

Framework for Evaluating the Feasibility/ Operability of Nonconvex Processes

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A large number of publications available on determining the feasible region and the operability limits for a design are all limited due to the assumption that the feasible space is convex, but almost all of the problems appearing in chemical engineering are nonconvex in nature. Determining the region where the design is feasible and safe to operate is of extreme importance. To address this problem, a novel algorithm was developed based on the idea of systematically evaluating the infeasibility areas using the outer approximation procedure introduced earlier, and the simplicial approximation approach to approximate the expanded feasible space constructed with the exclusion of the nonconvex constraints. This approach is general and deals with any nonconvex regions, as long as the nonconvex constraints are either concave or quasi-convex, as illustrated through a series of example problems. A new metric is introduced to accommodate the need for comparison between various designs.

Introduction

The determination of the range of feasible and safe operation for a given design is the subject of an extensive list of publications in the open literature during the past two decades. Grossmann and his coworkers have pioneered this field by introducing the flexibility and feasibility analysis approach in the early 1980s (Swaney and Grossmann, 1985a,b; Grossmann and Floudas, 1987). After that, a series of articles have mainly focused on improving and extending the use of such a metric in the design process. An alternative approach involved the introduction of the Resilience Index by Saboo, et al. (1985). In an attempt to determine the probability of feasible operation Straub and Grossmann (1993) introduced the Stochastic Flexibility index, which, however, required the determination of the boundary of the feasible region, identified through a series of optimization problems. A more detailed review of feasibility analysis can be found in Ierapetritou (2001a,b). The main shortcoming of all the approaches presented is the assumption of convexity made in order to guarantee that the determined feasible region does not include any infeasible points. On the other hand, a wide range of problems appearing in chemical engineering are nonconvex in nature and determining the region where the design is feasible and safe to operate is of paramount importance.

This article addresses the problem of evaluating the range of feasibility and operability of a given process for the case of general nonconvex regions. The basic idea is the identification and approximation of the infeasible region where the process cannot operate. The infeasible region is then approximated from the outside using the outer polytope approach introduced in Goyal and Ierapetritou (2002). By eliminating the nonconvexities, the expanded feasible region is approximated using the simplicial approximation approach, thus providing a complete representation of operability regions of the specific process. This approach constitutes the first attempt towards a characterization of nonconvex regions in a rigorous and systematic way.

The proposed framework is presented along with the introduction of new metric to represent the design feasibility for nonconvex regions. A number of case studies are presented to illustrate the applicability of the proposed approach to address the design under uncertainty, and the work is summarized and future directions are discussed.

Proposed Approach

The main focus of the proposed approach is to identify the nonconvex region of the feasible space by locating points on the boundary of the nonconvex region with the assumption

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that the nonconvex constraints can be identified *a priori*. The nonconvex region is then overestimated, using these points, utilizing the outer polytope approach proposed in Goyal and Ierapetritou (2002). The nonconvex constraints are then removed, one at a time, and the expanded region is approximated by a convex hull using the simplicial approximation approach and the QuickHull Algorithm (Goyal and Ierapetritou, 2002). The approximation of the expanded feasible region without the nonconvex constraints together with the overestimation of the infeasible space are used to define a new feasibility metric as explained in detail in the next subsection.

Approximation of the nonconvex feasible region

The design problem under uncertainty can be described by a set of inequality constraints $f_j(d, z, \theta) \leq 0$, $j \in J$ representing the plant operation and design specifications, obtained after eliminating the state variables using the equality constraints for ease in presentation, where d corresponds to the vector of design variables, z corresponds to the vector of control variables, and θ corresponds to the vector of uncertain parameters. Knowing the nature of the constraints, which is the only assumption made in the procedure, the nonconvex constraints can be identified and grouped in a sub-set NC such that $NC \subset J$. Using this information, the basic steps of the proposed approach in order to approximate the feasible space of operation are outlined below and shown graphically in Figure 1.

