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Dimitrios K. Varvarezos
Carnegie Mellon University

Ignacio E. Grossmann

Lorenz T. Biegler

Carnegie Mellon University.Engineering Design Research Center.

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D. Varvarezos, E. Grossmann, L. Biegler

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A Sensitivity Based Approach for Flexibility Analysis and Design of Linear Process Systems

Dimitrios K. Varvarezos, Ignacio E. Grossmann* and Lorenz T. Biegler
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

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* Author to whom all correspondence should be addressed.

Abstract

A novel solution approach that addresses uncertainty, flexibility evaluation and design of linear processes is presented, based on sensitivity analysis and linear programming. The idea is to evaluate the flexibility index of a process by successively expanding within a bounding search procedure a hyper-rectangle around a nominal point in the uncertainty parameter domain, thus expanding the limits of feasibility for an existing design. Sensitivity information, derived from the solution of a special form of the imbedded min-max problem, is utilized for the identification and investigation of the supporting active sets. Since the proposed approach automatically generates all the supporting active sets, it is incorporated within a design model for automatically generating flexibility constraints. As demonstrated by example problems, this approach identifies *all* critical points, including multiple equidistant ones, without enumerating (explicitly or implicitly) all possible active sets, and considering only the supporting active sets. Therefore, it offers an efficient and constructive way for the evaluation and design of linear processes.

1. Introduction

Addressing uncertainty at the design stage of a plant is a very significant problem for two reasons. On the one hand, it is only realistic to expect variations in the input and output streams of a chemical plant. These variations can be either the result of market forces (changing product demands) or natural occurrences (changing feed compositions or upstream equipment failures). On the other hand, uncertainty is always inherently present in the modeling parameters such as physical properties (kinetic, transfer or thermodynamic data) which are predicted or measured with a finite accuracy and often within a substantial margin of error. In addition to the above, even the models themselves may not be accurate and hence additional uncertainty has to be accounted for. To address these uncertainties, the common practice is to overdesign or perform ad-hoc case studies over the uncertain parameter domain. Over the last decade, considerable effort has been devoted to developing a systematic approach for designing flexible chemical plants (for a review on the state of the art, see Grossmann and Straub, 1992). The proposed approaches can be classified in two broad classes: (i) deterministic, in which the parameter uncertainty is described through bounds of expected deviations, and (ii) stochastic, that describes the uncertainty through a probability distribution function.

It is the purpose of this paper to develop a computationally efficient framework for addressing the evaluation of flexibility and the optimal design of a plant for a desired flexibility in the case of a linear deterministic model. The flexibility index by Swaney and Grossmann (1985a) is considered as well as the design model for fixed flexibility by Pistikopoulos and Grossmann (1988). Since a major difficulty is the identification of the active sets of constraints that limit flexibility, a new method for the flexibility analysis is proposed that is based on sensitivity analysis and has the feature of systematically identifying all the *supporting active sets* for a fixed design, which is further utilized in the flexibility design problem. The proposed approach uses the sensitivity analysis of the feasibility function with respect to the uncertain modeling parameters. This methodology addresses the problem in a rigorous way and at the same time reduces the combinatorial search involved in previous methods. The rest of the paper is organized as follows. In the next section we present the problem statement and a brief review of existing approaches to this problem. Sections 3 and 4 describe the development of the proposed method for evaluating flexibility. Section 5 states the detailed of the algorithm and section 6 illustrates the application to several example problems. Section 7 presents a brief account of the proposed method. In section 8 we extend these ideas to a design procedure for achieving a given flexibility, and we demonstrate the method with example problems. Finally present the conclusions of this work in section 9.

2. **Problem Statement and Background**

The model of the process can be described, in the case where the topology is fixed, by a set of equations and inequalities involving continuous variables of the form:

$$h(d,\mathrm{W}«\mathrm{O}= \qquad \text{(F0)}$$

$$g(d,z,x,0)<0$$

where the variables are defined as follows:

d e R^nd - denotes an *rid* vector of design variables that defines the structure and equipment sizes of the process

zeR''z - denotes an n_z vector of control variables that can be adjusted during plant operation

*xeR^n** - denotes an n_x vector of state variables that describes the behavior of the process

6eR^n° - denotes an *n$* vector of uncertain parameters.

For simplicity in the presentation and consistency with the existing literature (Grossmann and Floudas, 1987), it is assumed that the state variables in (FO) are eliminated from the equations and thus the model reduces to:

$$/,(z,6U)\leq 0 \qquad jeJ$$

Note, however, that in the development of the proposed methodology this projection will not be necessary.

For a given design d^N, the first important question is to determine whether this design is feasible for a realization of the uncertain parameters 0^, also known as the *feasibility problem* (Fl). The formulation of this problem (Halemane and Grossmann, 1983) is:

$$\psi(\theta,d) = \min_{z,u} u \qquad \text{(Fl)}$$

$$\text{s.t.} \qquad fj(z,0,d)\leq u \quad jeJ; \quad ueR^1$$

Note that problem (Fl) is an optimization problem where the objective is to find a point z*, for fixed d and 0, such that the maximum potential constraint violation is minimized. However, u is in principle a function of d and 9, and expressed in that form it represents the projected

feasibility function. The *projected feasibility function* y<0, *d)* is a key concept in the flexibility analysis and its construction is an important and challenging task (see Grossmann and Straub, 1991). As can be deduced from (Fl), *y/≤* 0 indicates feasibility and *y/>* 0, infeasibility.

