Determination of Operability Limits Using Simplicial Approximation

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Determining the boundaries of any process/design where feasible and safe operation is guaranteed has long been recognized as a major concern in process industries. Of additional value is identifying the range of operating conditions where the design is most profitable. Although there is a lot of discussion in the open literature regarding design feasibility in terms of uncertainty of process variables, these techniques are rather limited due to the underestimation of the feasible space. A new approach is presented based on the ideas of inner and outer approximation of the feasible region to identify the operating envelopes where process operation is feasible, safe, and profitable. A number of example problems are presented including two case studies to illustrate the applicability of this approach.

Introduction

The issue of determining the operating envelope for a feasible and safe operation is a concern for any industrial process plant. For example, in the air separation process which will be studied later, the feasibility of the optimal plant configuration is evaluated with respect to the flow rates of the liquid and gaseous oxygen produced that enables the determination of the capability range of the specific design. The same issues appear in the design of new materials where the constraints have the form of property functions targeting specific values. Of course, a hard constraint in any operability analysis of a product or a process is the reassurance of safe operation. Safety constraints can consequently be very limiting in terms of the available operating ranges. It is, thus, of major benefit to be able to identify as precisely as possible the feasible operating ranges to avoid limiting the operation to narrow conditions eliminating the ability to perform profit optimization studies. As would become apparent from the first case study presented, the issue of obtaining the feasible region of a design can be extended to the synthesis level where various process configurations are analyzed based mainly on their costs. The identification of feasibility in terms of operating conditions would greatly enhance the power of analytical tools for product/process design since it would improve the comparison of various design alternatives. In terms of addressing uncertainty issues, a flexibility and feasibility analysis approach proposed by Grossmann and coworkers (Swaney and Grossmann, 1985a,b) has been proven to be a powerful and, in most cases, the only approach available to identify the uncertainty ranges where the product/process is feasible to operate or function. However, as was first shown by Ierapetritou (2001), this approach can largely underestimate the actual feasible region. Thus, determining a feasible range more accurately will be of great value to analyze uncertainty in process and product design. This article presents a systematic framework for an accurate approximation of the feasible region or operating envelope of a given design based on the basic idea of approximating the feasible region from inside using the simplicial approximation approach and from the outside using the tangent planes at specific boundary points.

A number of articles have been published in the area of global optimization utilizing similar ideas of approximating the objective function and/or constraints either from inside or outside resulting in the development of successive approximation techniques. An interested reader is directed to the book by Horst and Tuy (1993).

The proposed framework including the presentation of the simplicial approximation, the proposed approach to generate the outer approximation of the feasible region, and the introduction of new metric to represent the design feasibility are presented. A number of case studies are presented to illustrate the applicability of the proposed approach to address the design under uncertainty, to identify the ranges of operating conditions where the alternative plant configurations for

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air separation are most profitable, and, finally, to determine the ranges of initial conditions where reduced kinetics models are valid. This is followed by a conclusion with discussion and future work directions.

Proposed Approach

To illustrate the basic concept of the proposed approach, it is assumed that the specific design is described by a set of inequality constraints $f_j(d,z,\theta) \le 0$ assuming that the equality constraints have been eliminated for ease in the presentation. In these constraints d represents the set of design variables, and z represents the set of control variables that can be adjusted to accommodate variations on the operating variables or uncertain parameters represented by the vector θ. The main idea of the proposed approach is to iteratively improve the approximation of the boundary of the feasible region by determining points at the boundary using a simplicial approximation approach (Director and Hachtel, 1977), which are used to inscribe a convex hull inside the feasible region that serves as a lower bound of the feasible space and then to determine the outer envelope by generating the tangent planes at these points. This serves as an upper bound of the feasible region and is also used to determine a new feasibility metric that accurately describes the design feasibility. For the case of a convex feasible region, the convex hull determined in this way is guaranteed to be inscribed within the feasible region. However, for the nonconvex case, there is no guarantee that this would be always the case. A study of the general nonconvex case is a subject of present research and would be published in a later publication.

Simplicial approximation of the feasible region

The *Simplicial Approximation Approach* (Director and Hachtel, 1977) 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 simplicies. 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 in the following steps:

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

(2) Using the set of m points on R, the convex hull of these points is then constructed. The convex hull is determined by applying the *Quickhull algorithm* (Barber et al., 1996). The convex hull is characterized by the set of m_H inequalities, describing the hyperplanes that complete the convex hull

$$h_k^T \boldsymbol{p} \le \boldsymbol{c_k}, \qquad k = 1, 2, \ldots, m_H \tag{1}$$

where h_k is a unit vector normal to kth hyperplane pointing outwards and c_k is a measure of the distance of the kth hyperplane from the origin.