(1) One nonconvex constraint from the set NC is selected and a point of infeasibility caused by that constraint is found by solving a modified feasibility problem. It has been shown by Grossmann and Halemane (1982) that the feasibility problem for a given design can be formulated as the max-min-max problem

$$\chi(d) = \max_{\theta \in T} \min_{z \in J} \max_{j \in J} f_j(d, z, \theta) \leq 0$$

$$T = \{\theta \mid \theta^L \leq \theta \leq \theta^U\} \quad (1)$$

where the function $\chi(d)$ represents a feasibility measure. This can be slightly modified to find a point inside the bounded infeasible region caused due the nonconvex constraint

$$\chi(d) = \min_{u, z, \theta} u$$

$$s.t. f_j(d, z, \theta) \leq u \quad j \in J - NC$$

$$f_j(d, z, \theta) \geq 0 \quad j \in NC$$

$$\theta^L \leq \theta \leq \theta^U, u \leq 0 \quad (2)$$

In the above formulation, the constraint

$$f_j(d, z, \theta) \geq 0 \quad j \in NC$$

is modified by reversing the sign of the inequality. This allows the determination of a point inside the infeasible region, which could be then used to approximate the infeasible region utilizing the simplicial approximation approach. Furthermore, the upper bound of u is set as zero to ensure the generation of a feasible point inside the nonconvex boundary.

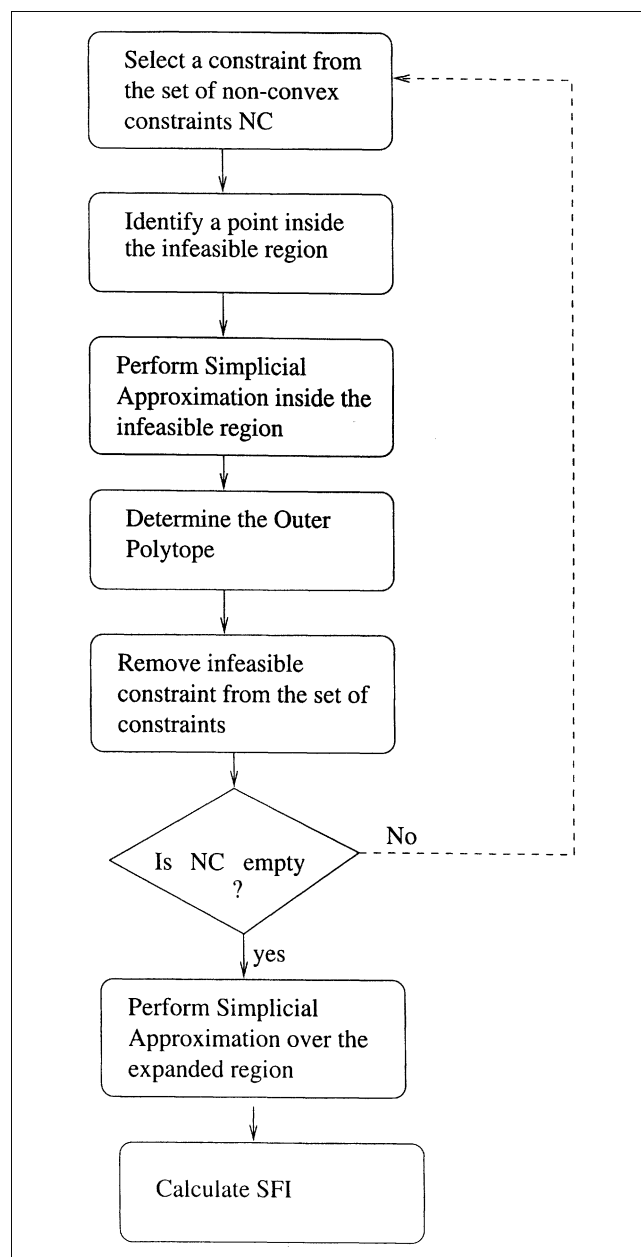


Figure 1. The overall algorithm for the proposed approach.

(2) The simplicial approximation technique is then applied to determine points on the boundary of the infeasible region. Since the sign of the nonconvex inequality is reversed, the region being approximated now becomes convex and can be approximated using simplicial approximation. To initiate the application of the simplicial approximation approach, $(n + 1)$ boundary points are required where n is the dimensionality of the uncertainty space. These additional n points are determined by performing simple line searches from the point found in step one.

(3) The convex polytope is generated using the simplicial points that correspond to an overestimation of the infeasible region.

(4) The nonconvex constraint is removed from the set NC .

(5) Steps 1–4 are repeated for every constraint in the set **NC**, one constraint at a time. Note that the proposed approach is independent of the selection sequence of nonconvex constraints as each nonconvex constraint is approximated, in the absence of other nonconvex constraints.

(6) When all the constraints belonging to the subset **NC** have been removed from the set **J**, the boundary of the feasible region is approximated without the nonconvex constraints using the simplicial approximation technique that results in a convex hull of the expanded feasible space. This is used for the evaluation of the Simplicial Feasibility Index (SFI) defined below.