The problem of evaluating flexibility, also known as the *flexibility index problem* (F2), is to determine the maximum deviation *8* that a given design d^N can tolerate, such that every point *9* in the uncertain parameter space: *T(8)* = J01 6^N - *8A6~* < 0 <0^N + <5A0$^+$} is feasible. Here, A9$^+$ and A8- are the expected deviations of uncertain parameters in the positive and negative direction. The formulation for this problem (Swaney and Grossmann, 1985a), is:

$$
\begin{aligned}
&F = \max\ 8 \\
&s.t.\ \max_{\theta \in T(\delta)} y/(0,d) \leq 0 \\
&\qquad 8 \geq 0 \qquad 8eR^{(}
\end{aligned}
\tag{F2}
$$

As seen from the implicit form of the *projected feasibility function* y(0,d)> problem (F2) cannot be directly solved unless \\|/ is determined. The simplest way around this problem (see Swaney and Grossmann, 1985b) is to determine the flexibility index in (F2) by vertex enumeration search in which the maximum displacement is computed along each vertex direction, thus avoiding the explicit construction of *y/.* This vertex enumeration scheme relies on the assumption that the critical points 0* lie at the vertices of T(8*), which is valid for the case of a linear model and in general only if certain convexity conditions hold. The drawback with this approach, however, is that it requires the solution of 2^no optimization problems, and therefore, it scales exponentially with the number of uncertain parameters. Recently, though, Kabatek and Swaney (1992) have developed an implicit enumeration procedure that does not require the exhaustive enumeration of all vertices.

An alternative method for evaluating the flexibility index that does not rely on the assumption that critical points correspond to vertices, is the active set strategy by Grossmann and Floudas (1987). In this method the key idea is that the feasible region projected into the space of d and 8, can be expressed in terms of active sets of constraints/}(z, 0, *d)* = w, je JA^k, k=l, nA& where nAS is the number of possible active sets of *fj.* These active sets are defined by all subsets of non-zero multipliers that satisfy the Kuhn-Tucker conditions of (Fl):

$$
\begin{aligned}
&\sum_{j \in J_A^k} \lambda_j^k = 1 \\
&55 \frac{\partial f_j}{\partial z} = 0
\end{aligned}
\tag{2.1}
$$

By reformulating problem (F2) for evaluating the flexibility index, and using (2.1) with 0-1 variables for the complementarity conditions and slacks, we get a mixed-integer optimization problem that can explicitly solve (F2) without having to find *a-priori* all the active sets. This method essentially amounts to solving an MINLP problem (or MILP if all constraints are linear) with $n_f = \text{card}\{J\}$ binary variables. In the worst case, this method scales exponentially with the number of projected constraints n_f.

At the design stage the goal is to design a plant with a desired flexibility F. This problem calls for the optimization of an objective function involving the design variables which invokes as a constraint a desired flexibility F, in the form of problem (F2). The formulation of the design problem is then:

$$
\begin{aligned}
&\min \ \phi(d) \\
&s.t. \ \ f_j(z,\theta,d) \le 0 \quad \forall j \in J, \quad \forall \theta \in T(F) \\
&\quad T(F) = \{\theta \mid \theta^N - F\Delta\theta^- \le \theta \le \theta^N + F\Delta\theta^+\}
\end{aligned}
\tag{F3}
$$

In order to address this design problem with explicit linear flexibility constraints, Pistikopoulos and Grossmann (1988) proposed a systematic enumeration procedure to identify all the n_{AS} active sets of constraints, provided that the corresponding sub-matrices in (2.1) are of full rank. In this way the following the design problem (F3) can be reformulated as:

$$
\begin{aligned}
&\min_d \ \phi(d) \\
&s.t. \quad \max_{\theta \in T(F)} \ \psi^k(\theta,d) \le 0 \qquad k = 1, n_{AS}
\end{aligned}
$$

where the projected feasibility function ψ^k for each active set is given by:

$$
\psi^k(\theta,d) = \sum_{j \in J_A^k} \lambda_j^k f_j(z,\theta,d) \quad k = 1, n_{AS} \tag{2.2}
$$

Since the number of active sets can become rather large, these authors also proposed a method that requires the solution of a sequence of MILP problems to identify subsets of active sets. Feasibility must be verified in this case and, if needed, proceed in an iterative fashion.

3. Flexibility Evaluation through Sensitivity Analysis

In order to develop a method for flexibility analysis that is computationally efficient, and still generate all supporting, or non-redundant, active sets and determine the flexibility index for a given design, we propose a sensitivity analysis based method. Here, we define as *supporting active sets* (ASs), all the active sets that define the segments (or supports) of the feasibility function \|/ within a hyper-rectangle with size F. This concept of the supporting active sets as well as the distinction between them and the redundant ones is illustrated in Figure 1. A major motivation is also to solve problem (F4) more efficiently without having to generate a-priori all active sets. The basic idea in the proposed method is to start with a nominal value of the uncertain parameters and then, based on the sensitivity information of the flexibility problem (Fl) with respect to the uncertain parameters, systematically expand within a bounding search procedure the flexibility boundaries from the inside out, identifying non-redundant active sets as defined by (2.2) for a fixed design d. Here, the main assumption is linearity in the performance models.