(3) Given the first approximation of ∂R, the largest hypersphere that can be inscribed in the convex hull is obtained. The distance from a point p^* inside the polytope to the kth hyperplane is

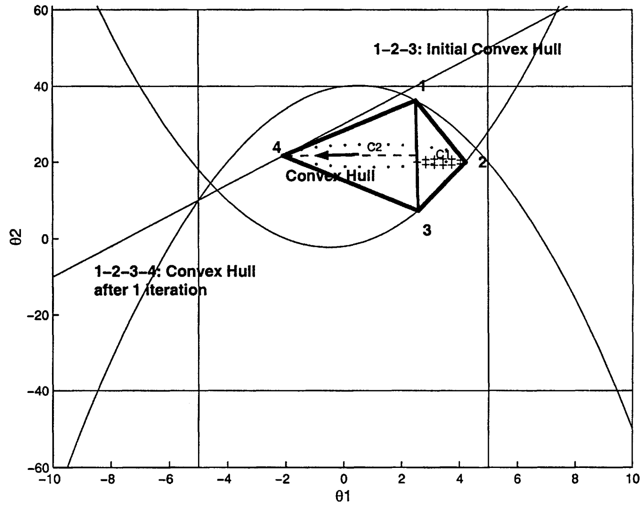

Figure 1. Steps in simplicial approximation.

Initial convex hull (1,2,3) and the resulting convex hull (1,2,3,4) after one iteration.

$$d_k = h_k^T \boldsymbol{p}^* - \boldsymbol{c_k} \tag{2}$$

Thus, the center and radius of the largest hypersphere can be estimated using the following linear program

$$\max r$$
$$h_k^T \boldsymbol{p}^* + \boldsymbol{r} \le \boldsymbol{c_k} \tag{3}$$

(4) The next step is to determine which is the largest of the m_H faces of the polyhedron that are tangent to the inscribed hypersphere. The largest face is the one in which the largest $(n-1)$ dimensional hypersphere can be inscribed. The largest face is of importance, because that is most likely the poorest approximation of the ∂R, since the best approximation corresponds to an infinite number of faces (points at the boundary), as shown in Figure 1. The tangent faces of the polyhedron are those with the zero slack variables in the solution of the linear program defined by Eq. 3. The center of the largest hypersphere inscribed in the jth face of the polyhedron, denoted by p_j^* must be on the jth hyperplane. The surface of a hypersphere of radius r_j can be described by

$$p_j^* + r_j h_j^{\perp} \tag{4}$$

where $h_j^{\perp}$ denotes a unit vector perpendicular to h_j, such that

$$\left(h_j^{\perp}\right)^T h_j = 0 \tag{5}$$

The largest such hypersphere is the one with the largest r_j that satisfies the constraints

$$h_k^T \left(p_j^* + r_j h_j^{\perp} \right) \le c_k,\ k = 1, 2, \ldots, m_h;\ k \ne j \tag{6}$$

which is equivalent to the constraint

$$h_k^T p_j^* + r_j \sin \theta_{jk} \le c_k \tag{7}$$

where θ_{jk} is the angle between h_k and h_j. Thus, a linear program has to be solved to determine p^* and maximize r subject to Eqs. 5 and 7. As described in Director and Hachtel (1977), this problem corresponds to the dual of the following (primal) linear program. Minimize the objective function

$$\Phi = \sum_{k=1}^{m_H+1} c_k \alpha_k \tag{8}$$

subject to the constraints

$$\begin{pmatrix} h_1 & h_2 & \cdots & h_j & \cdots & h_{m_H} & -h_j \\ \vdots & \vdots & & \vdots & & \vdots & \vdots \\ \sin\theta_{1j} & \sin\theta_{2j} & \cdots & 0 & \cdots & \sin\theta_{m_H j} & 0 \end{pmatrix} \times \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_{m_H+1} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 1 \end{pmatrix} \tag{9}$$

and $\alpha_k \ge 0$ for all k. Note that $c_{m_H+1} = -c_j$.

(5) A new boundary point is determined by making a one-dimensional search in the outwards normal direction, starting from the center of the largest inscribed hypersphere in the plane found at step 4.

(6) This new point is then added to the set of boundary points found in the previous iteration and a new convex hull is formed. Thus, an approximation to ∂R is improved in each step and a convex hull that approximates the feasible region is finally obtained.

The volume of the convex hull at each iteration is evaluated using the *Quickhull algorithm* (Barber et al., 1996), which shows an average time complexity of $O(*n \log m)$ for $n \le 3$ and $O(f_m)$ otherwise, where m is the number of points, n is their dimensionality and f_m is the maximum number of facets for m vertices. The simplicial convex hull obtained serves as a lower bound on the total feasible design space.