The convex outer polytope obtained over the infeasible region (step 3) provides an envelope of the region where the design is infeasible and the convex hull obtained in step 6 provides an overestimation of the operating envelope over the expanded feasible space. The volume of the overall feasible region could be obtained by subtracting the volume of the convex-polytopes from the volume of the simplicial convex hull. Note that the important outcome of the proposed approach is the determination of the envelopes of the infeasible operation, defined by the set of hyperplanes that constitute the convex outer polytope generated in step 3. Moreover, in step 6 the expanded feasible space without the nonconvex constraints is approximated. However, the proposed approach is limited to nonconvex constraints that are either concave or quasi-convex.

Based on these results, a new feasibility metric is introduced that describes the flexibility of a given process and can be used to compare different designs. This metric is the modification of the SFI introduced in Goyal and Ierapetritou (2002) to account for the infeasible region

This definition of SFI can be applied to calculate the percentage of feasibility for any nonconvex region. It can be used as a measure to quantify the feasibility/operability of different designs for a nonconvex process, as shown in the illustrating example in the next section (Computational Studies). For the case where the infeasible regions overlap, the SFI would result in an underestimation of the flexibility, depending on the degree of overlapping. In the next two subsections, the steps of the simplicial approximation approach and the convex outer polytope (Goyal and Ierapetritou, 2002) are outlined for completeness. In the next section a number of examples are presented to illustrate the applicability of the proposed approach.

Simplicial approximation of the feasible region

The *Simplicial Approximation Approach* is based on explicitly approximating the boundary ∂R of the feasible region R of an n -parameter design space by a polyhedron made up of n -dimensional simplices. It has been assumed that the constraint functions are locally convex, that is, that the sequence of points generated on ∂R are extreme points of a convex set. The procedure is described briefly in the following steps:

• Simplicial Convex Hull

(1) Determining any m points p_1, p_2, \dots, p_m on the boundary ∂R , where $m \geq n + 1$. One way to find the m points is to perform line searches as described in Ierapetritou (2001a).

(2) Use the set of m points on ∂R , to construct the convex hull of these points by applying the *QuickHull algorithm* (Barber et al., 1996).

$$\text{SFI} = \frac{\text{Volume of expanded convex hull} - \sum \text{Volume of infeasible convex polytopes}}{\text{Volume of the expanded convex hull}} \quad (3)$$

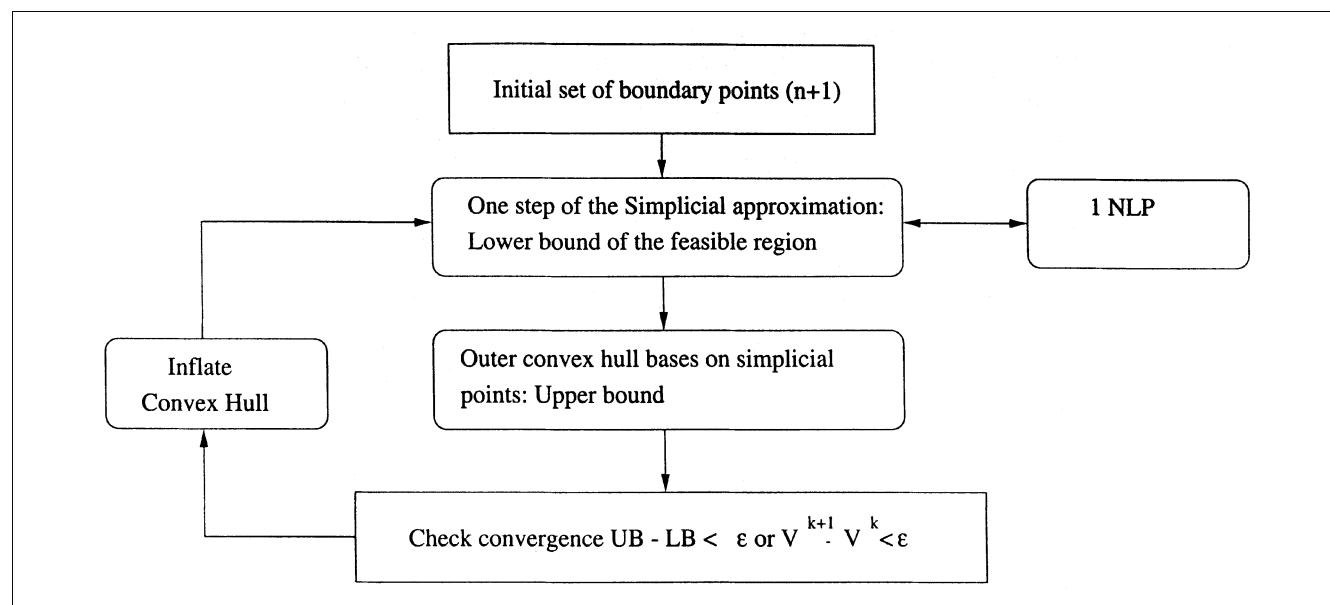


Figure 2. Overall algorithm for the simplicial approximation approach.