Sensitivity analysis with respect to the uncertain parameters can be used in determining the flexibility limits -or the flexibility index- of an existing or proposed design. The continuous uncertain parameters, 0, in the process operation problem are fixed at a nominal point *Oft* along with the existing design d^N. Considering model (FO) we can write the feasibility problem (PO) in a way similar to (Fl) as:

$$
\begin{aligned}
&\min w \\
&s.t.\quad h(x,z,d,\theta^N) = 0 \\
&\quad g(x,z,d^N,\theta^N) + s = u \\
&\quad x^L \leq x \leq x^u \\
&\quad z^L \leq z \leq z^u \\
&\quad s \geq 0
\end{aligned}
\tag{PO}
$$

For the linear case (PO) has the special form (PI):

$$
\begin{aligned}
&\min w \\
&s.t.\quad A[x^T|z^T]^T + C\theta^N + a = 0 \\
&\quad D[x^T|z^T]^T + E\theta^N + c + s = u \\
&\quad s \geq 0 \qquad u \in \Re^1
\end{aligned}
\tag{P1}
$$

where D incorporates all inequality constraints as well as bounds on x and z, so that there are no explicit bounds on them in (PI) (of course the bounds are still included, but expressed in terms of slack variables). In the above formulations we minimize the worst constraint violation so that if $w^* \leq 0$ the design is feasible for the given value of the uncertain parameters, θ^N. The main difference, however, between formulation (Fl) and the one proposed here, is the inclusion of the slack variables. It is interesting to note that the MILP formulation by Grossmann and Floudas (1987) also incorporates slacks. However, as shown in this paper the use of slack variables in the inequality constraints enables us to capture with the infinity norm all the trends in changes of the active set, through the sensitivity information rather than through the use of binary 0-1 variables. As will be seen later on, this is a key concept for the development of this method.

Sensitivity information with respect to the uncertain parameters, 9, can be obtained by means of differentiating the optimality conditions of the original feasibility problem (PI) with respect to 9 and setting them equal to zero. At the optimum of (PI) we have:

$$\bar{A}b + \bar{A}_N b_N + \bar{C}6^N + \bar{a} = 0 \qquad (3.1)$$

where b and bN are the basic and non-basic variables respectively, and $\bar{A}, \bar{C}$ *and* $\bar{a}$ are the augmented matrices and vectors that include the two type of equalities in (PI). If we differentiate the above with respect to 9 we have:

$$\bar{A}\frac{db}{de}^T + \bar{A}_N\frac{db_N}{d0}^T = -\bar{C} \qquad (3.2)$$

since the analysis is carried for the current basis the non-basic variables are fixed and thus they have zero sensitivity:

$$\wedge = 0 \qquad (3.3)$$

and so (3.2) becomes:

$$(3.4)$$

This information defines the optimal trends for all the basic variables with respect to the parameters 9, and since the models are linear, conditions (3.3) and (3.4) are exact for a given active set. Moreover, dependencies or correlation between the uncertain parameters can be also addressed through this sensitivity analysis, as shown in Appendix A. Note that from a flexibility analysis standpoint the solution of (PI) automatically identifies an active set, according to definition (2.1), since all the relevant multipliers X^k are given by the optimal solution of (PI).

The idea in the proposed method is to progressively generate and identify all the supporting active sets, in order of proximity to the nominal point 9^N. In order to accomplish that, we need to introduce the concept of the *allowable displacement distance,* 5, in the shortest directions pointing towards all neighboring active sets and infeasibility barriers. As stated earlier, sensitivity analysis provides all the information relevant to the optimal changes of all the basic variables of (PI) within this active set. Utilizing this information, we can express the feasible region of (PI) for a given active set in terms of the *allowable displacement distance, 8,* the basic slacks Sj and u.

For a given active set, ke AS, the corresponding feasible region FR projected in the parameter space, 0, and expressed parametrically with the scalar parameter 5 (8 ≥ 0), is given by the following set of constraints:

$$\left.\begin{array}{ll} 0 \le s_j^k + \dfrac{ds}{d\theta}^T_j (A0)^q 8 & V/eB* \\ 0 \ge u^k + \dfrac{du}{d6}^T (Ad)"S & \end{array}\right\} V? \qquad \text{(P2)}$$

where k denotes the optimum of (PI) for active set k, B the set of *basic slack variables* defined as B = {j I j: index of all slack variables Sj in (PI), currently basic} (note that only the slack variables are explicitly bounded in (PI)); $\dfrac{ds_j}{dd}$ are the sensitivities of the basic variables computed at the optimum of (PI) as presented earlier; (A0>1 are all vertex directions in the parameter space. Note also that in the above formulation the corresponding inequalities for the multipliers are not needed since their sensitivity is zero *(dX/dO* = 0 for linear programming problems) and therefore are satisfied for all 6.

Within active set k and for each *basic slack variable Sj,* we introduce $5^*_{s_j}$ to be the maximum feasible scaled displacements from 0^N in the space of the uncertain parameters, without making the current basic slack variables non-basic, and by considering all vertex directions and given displacements $AQ^{\pm}$. In the same context we define 5^*_u to be the scaled distance, within the current active set k, to an infeasibility barrier (where u > 0). For practical purposes we distinguish between 5^*_u and $S^k_{s_j}$ since they represent different measures:

$5^*_{s_j}$ is the shortest distance (within the current active set k) to an adjacent active set involving the currently basic variable SJ

5^*_u is the shortest distance to an infeasibility boundary (within the current active set k) following the direction of minimax constraint violation (u ≥ 0)

The proposed procedure for finding the flexibility index can be viewed as the progressive expansion of a hyper-cube (or hyper-rectangle in general) in the projected parameter space, centered at the nominal parameter point G^N. As this hyper-cube expands uniformly, it encounters adjacent active sets and points of infeasibility. As new active sets are encountered, problem (PI) is solved at the new critical point (0^C) and the corresponding sensitivities are evaluated (in fact in order to avoid degeneracy it should be solved at *6C+e* in the present direction). As we move to a new active set k+1 and in order to evaluate the new *allowable displacement distances* ($5^{*+1}_{s_j}$, 5^{*+1}_{u}), we have to project them back to the nominal point 6^N. The procedure is terminated when an infeasible point is encountered in this search so that the hypercube cannot expand further in a feasible manner. The following property relates the above *allowable displacement distances* to the lower bound on flexibility.

Property 1. The minimum among the distances $8^*_{s_j}$ *and* 5^*_u, is a lower bound to the flexibility index ($F^L = \min_j\{5^*_{s_j}, 5^*_u\}$). (The proof is given in Appendix B).