Scaling-inscribing a hyperellipsoid

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. After the appropriate scaling is performed, the procedure for inscribing the simplicial follows the same steps, as described in the previous subsection.

The scaling is performed in the following way. Assume that, after the mth step of simplicial approximation procedure $n+m+1$ boundary points, p_k, $k = 1,2,\ldots,n+m+1$ have been found. The lower and upper bounds for each parameter are determined as

$$p_i^L = \min_k p_{ik}$$

$$p_i^U = \max_k p_{ik}$$

for $i = 1,2,\ldots,n$ where p_{ik} is the ith coordinate of the kth boundary point. The scale factor for the ith component of the parameter vector is then given by

$$F_i = p_i^U - p_i^L, \quad i = 1, 2, \ldots, n$$

A scaled set of boundary points are now defined as

$$\hat{p}_k = \boldsymbol{F}^{-1} p_k, \quad k = 1, 2, \ldots, n$$

where $\boldsymbol{F}$ is the scale matrix defined as

$$\boldsymbol{F} = \text{diag}\, F_1, F_2, \ldots, F_n$$

Using this scaled set of points, the simplicial approximation procedure can be carried out and the final unscaled boundary points can be obtained as

$$p_k = \boldsymbol{F}\hat{p}_k \quad k = 1, 2, \ldots, n$$

Most of the examples shown in the next section have been scaled due to their asymmetric design space.

Convex polytope: the outer bound

In this section an algorithm is developed for the construction of a convex polytope around the simplicial convex hull. This provides (a) an upper bound to the feasible region and (b) an improved metric for design feasibility which is defined as the ratio of the volumes of the feasible convex hull and the outer convex polytope. Compared to the FCHR (Ierapetritou, 2001), this metric is much more accurate since the comparison is made with respect to the maximum design feasibility and the overall expected range. The proposed algorithm is based on the supporting hyperplane theorem of convex sets that states that if S is a convex set and $\boldsymbol{p}$ is a boundary point of S. Then, there exists a hyperplane containing $\boldsymbol{p}$ and containing S in one of its closed half-spaces. For any point $\boldsymbol{p_0}$ defined on the boundary of S, the tangent plane is defined as

$$[\nabla h(\boldsymbol{p_0})]^T \boldsymbol{p} = [\nabla h(\boldsymbol{p_0})]^T \boldsymbol{p_0}$$

where $h(\boldsymbol{p}) \le \boldsymbol{0}$ is an active constraint at point $\boldsymbol{p_0}$ and $\nabla h(\boldsymbol{p})$ is the gradient of the function $h(\boldsymbol{p})$. For a point $\boldsymbol{p_0}$ on the boundary, a tangent plane at $h(\boldsymbol{p_0})$ satisfies the supporting hyperplane theorem. The aim of the algorithm is to approximate the feasible region $\boldsymbol{R}$ by a polytope

$$\Re = \{x \mid \boldsymbol{Hp} \le \boldsymbol{c}\},\ \boldsymbol{H} \in \boldsymbol{R}^{m*n};\ \boldsymbol{c} \in \boldsymbol{R}^m$$

formed by intersection of m halfspaces in $\boldsymbol{R}^n$. The basic steps of the algorithm are as follows:

(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. The active constraints at a boundary point are the ones with a zero slack variable during the one-dimensional (1-D) line searches in the simplicial convex hull generation, so no additional optimization problems have to be solved to obtain the polytope, if the constraints are explicitly defined. In the case where the constraints are implicit, as, for example, the air separation case study which will be presented later, a different approach is used to calculate the slope of the tangent hyperplanes at each simplicial point. The basic idea is to numerically determine the derivatives at each simplicial point, considering small pertubations in the θ parameters by solving the feasibility problem (Eq. 10)

$$\psi(d,\theta) = \min_{z,u} u$$
$$\text{s.t.} \quad h_i(d,z,x,\theta) = 0; \quad i \in I$$
$$g_j(d,z,x,\theta) \le u \quad j \in J \tag{10}$$

where d corresponds to the vector of design variables, z is the vector of control variables, x is the vector of state variables, θ is the vector of operating variables or uncertain parameters, and $\psi(d,\theta)$, is the feasibility function (Swaney and Grossmann, 1985a). Values of θ for which $\psi(d,\theta) \le 0$ are feasible and the boundary of the region is determined implicitly by $\psi(d,\theta) = 0$. Computationally, this approach requires the solution of $k(n+1)$ nonlinear programs where k is the number of simplicial points and n is the dimension of the set of θ parameters.

(3) The points of intersection of the tangent half-planes are obtained.