(3) Given the first approximation of ∂R , determine which of the m_H faces of the polyhedron is the largest and, hence, the poorest approximate of the region. The largest facet is the hyperplane with the largest area.

(4) Determine a new boundary point by making a one-dimensional (1-D) search in the outwards normal direction, starting from the center of the largest hyperplane found at step 3.

(5) Add the new point to the set of boundary points and return to step 2.

• Outer Convex Polytope

(1) The points obtained by the generation of the simplicial convex hull are used as the initial boundary points.

(2) Tangent hyperplanes are generated at the points obtained at step 1.

(3) The points of intersection of the tangent half-planes are obtained using the Quick Hull Algorithm (Barber et al., 1996).

(4) A convex hull is generated using the QuickHull Algorithm (Barber et al., 1996) at the intersection points obtained above, forming the outer polytope which serves as an envelope of the simplicial convex hull.

The above obtained polytope serves as an upper bound (UB) for the feasible region and the simplicial convex hull as the lower bound (LB). The iterative procedure then proceeds until convergence is achieved between upper and lower bound and/or the volume (V^k at iteration k) of the convex hull, as illustrated in Figure 2. The volume of the convex hull at each iteration is evaluated using the *QuickHull algorithm* (Barber et al., 1996). When the feasible region is asymmetric in shape, inscribing a hypersphere could result in a poor approximation. This problem can be handled by scaling the uncertain or operating parameters and inscribing a hyperellipsoid (Director and Hachtel, 1977; Goyal and Ierapetritou, 2002).

Remark. Note that the step 3 of the approach was modified from the original approach of Goyal and Ierapetritou (2002), by determining the facet with the largest area, instead of determining the largest tangent hyperplane, as it was observed with experience that this change does not significantly effect the total number of simplicial iterations required for convergence, but eliminates the need to solve the $n+1$ ($n \geq 3$) linear program at each iteration for determination of the largest tangent hyperplane.

Computational complexity

Computationally, the proposed approach involves:

- The simplicial approximation procedure which requires the solution of $k+n+1$ simple line searches (NLP) where k is the number of iterations and n is the dimensionality of the problem. The $n+1$ line searches are needed to obtain the initial points.

- One nonlinear program is solved for each nonconvex constraint to get a feasible point inside the infeasible region.

- For the determination of the convex hull of the points obtained at the boundary of the feasible region, the QuickHull algorithm (Barber et al., 1996) is used that has an average time complexity of $O(n \log m)$ for $n \leq 3$ and $O(f_m)$ otherwise, where m is the number of processed points, n is their

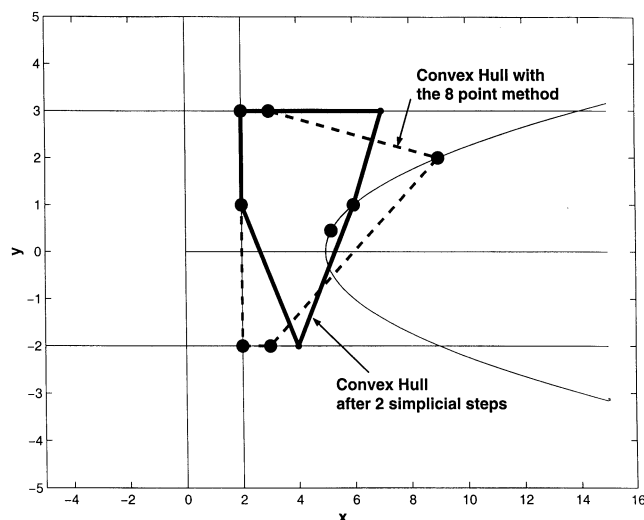


Figure 3. Convex hulls using the 8-point method and after 2 steps of the simplicial approximation approach, $d = 5$.

dimensionality and f_m is the maximum number of facets for m vertices.