The above property can be qualitatively explained based on the fact that (P2) is the projected feasibility region and all the active sets are generated in order of proximity to 9^N. Based on the above argument it can be also seen that the minimum of all generated 8_u^k> is an upper bound to the flexibility index $F^u = \min_{k=1,K}\{5^*_u\}$). The proposed flexibility evaluation procedure is terminated when $F^u = F^L = F$, or equivalently when $F = \min_j\{5_{5_j}, 8_U\} = S_u$. (These concepts are illustrated below and formally stated in Properties 2 and 3).

4. Computation of Feasibility Displacements

All changes in the active sets are captured through the sensitivity of the variables, provided that the solution of (PI) is non-degenerate. This is true, since any basis change implies that one non-basic variable will become basic and one basic variable will become non-basic. In the representation of the feasible region (P2) we can find all $(8_{S_j}, S_u)$ analytically with the following procedure. Note that (P2) can be re-written as:

$$\left.\begin{array}{l} -\delta\,\xi_q \le s_j^* \quad \forall j \in B \\ \delta\,\xi_q \le -u^* \end{array}\right\} \forall q \qquad \textbf{(P2.1)}$$

where $\xi_{jq} = \frac{ds_j}{d\theta}(\Delta\theta)^q$ or $\xi_q = \frac{du}{d\theta}(\Delta\theta)^q$. From the above it is clear that only one value of δ per variable bj can be a candidate for defining the shortest distance to a new active set. We can compute:

$$\delta_{s_j} = \frac{s_j^*}{-\min_q \xi_{jq}} = \frac{s_j^*}{-\sum_{p=1}^{n_\theta} \min\left(\frac{db_j}{d\theta_p}\Delta\theta_p^+,\ \frac{db_j}{d\theta_p}\Delta\theta_p^-\right)} \tag{4.1}$$

$$\delta_u = \frac{u^*}{\max_q \xi_q} = \frac{u^*}{\sum_p \max\left(\frac{du}{d\theta_p}\Delta\theta_p^+,\ \frac{du}{d\theta_p}\Delta\theta_p^-\right)} \tag{4.2}$$

As stated earlier, from Appendix B it follows that the largest δ that satisfies (P2) is a lowerbound to the flexibility index, given by: $\delta = F^L = \min_j \{\delta_{s_j}, \delta_u\}$ (4.3)

Property 2. The largest δ that satisfies (P2) is given by (4.3).

<u>Proof:</u> For the constraints in (P.2.1) we consider two cases where ξ_q is positive or negative. In the $\xi_q = 0$ case, any δ is a trivial solution to (P.2)\ In addition, if we consider the maximization of δ, (P.2.1) can be written as:

$$
\begin{aligned}
F = \max\ & \delta \\
\text{s.t. } & \delta \ge \frac{s_j^*}{|\xi_{jq}|} && \forall q \mid \xi_{jq} \ge 0; \quad \forall j \in B \\
& \delta \le \frac{s_j^*}{|\xi_{jq}|} && \forall q \mid \xi_{jq} < 0; \quad \forall j \in B \\
& \delta \le \frac{u^*}{|\xi_q|} && \forall q \mid \xi_q \ge 0 \\
& \delta \ge \frac{u^*}{|\xi_q|} && \forall q \mid \xi_q < 0
\end{aligned}
\tag{P2-2}
$$

Since the first and fourth set of inequalities are redundant (it is a maximization problem) they can be dropped, so that finally we have:

F^L = max S

$$s.t.\ \ 8 \leq \frac{s_J^*}{-\pi_q} T\text{-}\wedge \qquad VjeB \qquad \textbf{(P2.3)}$$

$$S \leq \frac{-u^*}{\max_q(\xi_q)}$$

By using (P2.3) with the definitions (4.1) and (4.2), we conclude that the maximum 5 in (P2) isgiven by (4.3) r.

From the above analysis it is clear that each 8_{S_j} has an associated *critical direction* D_{s_j} in the parameter space, defined for each variable sj as a vector with elements:

$$D\wedge sign(A0_{jtPmia}l \qquad p = l,n_e \qquad \textbf{(4.4)}$$

where $A0_{j\%Pwlm}$ refers to the corresponding terms of $\min\left\{\frac{ds_j}{d\theta_p}\text{-}40\theta^*, \frac{ds\text{-}}{d\theta_p}{}^L A0\theta\right\}$. Note that if the sensitivity $\frac{ds_j}{d0_p}$ is zero, any (e.g. +1 or -1) direction along this axis can be selected. This is equivalent to multiple vertices having the same flexibility. Note, form (P2.1), that the number of 8's considered in each active set is/i£ + 1 (where nB is the number of *basic slack variables* Sj in **(PD).**

5. Algorithm for Flexibility Evaluation

The proposed method can be viewed as a constructive approach to the evaluation of flexibility. Starting from a nominal point and zero flexibility, we expand the boundaries of feasible operation as we move from the nominal point outwards with the implicit solution of problem (P2), going through all the changes in *supporting* active set whose lower bound $F^L \leq F$. At each active set k that is generated we evaluate $5^*_{s_j}$ *and* 8^k_u. If at any point $8_u{}^k$ is the smallest, the lower and the upper bound become identical and the search is stopped. Otherwise, we order the displacements for all past active sets in a list A, in ascending order, keeping only the elements $\delta^*_{s_j}$ that are lower than the current upper bound on the flexibility F^u. Each time we visit a new active set, we update the lower bound on the flexibility F^L. Eventually, as shown later in Property 3, $F^u = F^L = F$.