(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 the upper and lower bound and/or the volume (V^k at iteration k) of the convex hull, as illustrated in Figure 2. In the next section, the design under uncertainty problem is addressed using three example problems from the literature, followed by an air separation process synthesis case study that targets the evaluation of the feasible range of operating conditions of various products and the problem of evaluating the range of initial conditions for a specific reduced kinetic model.

Remark 1. The complete optimization problem requires the solution of k nonlinear and $k(n+1)$ linear programs. If the constraints are implicit in nature, $k(n+1)$ additional nonlinear programs have to be solved (Figure 2). It should be noted that the computational time (CPU) needed for all of the optimization problems solved in the next section is very small and, hence, is not a significant factor.

Remark 2. The proposed approach has also been proved to be independent of the nominal point as shown in the illustrating example in the next section.

Case Studies

Uncertainty consideration

Illustrating Example. The first case study considered in this section involves the following set of constraints

$$f_1 = \theta_2 + \theta_1^2 - \theta_1 - 40 \le 0$$
$$f_2 = \theta_1^2 + \theta_1 - \theta_2 - 2 \le 0$$
$$f_3 = \theta_2 - 4 \times \theta_1 - 30 \le 0$$

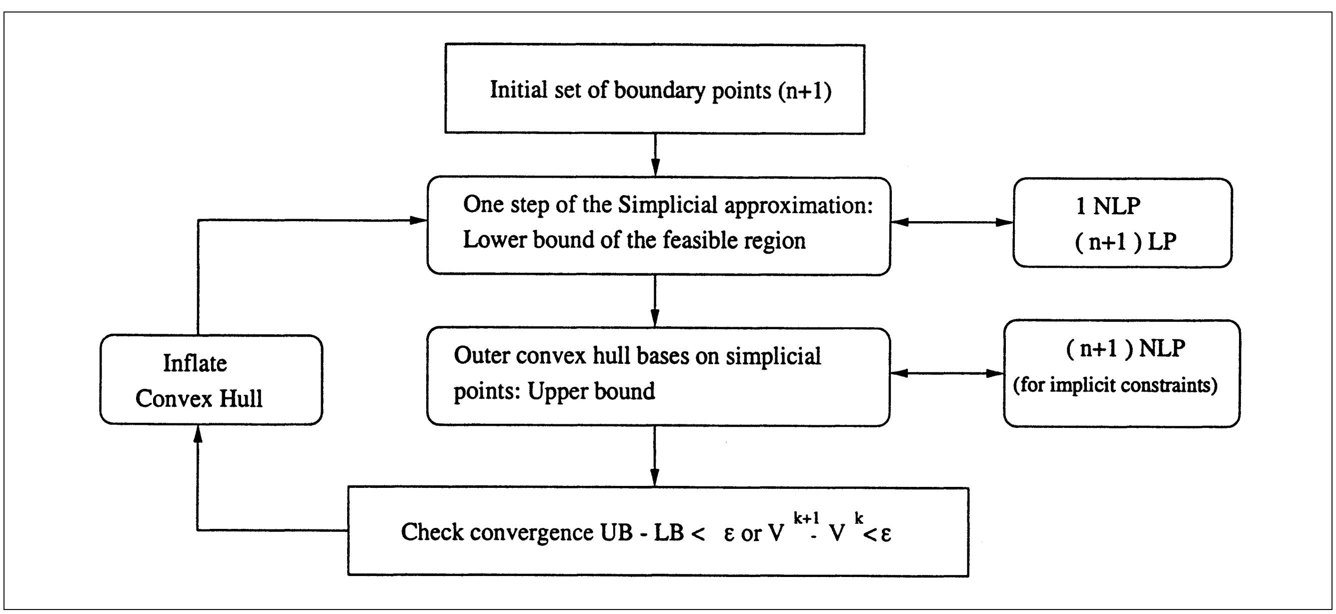

Figure 2. Overall algorithm for the proposed approach.

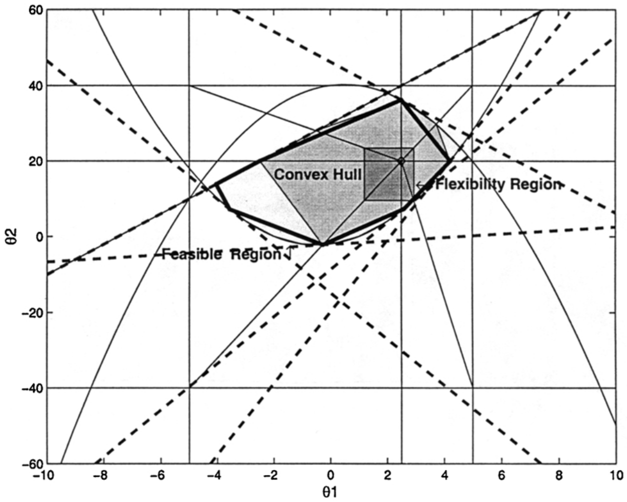

Figure 3. Simplicial convex hull for Case Study 1 with nominal points of (θ1, θ2) = (2.5, 20).