All computations in this article are performed on a Dell 933 Mhz Pc with a Linux operating system and a convergence parameter of 10^{-2} . It should be noted that the computational time (CPUs) needed for all of the optimization problems solved in the next section is very small and, hence, is not reported.

Computational Studies

Illustrating example

The first example considered in this section involves the following set of constraints

$$f_1 = 2 - x \leq 0$$

$$f_2 = -y - 2 \leq 0$$

$$f_3 = y - 3 \leq 0$$

$$f_4 = x - d - y^2 \leq 0$$

The design is described by the parameter d whereas x, y are the uncertain parameters. A nominal point of $(x, y) = (3, 1)$ is considered with expected deviations of $\Delta x^- = 1$, $\Delta x^+ = 12$, $\Delta y^+ = 2$ and $\Delta y^- = 3$ and the value of design d is set to 5. The feasible region is first approximated using the method proposed by Ierapetritou (2001a). This results in a convex hull which is shown in Figure 3 with the dotted edges. The convex hull obtained was an inaccurate approximation of the feasible region as it contains infeasible points due to the nonconvex nature of the problem. Then, the simplicial approximation approach outlined in Goyal and Ierapetritou (2002), was used. The algorithm was terminated after two simplicial iterations as part of the infeasible region was included in the convex hull. The result is shown in Figure 3 as the polytope with the dark edges. Thus, both these approaches failed to approximate the nonconvex region correctly.

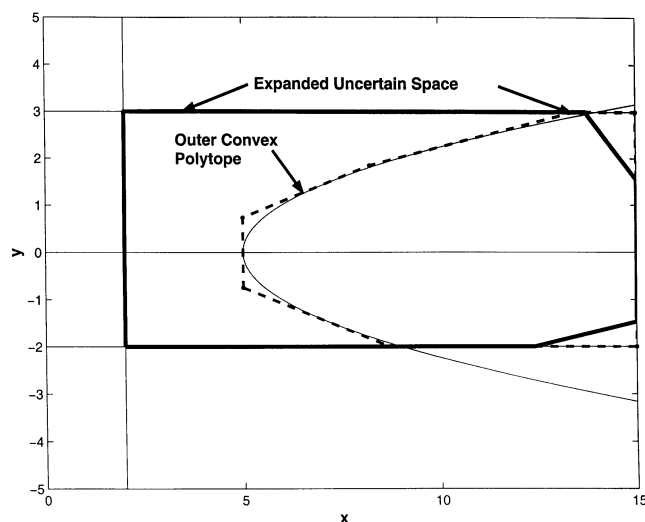


Figure 4. Convex polytope and overall convex hull for illustrating example, $d = 5$.

The proposed algorithm was then used to evaluate the feasible region. The constraint f_4 was identified as the only nonconvex constraint and was added to the set \mathbf{NC} . The proposed approach was then applied resulting in the outer convex polytope around the infeasible region with a volume of 39.131 units. f_4 was then removed from the set of constraints, and the simplicial approximation over the region gives an expanded convex hull with a volume of 63.77 units. The outer polytope is shown in Figure 4 with the dotted edges, and the convex hull of the expanded feasible region is shown with dark edges. This results in a feasible region with the volume of 24.639 units and a SFI of 0.386. Note that the proposed approach correctly approximates the region of feasible and infeasible operation in contrast with the existing approaches that require feasible region convexity. To validate the approximation, the true value of SFI was determined by calculating the area of the infeasible and expanded region through integrating over the curves and was found to be 0.4, a close approximate with an error of 3.5%. Computationally, the proposed approach required five simplicial iterations for the approximation of the infeasible region using the outer polytope approach and seven simplicial iterations for the approximation of the expanded overall feasible region. The number of problems solved and the number of iterations required for convergence are shown in Table 1. The value of the SFI can be moved closer towards the actual value by decreasing the convergence parameter, but at the price of a larger number of optimization problems being solved.

To illustrate the applicability of the metric introduced (SFI), a different design is examined with $d = 7$ and the proposed approach was applied to approximate the new feasible region. This resulted in an outer convex polytope around the infeasible region with a volume of 29.355 units and an expanded convex hull with a volume of 63.77 units. The outer polytope is shown in Figure 5 with the dotted edges, and the convex hull of the expanded feasible region is shown with dark edges. The resulted feasible region was then determined to correspond to a volume of 34.415 units and SFI of 0.543.