It is important for this method to guarantee that it will never go back to an active set already visited. This is ensured by an added provision according to which at any active set k, the variable that just entered the basis (SJ') is not considered in the analysis. Therefore, the new basis is one that has not been examined before. Since the new point 9^C is defined as marginally into the new active set, variable Sj' has just entered the basis and therefore has a marginally positive value which in turn gives rise to a corresponding 8 of value £. The above provision can also be seen as an anti-cycling scheme (although it is an obvious step in the construction of this method). Formal proof of the above is provided in Property 3. The above concepts are illustrated in the following example.

Example 1. In order to demonstrate this method we introduce an example problem consisting of three inequality constraints, one unbounded control variable z and one uncertain parameter 0. In this problem (El), we need to find the flexibility index for a nominal value $0^N = 2$ and symmetric deviations of $A0 = \pm 2$ (see Fig. 2).

$$\left.\begin{array}{l} f_x = z - 0 - 2.667 \le 0 \\ f_2 = -z - \frac{\theta}{3} + 2.667 \le 0 \\ f_3 = z + 0 - 5.333 \le 0 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} z - \theta - 2.667 + s_1 - u = 0 \\ -z - \frac{Q}{2} + 2.667 + s_2 - u = 0 \\ z + \frac{\theta}{3} - 5.333 + s_3 - u = 0 \end{array}\right. \qquad \text{(El)}$$

Solving the above by minimizing u with $0^N = 2$ we have:

$$\{6=2\}: \Rightarrow \left\{\begin{array}{l} u = -0.667 \\ s_1 = 1.333 \\ s_2 = 0. \\ s_3 = 0. \\ z = 2.667 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \textit{Basic Variables: } [s_1, u] \\ \textit{Sen****} \frac{ds_1}{d\theta} = \frac{du}{d\theta} = \frac{1}{3} \\ \textit{Distance: } S_{s_1} = \frac{1}{3};\ S_u = 1] \\ \textit{Directions: } D_{s_1} = -1;\ D_u = 1 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} F^L = \delta_{s_1} = 0.333 \\ F^U = \delta_u = 1 \end{array}\right\}$$

which gives rise to active set $(AS)^1$ ={f2, f3} with a lower bound for the flexibility index F^L = 0.333. As seen in Figure 2, the limiting point is then A (0 = 1.333) which is at the boundary of a change to the active set $(AS)^2$ = {fi, f2l- Now we can move to the critical parameter point 0^C = 1.333 and solve again the feasibility problem that gives:

$$\left\{\begin{array}{l}\theta = 2 + \frac{1}{3}2(-1) - \varepsilon = \\ \quad = 1.333 - \varepsilon\end{array}\right\} \Rightarrow \left\{\begin{array}{l} u = -0.889 \\ s_1 = 0. \\ s_2 = 0. \\ s_3 = \varepsilon \\ z = 3.111\end{array}\right\} \Rightarrow \left\{\begin{array}{l} \textit{Basic Variables: } [s_3^*, u] \\ \textit{Sensitivity: } \frac{ds_3^*}{d\theta} = -2;\ \frac{du}{d\theta} = \frac{2}{3} \\ \textit{Distance: } \delta_{s_3} = \frac{\varepsilon^*}{4};\ \delta_u = \frac{2}{3} \\ \textit{Proj.Dist. } \delta_{s_3} = \frac{1^*}{3};\ \delta_u = 1 \\ \textit{Directions: } D_{s_3} = 1^*;\ D_u = -1 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} F^L = \delta_u = 1 \\ F^U = \delta_u = 1\end{array}\right\} \Rightarrow F = 1$$

which gives rise to the active set $(AS)^2$ with a lower bound on the flexibility index $F^L = 1$, hence the procedure converges. The asterisk (*) above, refers to the fact that this variable need not be considered since it refers to a variable non-basic in the previous iteration and hence it points towards the active set already visited (the relevant numbers are shown here only for demonstration). Note that for the non-degenerate case, only one basic variable is exchanged between active sets. This information is not relevant to our search since we have already analyzed the corresponding active set (f2, f3). However, the projection of the distance from θ^C to θ^N is necessary in order to establish a common reference point. The above procedure can be also seen graphically on Figure 2.

The algorithm for the above method can be summarized as follows:

***Algorithm I* - Evaluation of the Flexibility Index for a given design**

Step 0. Set iteration count k= 1. Set $\theta^N = \theta^C$. Set $F^L = 0$ and $F^u = \infty$. Set $\bar{B}^k = 0$ and $A^k = 0$.

Step 1. Solve (P1) based on θ^C, define the corresponding active set $(AS)^k$, and evaluate the sensitivities $\frac{ds_L}{d\theta_p}$ using (3.4).

Step 2. Solve (P2) and evaluate all $\bar{\delta}^k_{s_j}, \bar{\delta}^k_u$ as well as $D^k_{s_j}, D^k_u$ for u and all the basic variables $s_j \in \bar{B}^k$ = {j | j: index of a basic slack variable s_j in current active set $(AS)^k$ that also satisfies $s_j \in \bar{B}^{k-1}$ (k>1)}, using (4.1), (4.2) and (4.4). (Note that the definition of $\bar{B}^k$ excludes variables that were non-basic in the previous iteration, and hence prohibits revisiting active sets already considered).

a. Based on the values of $\bar{\delta}^k_{s_j}$ and $\bar{\delta}^k_u$ evaluate the equivalent $\delta^k_{s_j}$ and δ^k_u based on the nominal point (by projecting into the original θ^N if necessary, i.e. in case $\theta^P \neq \theta^N$ and $D^k_{s_j} \neq D^{k-1}_c$). The projection step will be detailed below.

b. Set $F^u = \delta_U = \min\{S_u^*, F^u\}$. Update the set of candidate allowable distances $A^k = \{d_c \mid S'_{s_c} * S^l_c$ and $S'_c < F^u; l = 1, k\}$. Set $F^L = \delta^k_c = \min\{d_c^*, \delta_U\}$ and the associated critical direction D_c^k. If $F^u = F^L$ terminate with $F = F^\wedge = F^L$.

c. Evaluate the new θ^C as follows: $\theta^C = \theta^N + \delta^k_c \Delta d^k_c$. Set $k \leftarrow k+1$. Go to step 1.