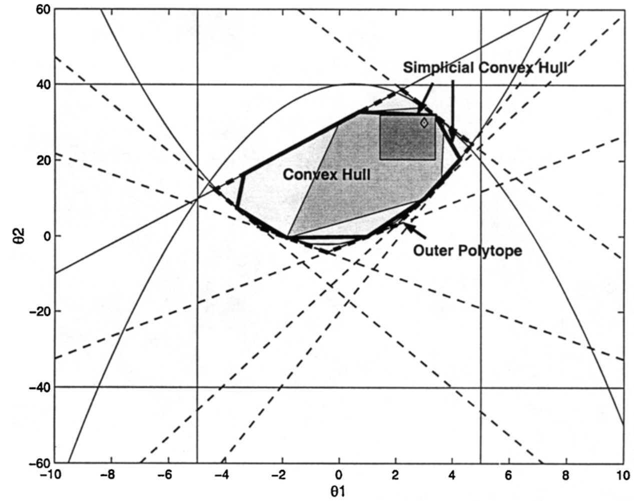

Figure 4. Simplicial convex hull for Case Study 1 with nominal points of (θ1, θ2) = (3, 30).

A nominal point of $(\theta_1, \theta_2) = (2.5, 20)$ is considered with expected deviations of $\Delta\theta_1^- = 7.5$, $\Delta\theta_1^+ = 2.5$, $\Delta\theta_2^+ = 20$, and $\Delta\theta_2^- = 60$. The flexibility index is evaluated first and is found to be equal to $F = 0.174$, as described by the rectangular region in Figure 3. The convex hull is then constructed by the approach of Ierapetritou (2001) and is found to have the volume of 148.7 units and a FCHR = 0.19, which is shown as the light shaded area in Figure 3. The proposed approach is then applied resulting in the inscribed convex hull shown in Figure 3 by the polytope with the dark edges with a volume of 172.59 units and the outer convex polytope with a volume of 209.8 units, resulting in a feasibility metric of 0.8226. The outer polytope is shown in Figure 3 with the dark dotted edges. Computationally, the proposed approach requires the solution of seven nonlinear and five linear programs for all iterations and converges in four simplicial iterations. All computations in this article are performed on a Dell 933 Mhz Pc with a Linux operating system and a convergence parameter of 10^{-4}. On average, the NLPs required 25 iterations per run and the LPs converge in five iterations. Note that the number of linear programs required in this problem are considerably lower due to the low dimensionality of the problem that allows the determination of the largest tangent plane in each simplicial iteration directly from the Qhull algorithm (Barber et al., 1996) by computing the area of each facet of the convex hull. To illustrate the independence of the proposed technique from the nominal point location, the nominal points were changed from $(\theta_1, \theta_2) = (2.5, 20)$ to $(\theta_1, \theta_2) = (3, 30)$ and the analysis was performed again. It is observed that both the flexibility index and the convex hull generated by the approach of Ierapetritou (2001) showed a change to 0.195 and FCHR = 0.145, which are shown in Figure 4 as the rectangular and the light shaded region, respectively. The simplicial approximation approach results in a slight increase in volume of the inscribed convex hull to 178.56 units, and the outer convex polytope volume slightly decreased to 204.83 units, as shown in Figure 4. This gives rise to a new feasibility metric of 0.872, as compared to 0.823 obtained using different nominal points. Moreover, one can notice by comparing Figure 3 and Figure 4 that, although the inscribed convex hull region is approximately the same, the flexibility region and the region inscribed following the approach of Ierapetritou (2001) are very much different. Thus, it is shown that the proposed approach offers the additional advantage of being almost independent of the nominal points, as compared to the existing approaches.