Table 1. Computational Results

Example 1	No. of Problems Solved	Total Iter.	SFI	Error (%)
NLP (Feasibility Problem)	1	2		
NLP (1-D Line Search)	18	54	0.386	3.5
Example 2				
NLP (Feasibility Problem)	2	26		
NLP (1-D Line Search)	25	245	0.83	1.5
Example 3				
NLP (Feasibility Problem)	1	15		
NLP (1-D Line Search)	21	150	0.978	0.2
Example 4				
NLP (Feasibility Problem)	1	52		
NLP (1-D Line Search)	8	300	0.184	8

The actual value of SFI was determined to be 0.55, thus having an error of 1.3%. The proposed approach thus correctly predicts that, with the change of the design variable, the feasible region increases and thus the proposed metric can be effectively used to compare the feasibility of different designs.

Multiple nonconvex constraints

The second example considered here contains two nonconvex constraints and is defined by the following set of constraints

$$f_1 = \theta_2 - 2\theta_1 - 15 \leq 0$$

$$f_2 = \frac{\theta_1^2}{2} + 4\theta_1 - 5 - \theta_2 \leq 0$$

$$f_3 = 10 - \frac{(\theta_1 - 4)^2}{5} - \frac{\theta_2^2}{0.5} \leq 0$$

$$f_4 = \theta_2 - 15 \leq 0$$

$$f_5 = \theta_2(6 + \theta_1) - 80 \leq 0$$

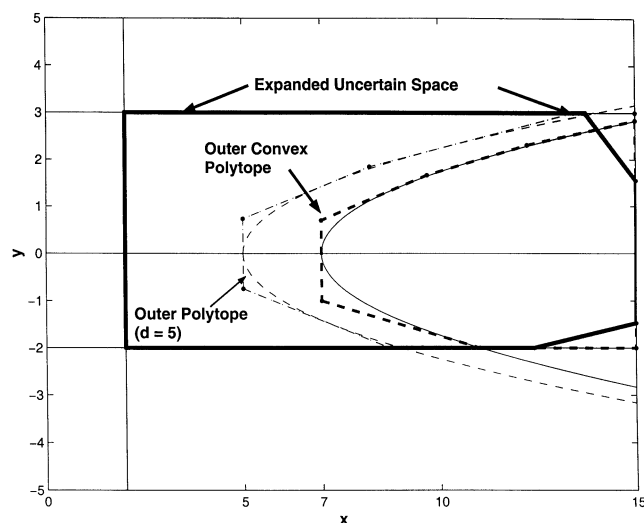


Figure 5. Convex polytope and overall convex hull for illustrating example, $d = 7$.

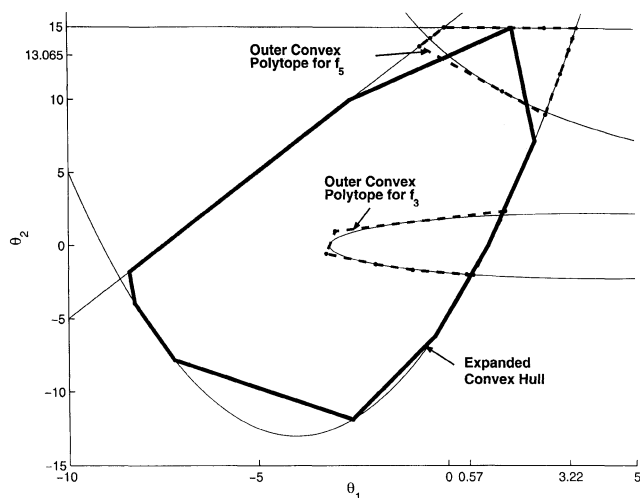


Figure 6. Convex polytopes and overall convex hull for example 2.

A nominal point of $(\theta_1, \theta_2) = (-2.5, 0)$ is considered with expected deviations of $\Delta\theta_1^- = -7.5$, $\Delta\theta_1^+ = 7.5$, $\Delta\theta_2^+ = 15$, and $\Delta\theta_2^- = -15$. The constraints f_3 and f_5 are identified as the nonconvex constraint and added to the set NC. The proposed approach is then applied for both the nonconvex constraints, one at a time, resulting in the outer convex polytope around the infeasible region generated due to f_3 with a volume of 12.931 units and for the infeasible region due to f_5 with a volume of 14.045 units. Both these constraints are then removed from the set of constraints and the simplicial approximation over the region gives an expanded convex hull with a volume of 156.66 units. The outer polytopes is shown in Figure 6 with the dotted edges, and the overall convex hull is shown with dark edges. This results in a feasible region with the volume of 129.69 units and a SFI of 0.83. The actual value of SFI was determined to be 0.842, thus having an error of 1.5%.