~~Projection Scheme~~: The projection of $\bar{\delta}^k_{s_j'}$ to $\delta^k_{s_j'}$ (step 2a) is done through the simultaneous solution of $(AS)^k$ and the fixed bound on the candidate variable S_j' (this is the variable that will define a new active set) along the direction $D^k_{s_j'}$. The reason for this projection is to scale the $\bar{\delta}^k_{s_j'}$ from the local analysis of the current active set, back to our nominal point, θ^N. The corresponding system of linear equations to be solved is:

$$
\begin{aligned}
&A\left[x^T | z^T\right]^T + C\theta + a = 0\\
&D\left[x^T | z^T\right]^T + E\theta^N + c + s = u\\
&\theta = \theta^N + \delta\,(\Delta\theta)^k\\
&s_j = 0 \qquad \forall j \in AS^*\\
&s_j' = 0
\end{aligned}
\tag{5.1}
$$

where the parameters θ are given parametrically with respect to δ.

System (5.1) (which essentially describes the possible intersection of the current active set with the new one that involves S_j') is a square system with a unique solution that corresponds to the projected $\delta^k_{s_j'}$. If, however, the solution of the above system does not exist this indicates that $S^k_{s_j'} = \infty$, so this variable does not participate in any adjacent active set. Note here, that if there are multiple $\bar{\delta}^k_{s_j'}$ with the same critical direction $D^k_{s_j}$ only the smallest needs to be considered for the projection step. The information for the rest is redundant, since it corresponds to a different active set.

If the predicted direction $D^k_{s_j'}$ coincides with the previous direction $(D^k_{s_j'} = D_c^{k-1})$ and $\bar{\delta}^k_{s_j'}$ is the minimum in this direction, then the corresponding projected δ is simply the sum of $\bar{S}^k_{s_j'}$ and S_c^{k-1}, as in Example 1:

$$
\delta^k_{s_j'} = \bar{\delta}^k_{s_j'} + \delta^{k-1}_c
\tag{5.2}
$$

In order to show that the method will not cycle, provided that the active sets are non-degenerate, we first need to show that the lower bound on the flexibility index F^L will monotonically increase in each iteration.

Property 3. The lower bound on the flexibility index generated by Algorithm I is monotonically increasing, provided that the active sets encountered are not degenerate.

Proof: From the projection scheme and the definition of A^k it is guaranteed that all encountered active sets are ordered and examined in order of proximity to the nominal point. When a new active set is encountered, 8_c^k is increased slightly by 6 in order to avoid solving (PI) at the intersection of the two active sets. Since u is a continuous function of 6 (Swaney and Grossmann, 1985a) the above procedure for visiting a new active set is valid. Therefore, any active set k examined lies by definition *strictly* beyond active set k-1, so that:

$$\delta_c^{k-1} < \delta_{s_j}^k, \delta_u^k \tag{5.3}$$

By definition,

$$(F^L)^{k-l} = 8^k{}_c{}^{-l} < 8^l{}_{sj9} 8^l{}_u \qquad l = U - 1$$

and also

$$(F^L)^k < 8^l{}_{sj9} 8^l{}_u \qquad l = l_9 k$$

By combining the above with the definition of A^k we finally get:

$$(F^L)^{k-l} < (F^L)^k.$$

We are now left to eliminate the case $(F^L)^{k\sim l} = (F^L)^k$. Since the previous active set cannot be considered (note the strict inequality sign in (5.4) and the corresponding reasoning), in order for the equality to hold, two active sets in the same iteration have to be at exactly the same distance from the nominal point. This case, however, implies that the solution of (PI) in that point is not unique. In that case we can arbitrarily order the active sets through a lexicographic method. Hence, the equality case is excluded, by the above ordering argument, so that we conclude:

$$(F^L)^{k-l} < (F^L)^k \qquad \text{r.}$$

Corollary 1. If the lower bound on the flexibility index increases monotonically in each iteration, Algorithm I will not cycle.

Proof: Cycling requires that the method will encounter the same active set and hence the same flexibility bound at least twice. From Property 2 this cannot happen r.

The above method will converge to the flexibility index F, since it systematically generates a strictly increasing (for non-degenerate cases) sequence of lower bounds to F, as shown in Property 3. These lower bounds will converge to the upper bound given by $F^u = 5_U$ = min{$§u^k$}. The convergence property for this method is shown below in Property 4.

Property 4. The method described in Algorithm I will converge to the flexibility index of the corresponding problem.

Proof: The proposed method creates a sequence of lower bounds of the flexibility index. It also generates upper bounds for F. We have to show that the two bounds will converge so that F^u = F^L = F. Since there is a finite number of active sets and since every one is considered at most once, there exists an active set k' for which there are no other active set directions so that $A^{k'}$ = 0, and hence $F^L = 8_U$. But also by definition $F^u = 5_U$, so that $F^u = F^L$ = F. r.

Note also that although in this development we assumed non-degenerate active sets this is not a restricting element. In particular, the case of degeneracy could be addressed by the introduction of an ordering lexicographic method for all the relevant basic variables Sj. This provision will enable the ordering of the active sets in a degenerate case. Also in that case all degenerate active sets should be excluded from $\overline{B}^k$ (where for example active sets k-1 and k-2 are degenerate). In this work, however, only non-degenerate cases are considered.