3-D Case. The second case study considered here is an example from Ierapetritou (2001) with three uncertain parameters. The constraints describing the feasible region of the design (d_1, d_2) have the following form

$$f_1 = -z - \theta_1 + 0.5 \times \theta_2^2 + 2.0 \times \theta_3^2 + d_1 - 3 \times d_2 - 8 \le 0$$

$$f_2 = -z - \theta_1/3 - \theta_2 - \theta_3/3 + d_2 + 8/3 \le 0$$

$$f_3 = z + \theta_1 \times \theta_1 - \theta_2 - d_1 + \theta_3 - 4 \le 0$$

where z is the control variable, and θ_1, θ_2, θ_3 are the uncertain parameters with the nominal value of $\theta_1^N = \theta_2^N = \theta_3^N = 2$ and expected deviations $\Delta\theta_1^{\pm} = \Delta\theta_1^{\pm} = \Delta\theta_1^{\pm} = 2$. All the constraints are jointly convex on (θ) and (z). The design examined here corresponds to $(d_1, d_2) = (3,1)$. Using the approach of Ierapetritou (2001), the feasible region is approximated with a convex hull of volume of 12.16 units and a FCHR = 0.19, which is shown as the light shaded area in Figure 5. The proposed approach is then applied resulting in a feasible region, approximated by a convex hull that has an increased volume of 14.69 units and is shown in Figure 5 by the polyhedron with the darker edge and the outer convex polytope that has a volume 25.29 units. This is shown in Figure 5 with the dark dotted edges, resulting in a new feasibility metric of 0.581. Computationally, the proposed approach requires the solution of 14 nonlinear and 44 linear programs and converges in ten simplicial iterations. The NLPs on average converge in ten iterations per run and the LPs converge in seven.

Pump Design Problem. The third case study considered is the pump and pipe example in Swaney and Grossmann

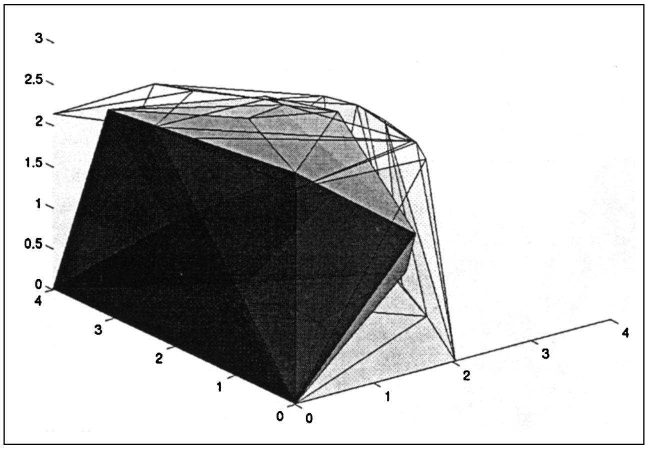

Figure 5. Simplicial convex hull for a 3-D feasible region.

(1985a). This problem involves a centrifugal pump which transports liquid at a flow rate m from its source at pressure P_1 through a pipe to its destination at a 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 design corresponds to the values of $D = 0.0762$ m, $H = 1.3$ kJ/kg, $W = 31.2$ KW, and $C_v^{\max} = 0.0577$. The valve coefficient C_v is the control variable. m, P_2, k, η are considered as uncertain parameters in this problem with expected deviations and nominal points, as shown in Table 1.

After elimination of the state variables, the constraints for this problem are expressed as

$$f_1 = P_1 + \rho \times H - \frac{m^2}{\rho \times c_v^2} - k \times m^{1.84} \times D^{-5.16} - P_2 - \epsilon \leq 0.0$$

$$f_2 = -P_1 - \rho \times H + \frac{m^2}{\rho \times c_v^2} + k \times m^{1.84} \times D^{-5.16} + P_2 - \epsilon \leq 0.0$$

$$f_3 = m \times H - \eta \times \hat{W} \leq 0.0$$

$$f_4 = c_v - c_v^{\max} \leq 0.0$$

$$f_5 = -c_v + r \times c_v^{\max} \leq 0.0$$

Since the above problem is nonconvex, the following exponential transformation is applied

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

where m', C_v', k' are the new transformed variables. The problem is further transformed using two new variables, $x = 2m' - 2C_v'$ and $y = k' + 1.84m'$, so that the constraints can now be expressed as

$$f_1 = -1{,}380 + 0.001\exp(x) + 0.587641\exp(y) + P_2 \geq 0$$

$$f_2 = -1420 + 0.001\exp(x) + 0.587641\exp(y) + P_2 \leq 0$$

$$f_3 = 1.3\exp(m') - 31.2\eta \leq 0.0$$

$$f_4 = \exp(c_v') - c_v^{\max} \leq 0.0$$

$$f_5 = -\exp(c_v') + 0.05c_v^{\max} \leq 0.0$$

The problem is, thus, transformed to a convex model and can be solved using a local optimization solver. The proposed approach is then applied resulting in a feasible region approximated by a convex hull of volume 24.38 unit and an outer convex polytope with the volume 36 units and a new feasibility metric of 0.65. Although, the dimensionality of the problem is high, the computational requirement does not increase drastically and, in particular, 14 nonlinear and 50 linear programs have to be solved and the procedure converges in nine simplicial iterations. The NLPs on an average converge in 25 iterations per run and the LPs in twelve.