Computationally, the proposed approach required five simplicial iterations for the approximation of the outer polytope due to the constraint f_3 , four simplicial iterations for the approximation of the outer polytope due to the constraint f_5 , and seven iterations for the expanded convex hull for convergence. The number of problems and iterations used to obtain convergence are shown in Table 1. Note that the proposed approach correctly approximates the region of infeasible operation for both the nonconvex constraints. Computationally, the number of nonlinear problems increases with the increased number of nonconvex constraints. However, this additional complexity is fairly small since only one additional nonlinear feasibility problem is solved for each additional nonconvex constraint and the change in the number of simplicial steps is small. For example, the total number of simplicial iterations required for convergence for the illustrating example was 12 compared to 16 needed for example 2, which has one additional nonconvex constraint.

Three uncertain parameters

The third example considered involves three uncertain pa-

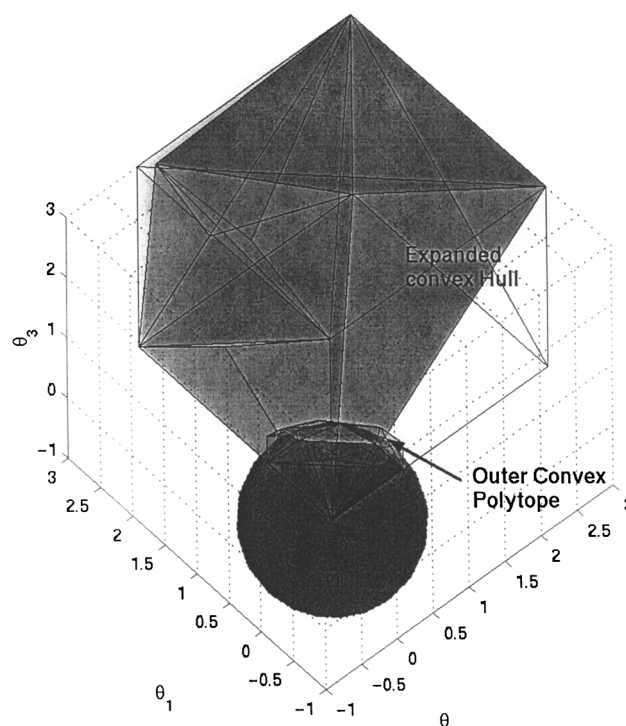


Figure 7. Convex polytopes and overall convex hull for example 3.

rameters and is described by the following set of constraints

$$f_1 = \theta_1 - 3 \leq 0$$

$$f_2 = \theta_2 - 3 \leq 0$$

$$f_3 = \theta_3 - 3 \leq 0$$

$$f_4 = \theta_1^2 + \theta_2^2 + \theta_3^2 - 1 \geq 0$$

$$\theta_1, \theta_2, \theta_3 \geq 0$$

A nominal point of $(\theta_1, \theta_2, \theta_3) = (1.5, 1.5, 1.5)$ is considered with expected deviations of $\Delta\theta_1^- = -1.5$, $\Delta\theta_1^+ = 2.5$, $\Delta\theta_2^+ = 2.5$ and $\Delta\theta_2^- = -1.5$ and $\Delta\theta_3^+ = 2.5$ and $\Delta\theta_3^- = -1.5$. The constraint f_4 , which is the equation of a sphere cutting the cube defined by constraints f_1, f_2, f_3 , is identified as the nonconvex constraint and added to the set NC. The proposed approach is then applied resulting in the outer convex polytope around the infeasible region with a volume of 0.577 units. f_4 is then removed from the set of constraints and the simplicial approximation over the expanded feasible region gives a convex hull with a volume of 26.45 units. The outer polytope is shown in Figure 7 as the polytope around the portion of the sphere cutting the cube and the expanded convex hull is the polytope inside the cube. This results in a feasible region with the volume of 25.88 units and a SFI of 0.978. The actual value of SFI was determined to be 0.98, thus having an error of 0.2%.