6. Flexibility Evaluation Examples

In order to demonstrate the proposed sensitivity based feasibility index method and illustrate the steps of the algorithm we consider the following example problems.

Example 2. This is a four heat exchanger network design problem with five inequality constraints, one non-negative control variable (Q_c) and two uncertain parameters, 6 = [Ti, T2F, with symmetric deviations (Grossmann, 1987). This is a small version of Example 3 to better illustrate the steps of the algorithm. The process model in projected form is described as follows:

$$0.667Q_c - 350 + s_1 - u = 0$$

$/_2$: - r_i - r_2 + 0.5£ + 923.5 + s_2 - w = 0

$/_3$: - 2r_1 - r_2 + a + ii44 + 5_3 - « = **o** (E2)

$/_4$: - 2r_i - r_2 + & + 1274 + s_4 - M = 0

$$f_5:\ 2r_i + T_2 - Q_c - 1284 + s_5 - u = 0$$

$$f_6: -Q_c + s_6 - u = 0$$

Nominal point: $6^N = [388,583]^r$. Expected symmetric deviations $A0 = [\pm 10, \pm 10]^T$.

First iteration:

Starting from the nominal point we solve (PI) and obtain the optimal solution. Based on this and using (3.4) we obtain the sensitivities for all the basic slack variables and u. Using (4.1) and (4.2) we find the allowable displacement for all Sj and u, along with the corresponding critical directions D_{s_j} using (4.4). Based on that we find F^u and &.

$$
\theta^N = \begin{pmatrix} 388 \\ 583 \end{pmatrix} \Rightarrow
\left(\begin{array}{ll} s_4=0; & A_4=0.5 \\ s_5=0; & A_5=0.5 \\ s_1 = 10.36 & \\ s_2=2.50 & \\ s_3 = 130.0 & \\ s_6 = 75.0 & \\ u = -5.0 & \end{array}\right)
\overset{(3.4)}{\Rightarrow}
\left(\begin{array}{l} \dfrac{ds_1}{d\theta} = \begin{pmatrix} 0.33 \\ 0.67 \end{pmatrix} \\ \dfrac{ds_2}{d\theta} = \begin{pmatrix} 0 \\ 0.5 \end{pmatrix} \\ \dfrac{ds_3}{d\theta} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \dfrac{ds_6}{d\theta} = \begin{pmatrix} 2.0 \\ 1.0 \end{pmatrix} \\ \dfrac{du}{d\theta} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{array}\right)
\overset{(P2)}{\Rightarrow}
\left(\begin{array}{ll} S_s = 1.04 \quad D, & = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \\ S_{S2} = 0.50 D_{Si} & = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\ \delta_{s_3} = \infty & \\ \delta_{s_6} = 2.50 \quad D_{s_6} & = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \\ 8_{,}, = \infty & \end{array}\right)
\Rightarrow
\left(\begin{array}{l} \delta_c^1 = 0.5 \\ D_c^1 = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\ F^L = 0.5 \\ F^U = \infty \end{array}\right)
$$

which gives rise to active set $(AS)^1$ = {£4, *f$)* with $F^L = 0.5$. Also, note that since the resulting critical direction $(0,-1)^T$ is not uniquely defined. Here $(1,-1)^T$ and $(-1,-1)^T$ are both acceptable and we can select an of the two. Although, this selection will not affect the continuation of this method as far as the final result is concerned, in order to demonstrate the projection scheme we will examine both instances below (graphically presented in Figure 3 as AB and AB'):

***Second iteration* - Case I: $(D^0)^1 = (-1, -1)^T$:**

We follow a procedure similar to the one in the first iteration. The only difference is that here, since (P2) was solved at a parameter point different than 0^N we need to project the allowable distances $\overline{S}^*_{s_j}$, to $5^*_{s_j}$ using (3.12).

$$e^N = \begin{pmatrix}388\\583\end{pmatrix} + 0.5^+ \begin{pmatrix}-1O\\-10\end{pmatrix} \Rightarrow \begin{pmatrix} \wedge = 0; \quad \lambda_2 = 0.67 \\ s_5 = 0; \quad A_5 = 0.33 \\ 5, = 5.35 \\ 5_3 = 130.0 \\ S_4 = £ \\ s_6 = 59.97 \\ M = -5.0 \end{pmatrix} \overset{(3.4)}{\Rightarrow} \begin{pmatrix} \frac{ds_1}{d\theta} = \begin{pmatrix}0.33\\0.56\end{pmatrix} \\ \frac{ds_3}{d\theta} = \begin{pmatrix}0\\-0.67\end{pmatrix} \\ \frac{ds_4}{d\theta} = \begin{pmatrix}0\\-0.67\end{pmatrix} \\ \frac{ds_6}{d\theta} = \begin{pmatrix}2.0\\1.0\end{pmatrix} \\ \frac{du}{d\theta} = \begin{pmatrix}0\\-0.33\end{pmatrix} \end{pmatrix} \overset{(P2)}{\Rightarrow}$$

$$\overset{(P2)}{\Rightarrow} \begin{pmatrix} \bar{\wedge}, = 0.6 \quad D_{s_1} = \begin{pmatrix}-1\\-1\end{pmatrix} U \; S_{Si} = 1.10 \\ \bar{\delta}_{s_3} = 19.5 \quad D_{s3} = \begin{pmatrix}0\\1\end{pmatrix} \to \delta_{s_3} = \infty \\ \bar{\delta}_{s_6} = 2.0 \quad D_{s_6} = \begin{pmatrix}-1\\-1\end{pmatrix} \to \delta_{s_6} = \infty \\ \bar{\delta}_{u} = 1.50 \quad D_{u} = \begin{pmatrix}0\\-1\end{pmatrix} \to \delta_{u} = \infty \end{pmatrix} \Rightarrow \begin{pmatrix} \delta_c^2 = 1.10 \quad D_c^2 = \begin{pmatrix}-1\\-1\end{pmatrix} \\ F^L = 1.10 \\ F^U = \infty \end{pmatrix}$$