Air separation plant: determination of operating envelopes

The case study presented in this section is the optimization of an air separation unit (ASU) for the cryogenic separation of air into gaseous and liquid oxygen and nitrogen products. The main product of the plant is gaseous oxygen with coproducts of liquid oxygen, liquid nitrogen and gaseous nitrogen. An ASU consists of four unit operations: heat exchanger, refrigeration, distillation and compression. Depending on the size and type of equipment used for each process a number of different options and suboptions are available, representing various unit operations decisions. The number of options and suboptions for each unit are as shown in Table 2.

The objective of the problem is to determine the minimum cost of production of gaseous oxygen that meets the given production rate of gaseous oxygen at a specified pressure and composition by the appropriate selection of equipment and operating conditions. The model constraints represent the mass and energy balance equations along with variable bounds. The optimization problem is a mixed integer nonlinear programming problem and is solved using branch and bound solution procedure. Details of the model equations are available in Sirdeshpande et al. (2001). By selecting a specific case of a product requirement, the above optimization problem is solved to determine the design as shown in Table 3. The feasibility of this design is then examined in terms of the flow rate of gaseous oxygen F_{GOX} and the flow rate of liquid

Table 1. Uncertain Parameters: Example 4

Parameter	P_2 (kPa)	m (kg/s)	η	k (kPa)(kg/a)$^{-1.84}$(m$^{5.16}$)
Nominal Value	800	10	0.5	9.101×10^{-6}
Positive Dev.	200	2	0.05	$0.45505.101 \times 10^{-6}$
Negative Dev.	500	5	0.05	$0.45505.101 \times 10^{-6}$

Table 2. Options for the Unit Operations in the ASU

Unit Operation	No. of Main Options	No. of Suboptions
Heat Exchanger	2	
Distillation Col.	4	4
Refrigerator	4	2
Compressor	4	2

Table 3. Optimized Equipment Selection for the BOC ASU

	Main Option	Suboption
Heat Exchanger	2	
Distillation Column	4	1
Refrigerator	2	3
Compressor	4	1

oxygen F_{LOX}. The nominal point for the operating variables corresponds to $F_{GOX} = 800 Mtpd$ and $F_{LOX} = 170 Mtpd$ with expected deviations of $\Delta F_{GOX}^{+} = 400$ Mtpd, $\Delta F_{GOX}^{-} = 270 Mtpd$, $\Delta F_{LOX}^{+} = 64 Mtpd$ and $\Delta F_{LOX}^{-} = 70 Mtpd$. The design pressure is $P_{GOX} = 9$ atm and the desired product purity of oxygen = 95%. The feasible region is first approximatied by the approach of Ierapetritou (2001) and the convex hull is found to have the volume of 62,221.39 units and a FCHR = 0.69 and is shown as the dark shaded area in Figure 6. The proposed approach is then applied resulting in a feasible region, approximated by a convex hull that has an increased volume of 63,563.72 units. This is shown in Figure 6 by the polyhedron with the darker edge and the outer convex polytope that has a volume of 72,358.4 units, as shown in Figure 6 with the dark dotted edges, thus resulting in a new feasibility metric of 0.879. Note that, for this case study, since the constraints are not explicitly defined, the derivatives of the boundary of the feasible regions at the simplicial points are determined numerically using the procedure described earlier. The computational requirement for this case study required the solution of 44 nonlinear and nine linear programs and converges in eight simplicial iterations. The NLP for each simplicial iteration converge in an average of seven iterations per run, and the NLP for determining the derivatives converge in 150 iterations per run and the LPs converge in seven. Note that the result constitutes an excellent representation of the actual feasible region compared with the flexibility index method. Another important outcome of this approach is the description of the feasible space by a set of linear equations, which describe the half-planes that form the convex hull. By obtaining this information, there is no need to work with the original nonlinear model in order to evaluate the feasibility of any given point in the (F_{GOX}, F_{LOX}) operating space.

Reduced kinetics model: identification of range of validity

The problem addressed in this section is to evaluate the range of validity in terms of the initial conditions of a reduced kinetic model (Sirdeshpande et al., 2001). The system studied is the H_2/O_2 combustion problem at low pressure and is assumed to take place in an isobaric batch reactor with premixed reactants and well mixed contents operating isothermally and adiabatically. Details of the model reduction process are available in Sirdeshpande et al. (2001) and Androulakis (2000). After the reduction has been performed, it is of great interest to evaluate the range of conditions under which the reduced model could be used with a required accuracy. In other words to evaluate the range of initial conditions that would result in output species profiles that are in close agreement with the profiles generated by the full mechanism. Considering the initial oxygen mole fraction X_{O_2} and initial temperature T_0 as the conditions of interest with the following bounds