Computationally, the proposed approach required seven simplicial iterations for the outer polytope and nine iterations for the expanded convex hull for convergence. The number of problems solved and iterations used to obtain con-

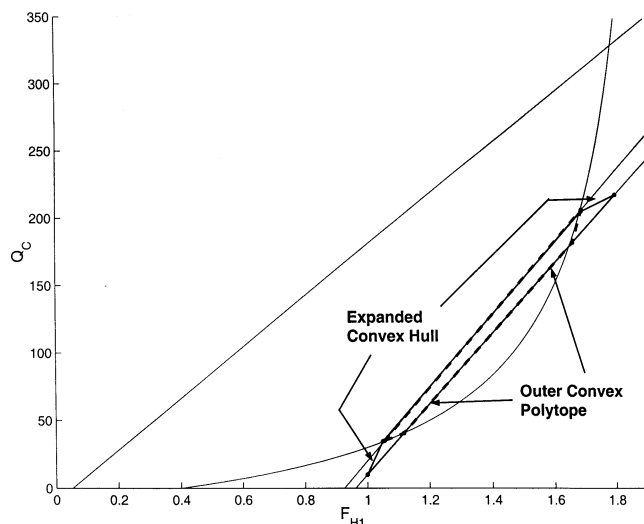


Figure 8. Convex polytopes and overall convex hull for example 4.

vergence are shown in Table 1. Note that the computational requirement of the proposed approach does not increase much with the number of uncertain parameters involved. Comparing with the illustrating example that also included one nonconvex constraint, the number of simplicial iterations and the number of 1-D line search NLP's increases slightly from 12 to 16 and 18 to 21, respectively. Thus, the scaling properties of the proposed approach are very promising for addressing large-scale problems.

Disjoint feasible region

The last example considered is the heat exchanger network given in Grossmann and Floudas (1987). The following set of constraints describe the process

$$f_1 = -25F_{H1} + Q_c - 0.5Q_c F_{H1} + 10 \leq 0$$

$$f_2 = -190F_{H1} + Q_c + 10 \leq 0$$

$$f_3 = -270F_{H1} + Q_c + 250 \leq 0$$

$$f_4 = 260F_{H1} - Q_c - 250 \leq 0$$

The uncertain parameters is the heat flow rate of steam, F_{H1} , which has a nominal value $F_{H1}^N = 1.4 \text{ kW/K}$ and an expected deviation of $\Delta F_{H1}^+ = 0.4 \text{ kW/K}$ and $\Delta F_{H1}^- = 0.4 \text{ kW/K}$. The feasible region of this network is illustrated in Figure 8 and consists of two disconnected domains, which are identified by the proposed approach. The constraint f_1 is identified as the nonconvex constraint causing the division of the feasible region and is added to the set NC. The proposed approach is then applied resulting in the outer convex polytope around the infeasible region with the area of 8.16. f_1 is then removed from the set of constraints and the simplicial approximation over the expanded region gives an overall convex hull with the area of 10 units. The outer polytope is shown in Figure 8 with the dotted edges and the overall convex hull is shown with dark edges. This results in a disjoint feasible

region with the volume of 1.84 units and a SFI of 0.184 compared to the actual value of 0.2.

Due to the 1-D nature of the problem, line searches were sufficient to locate points on the boundary instead of applying steps of the simplicial approximation approach. The proposed approach results in the set of linear inequalities that corresponds to the equations of the hyperplanes defining the outer polytope of the infeasible region, as well as the linear approximation of the expanded region thus providing a complete picture of process feasibility. Computationally, the proposed approach required two simplicial iterations for the outer polytope, and for the overall convex hull for convergence due to the low dimensionality of the problem. The number of problems and iterations used to obtain convergence are shown in Table 1.

Summary and Discussion

A new approach is presented to identify the operating envelopes where process operation is feasible for any nonconvex problem. The basic idea of the proposed approach is to identify a point inside the infeasible region resulting due to the nonconvexities and then to iteratively improve the approximation of the boundary of the infeasible region by determining points at the boundary using a simplicial approximation technique which is then used to determine the outer envelope by generating the tangent planes at these points. This serves as an overestimation of the infeasible region. The nonconvex constraint is then removed and the expanded feasible region is approximated using the simplicial approximation approach. The convex hull is then computed using the *QuickHull Algorithm*. The outcome of the application of the *QuickHull Algorithm* is not only the computation of the convex hull described by a set of linear constraints, but also its volume. The volumes of the convex hull over the expanded region and the infeasible region are used to estimate a new metric for quantifying process/design feasibility for the case of nonconvex processes. The work presented in this article addresses the problem of quantifying feasibility for the general nonconvex regions in a novel and systematic way, as long as the nonconvex constraints are concave or quasi-convex in nature. To our knowledge, no work has been published to address this problem, but rather convexity assumption has to be always assumed. The only assumption made here is that the source of nonconvexity is known. Work is underway towards the direction of identification of nonconvexities, given a general nonconvex region and applying the proposed approach to general nonconvex constraints.

Acknowledgments

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