2} + T_{w1} \leq 0.0$$
$$g_7 = -T_1 + T_{w2} \leq -11.1$$
$$g_8 = -T_2 + T_{w1} \leq -11.1$$

Note that the functions are monotonic in control variables. Based on the modified active set strategy[5], the following active set of constraints have been identified.

Active set 1: $\{g_1, g_2, g_4, g_7\}$

Active set 2: $\{g_1, g_2, g_3, g_7\}$

Active set 3: $\{g_1, g_2, g_3, g_8\}$

Active set 4: $\{g_1, g_2, g_4, g_8\}$

Active set 5: $\{g_1, g_2, g_7, g_8\}$

Active set 6: $\{g_1, g_3, g_7, g_8\}$

Active sets 1 and 4 lead to infeasible subproblems since for active set 1, $T_1 = 311, T_{w2} = 299.9$ that results in $T_2 \geq 311.1, T_2 \leq 311$, and for active set 4, $T_1 = 311, T_2 = 311.1$, which contradicts constraint g_5. However, active sets 2, 3, 5 and 6 correspond to nonconvex NLPs. For this case either one of the modified methods of Section 6 can be applied. In this section both alternatives are employed and a comparison of results is provided.

First, the different NLPs are solved using $\boldsymbol{\alpha}$**BB**[1;2;3;4] global optimization algorithm.

Active Set 2

$$g_3 = 0 \Rightarrow T_1 = 389$$
$$g_7 = 0 \Rightarrow T_{w2} = 377.9$$

The set of nonlinear equalities $g_1 = 0, g_2 = 0$ is then solved using $\boldsymbol{\alpha}$**BB** leading to flexibility value of $F_2 = 0.064$, in 0.01 CPUs.
Active Set 3

$$g_3 = 0 \Rightarrow T_1 = 389$$
$$g_8 = 0 \Rightarrow T_2 = 311.1$$

Again in this case the remaining set of nonlinear equalities $g_1 = 0, g_2 = 0$ is then solved using $\boldsymbol{\alpha}$**BB** leading to flexibility value of $F_3 = 0.064$, in 0.02 CPUs.
Active Set 5

$$g_7 = 0 \Rightarrow T_{w2} = T_1 - 11.1$$
$$g_8 = 0 \Rightarrow T_2 = 311.1$$

The set of nonlinear equalities $g_7 = 0, f_1 = 0, f_2 = 0$ is then solved using $\boldsymbol{\alpha}$**BB** leading to flexibility value of $F_5 = 6.001$, in 0.04 CPUs.
Active Set 6

$$g_3 = 0 \Rightarrow T_1 = 389$$
$$g_7 = 0 \Rightarrow T_{w2} = 377.9$$
$$g_8 = 0 \Rightarrow T_2 = 311.1$$

From the solution of the nonlinear equality $g_1 = 0$ using $\boldsymbol{\alpha}$**BB** a flexibility value of $F_6 = 1.25$ is obtained, in 0.02 CPUs. Since F corresponds to the smallest value from the values obtained from the different active sets, $F = 0.064$.

Then, the second proposed approach of section 6 is applied. Following this approach the local solution of different NLPs result in an upper bound of 0.064, whereas the convexified problems yield a lower bound of 0.0207. At the second iteration branching is performed by bisecting the range of uncertain parameters $22.68 \leq F_0 \leq 68.04$, $10.8 \leq k_0 \leq 13.2$. In this iteration considering the bisection of F_0 range, the upper bound does not change whereas the lower bound increases to 0.064 which is the global solution to flexibility problem. Note that following the second procedure the global solution is obtained at the second iteration and requires the local solution of four nonconvex and four convexified constraints at each iteration. On the other hand, the first approach requires the global solution of 4 nonconvex problems that involve the local solution of nonconvex and convexified subproblems.

7.5 Example 5

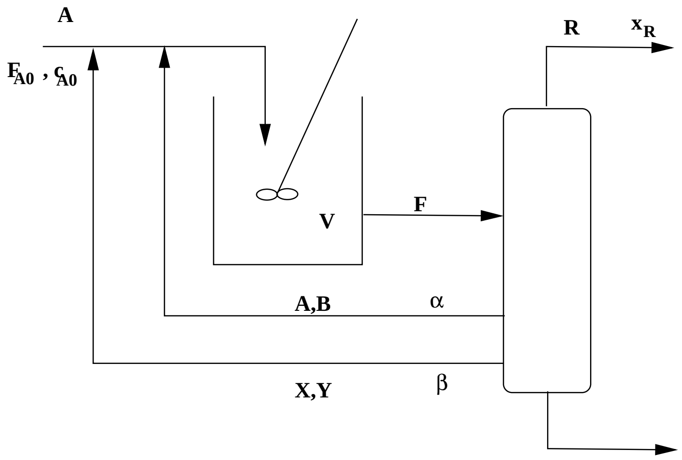

Figure 8: Chemical Reaction Process for Example 5

In this example the prototype chemical process with recycle shown in Figure 8, presented by Ostrovsky et al.[10], is examined. The system consists of a CSTR of volume $V(m^3)$, where Denbigh's reaction takes place with first order irreversible kinetics. As described by Ostrovsky et al.[10], the steady state process operation assuming isothermal conditions can be described by the following set of nonlinear constraints:

$$\begin{aligned}
h_1 &= F_{A0} - x_A F(1-\alpha) - V(k_B + k_X)c_{A0}x_A = 0.0 \\
h_2 &= -Fx_B(1-\alpha) + Vc_{A0}[k_B x_A - (k_R + k_Y)x_B] = 0.0 \\
h_3 &= -Fx_X(1-\beta) + Vc_{A0}k_X x_A = 0.0 \\
h_4 &= -Fx_Y(1-\beta) + Vc_{A0}k_Y x_B = 0.0 \\
h_5 &= -Fx_R + Vc_{A0}k_R x_B = 0.0 \\
h_6 &= x_A + x_B + x_X + x_Y + x_R = 1.0
\end{aligned}$$

$$
\begin{aligned}
g_1 = F_R - F x_R &\leq 0.0 \\
g_2 = 1 - \beta &\geq 0.0 \\
g_3 = 1 - \beta &\leq 1.0 \\
g_4 = 1 - \alpha &\geq 0.0 \\
g_5 = 1 - \alpha &\leq 1.0
\end{aligned}
$$

where the last constraint describes the minimum production requirement for product R. The values of problem parameters are:

$$F_{A0} = 100\text{mol/hr}, c_{A0} = 100\text{mol/m}^3, F_R = 70\text{mol/hr}$$

The rate constants k_B, k_X, k_Y, k_R correspond to the uncertain parameters with nominal values and expected deviations as shown in Table IV.

Parameter	$k_B[h^{-1}]$	$k_X[h^{-1}]$	$k_Y[h^{-1}]$	$k_R[h^{-1}]$
Nominal Value	0.4	0.02	0.01	0.1
Positive Deviation	0.08	0.004	0.002	0.02
Negative Deviation	0.08	0.004	0.002	0.02

Table IV: Uncertain Parameters - Example 5

The volume of the reactor is considered known and equal to the value obtained for the nominal values of the uncertain parameters, $V = 12.3m^3$. For this reactor, the feasibility test and the flexibility index problems are addressed.

For the feasibility test problem, the active set strategy[5], is employed. Since the description of the problem involves 6 equality, 5 inequality constraints and 8 variables, this results in 2 degrees of freedom and thus 3 active constraints in the active sets. The following active sets are identified:

Active set 1: $\{g_1, g_2, g_4\}$

Active set 2: $\{g_1, g_2, g_5\}$

Active set 3: $\{g_1, g_3, g_4\}$

Active set 4: $\{g_1, g_3, g_5\}$

Note that constraints g_2, g_3 correspond to bound constraints for $1-\beta$ and cannot be active simultaneously. The same holds true for constraints g_4, g_5. At the first step of the proposed procedure the nonlinear NLPs that correspond to 4 active sets are solved locally to obtain an upper bound to feasibility function $\chi(\mathbf{d})$. The local solution for the corresponding NLPs results in the following values for feasibility function, $\chi(\mathbf{d})$:

Active set 1: $\chi^1(\mathbf{d}) = -0.00052$, in 2.07 CPUs

Active set 2: $\chi^1(\mathbf{d}) = -0.85$, in 0.04 CPUs

Active set 3: $\chi^3(\mathbf{d}) = -0.0092$, in 0.38 CPUs

Active set 4: $\chi^4(\mathbf{d}) = -0.938$, in 0.08 CPUs

Since $\chi(\mathbf{d})$ corresponds to the maximum of these values, after the first step the upper bound of the global solution for $\chi(\mathbf{d}) = -0.00052$ which suggest that the design is feasible for the whole T range and the procedure stops, no further iterations are required.

For the flexibility index problem, at the first step the four NLP problems that correspond to four different active sets are solved using the local optimization package MINOS that leads to the following results:

Active set 1: Infeasible

Active set 2: $\mathrm{F}^2(\mathbf{d}) = 7.62$, in 1.38 CPUs

Active set 3: $\mathrm{F}^3(\mathbf{d}) = 3.27$, in 1.42 CPUs

Active set 4: $\mathrm{F}^4(\mathbf{d}) = 7.62$, in 2.03 CPUs

Since the design flexibility corresponds to the minimum of these values, at the end of step 1, the upper bound of the design flexibility is $F^U = 3.27$. In the next step the basic principles of the $\boldsymbol{\alpha}$**BB** deterministic global optimization algorithm[1;2;3;4], are used to convexify the NLPs for the different active sets which then can be solved using local optimization techniques in order to obtain a lower bound to the global solution of the flexibility index problem. The solution of the convexified problems are:

Active set 1: Infeasible

Active set 2: $F^2(\mathbf{d}) = 7.52$, in 2.46 CPUs

Active set 3: $F^3(\mathbf{d}) = 3.09$, in 2.94 CPUs

Active set 4: $F^4(\mathbf{d}) = 7.51$, in 3.57 CPUs

and consequently $F^L = 3.09$. The procedure continues providing the bounds as shown in Table V. The approach requires 6 iterations to converge to global value of design flexibility $F = 3.27$.

Iteration	F^L	F^U
1	3.09	3.27
2	3.23	3.27
3	3.23	3.27
4	3.23	3.27
5	3.24	3.27
6	3.267	3.27

Table V: Progression of the bounds for Example 5

8 Conclusions

In this paper, a novel global optimization framework is presented for addressing the feasibility test and the flexibility index problems in a rigorous and efficient way. The approach is based on a convexification/ relaxation of the feasible region, coupled with convex underestimation schemes within a branch and bound global optimization framework. Valid upper and lower bounds are iteratively generated through the global solution of the problem described by the convexified set of constraints and the local solution of the original formulation. The proposed approach is general and can address twice continuously differentiable nonconvex constraints. A number of computational studies are presented to illustrate the applicability of the proposed approach to problems involving different type of constraints.

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