$$\Delta X_{O_2}^{+} = 0.85,\ \Delta X_{O_2}^{-} = 0.15,\ \Delta T_0^{+} = 250,\ \Delta T_0^{-} = 400$$

around a nominal point $X_{O_2} = 0.15$ and $T_n = 1{,}250$ K, the proposed approach can be applied to evaluate accurately the range of validity of a given mechanism. First, to determine the feasible region of the design of this reduced mechanism, a grid search procedure is performed on the entire feasible range of operation to obtain the boundary of the feasible region. The range of validity is approximated by the simplicial approximation approach, and the convex hull obtained is shown in Figure 7 as the polyhedron with dark edges and represents 89.26% of the overall considered range. Compared to the flexibility index approach that results in the retangular region shown in Figure 7, the proposed approach determines the range of validity much more accurately. Thus, the outer envelope is not obtained in this case study. Also, a large increase is achieved compared to the proposed approach of Ierapetritou (2001) that obtained a FCHR of 0.351, and, thus, represents only 35.1% of the overall space of vari-

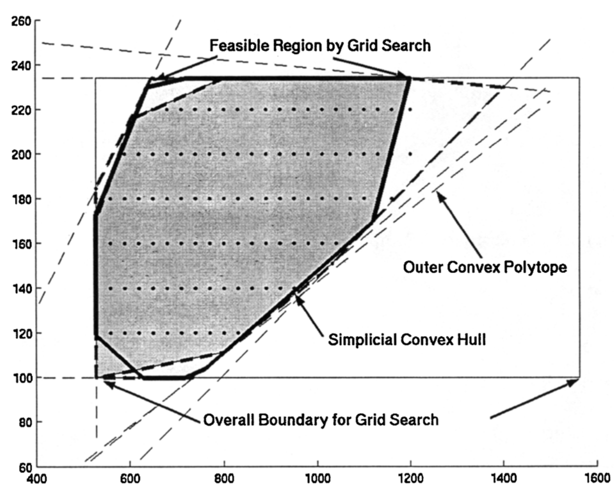

Figure 6. Simplicial convex hull for the BOC case study.

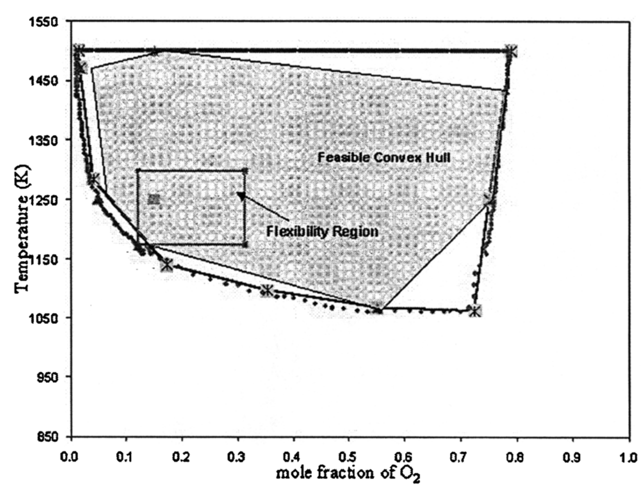

Figure 7. Simplicial convex hull for the kinetics case study.

ability of the initial conditions. Computationally, the proposed approach required the solution of eight nonlinear and six linear programs and converged in five simplicial iterations. The differential equations were solved using LSODE (Hindmarsh, 1983), and the thermophysical properties and reaction rates appearing in the ODs were evaluated using the CHEMKIN-III package. The NLPs on an average required twelve iterations per run and the LPs required five.

Discussion and Future Directions

A new approach is presented to identify the operating envelopes where process operation is feasible. The basic idea of the proposed approach is to iteratively improve the approximation of the boundary of the feasible region by determining points at the boundary using the simplicial approximation approach (Director and Hachtel, 1977), which are used to inscribe a convex hull inside the feasible region that serves as a lower bound of the feasible space and then to determine the outer envelope by generating the tangent planes at these points. This serves as an upper bound of the feasible region and is used to determine a new feasibility metric that accurately describes the design feasibility. The convex hull is computed using the *Quickhull Algorithm,* which is an incremental algorithm for evaluating the convex hull given a set of points. 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. In all the case studies considered in this article we found that the proposed approach results in a much better description of the feasible space and was independent of the nominal point. Work is currently underway regarding the extension of the approach to a nonvonvex case and to a tighter convergence of the feasible region between the simplicial hull and its outer convex envelope. Another area of future research is the effect on the accuracy of the results by using the largest hyper-plane and not the largest tangent hyper-plane, as that would greatly reduce the number of linear programs that have to be solved.

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