Projection step $\bar{S}_{Si}$ -» 5^: Since D_{Si} s $(D^c)'$, which means that the predicted direction is the same with the previous critical direction, we evaluate the projected 8 by simply adding 8 to the previous critical (SP)[1], so $8_{Si} = (8^c)^l + \bar{8}_{Si} = 0.5 + 0.6 = 1.1$

Second iteration - Case II: $D_c^1 = (1, -1)^T$:

$$e^N = \begin{pmatrix} 3.88 \\ 5.83 \end{pmatrix} + 0.5 \begin{pmatrix} 10 \\ -10 \end{pmatrix} \overset{(P1)}{\Rightarrow} \begin{pmatrix} s_2 = 0; \quad \lambda_2 = 0.67 \\ s_5 = 0; \quad \lambda_5 = 0.33 \\ s_1 = 8.69 \\ s_3 = 130.0 \\ s_4 = \infty \\ s_6 = 80.01 \\ u = -5.0 \end{pmatrix} \overset{(3.4)}{\Rightarrow} \begin{pmatrix} \frac{ds_1}{d\theta} = \begin{pmatrix} 0.33 \\ 0.56 \end{pmatrix} \\ \frac{ds_3}{d\theta} = \begin{pmatrix} 0 \\ -0.67 \end{pmatrix} \\ \frac{ds_4}{d\theta} = \begin{pmatrix} 0 \\ -0.67 \end{pmatrix} \\ \frac{ds_6}{d\theta} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \frac{du}{d\theta} = \begin{pmatrix} 0 \\ -0.33 \end{pmatrix} \end{pmatrix} \overset{(P2)}{\Rightarrow}$$

$$\overset{(P2)}{\Rightarrow} \begin{pmatrix} \bar{\delta}_{s_1} = 0.98 \quad D_{s_1} = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \rightarrow \delta_{s_1} = 1.10 \\ \bar{\delta}_{s_3} = 19.5 \quad D_{s_3} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \delta_{s_3} = \infty \\ \bar{\delta}_{s_6} = 2.67 \quad D_{s_6} = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \rightarrow \delta_{s_6} = \infty \\ \bar{\delta}_u = 1.50 \quad D_u = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \rightarrow \delta_u = \infty \end{pmatrix} \Rightarrow \begin{pmatrix} \delta_C^2 = 1.10 \quad D_c^2 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \\ F^L = 1.10 \\ F^U = \infty \end{pmatrix}$$

Projection step $\bar{\delta}_{s_1} \rightarrow \delta_{s_1}$: we have to solve (5.1) to find the intersection of the current active set with the intersection with the new active set defined by the removal of s_1 from the basis, along direction D_{s_1}. The corresponding system of equations to be solved as defined by (5.1) is:

$$\begin{pmatrix} s_2 = 0; \quad s_5 = 0; \quad s_1 = 0 \\ \theta = \theta^N + \delta_{s_1} \begin{pmatrix} -10 \\ -10 \end{pmatrix} \end{pmatrix} \overset{(E3)}{\Rightarrow} \delta_{s_1} = 1.1$$

Graphically this step from $\bar{\delta}_{s_1} = 0.98$ to $\delta_{s_1} = 1.1$ is given by segments B'C'C in Figure 3.

Third iteration:

$$\theta^N=\begin{pmatrix}388\\583\end{pmatrix}+(1.1+\varepsilon)\begin{pmatrix}-10\\-10\end{pmatrix}\overset{(P1)}{\Rightarrow}\begin{pmatrix}\$,=0; & A,=0.43\\ s_2=0; & A_2=0.57\\ s_3=134.0 & \\ s_4=4.01 & \\ s_5\ =\pounds & \\ s_6=41.93 & \\ w=-3.0 & \end{pmatrix}\overset{(3.4)}{\Rightarrow}\begin{pmatrix}\frac{ds_3}{dO}=\begin{pmatrix}0.14\\ \wedge\text{-}0.43\end{pmatrix}\\ dd=\begin{pmatrix}0.14\\ 1,\text{-}0.43\end{pmatrix}\\ \frac{ds_5}{d\theta}=\begin{pmatrix}\text{f-}0.43'\\ 1\text{-}0\text{-}72,\end{pmatrix}\\ \frac{ds_6}{dd}=\text{foil}\\ \frac{du}{d\theta}=\begin{pmatrix}-0.14\\ ,\text{-}0.57\end{pmatrix}\end{pmatrix}\overset{(P2)}{\Rightarrow}$$

$$\overset{(P2)}{\Rightarrow}\begin{pmatrix}\bar{5},3=23.5 & D_{s_3}=\begin{pmatrix}-1\\1\end{pmatrix}\rightarrow\delta_{s_3}=\infty\\ \bar{5}_{Si}=0J & D_{s3}=\begin{pmatrix}-1\\1\end{pmatrix}\rightarrow\delta_{s_5}=\infty\\ \bar{S}_{s_6}=2.26 & D_{s_6}=\begin{pmatrix}-1\\-1\end{pmatrix}\rightarrow\delta_{s_6}=\infty\\ \bar{\delta}_u=0.42 & D_u=\begin{pmatrix}-1\\-1\end{pmatrix}\rightarrow\text{•}5.=1.52\end{pmatrix}\Rightarrow\begin{pmatrix}\text{'S-L52} & \text{flf-l}\begin{pmatrix}-1\\-1\end{pmatrix}\\ \left.\begin{matrix}F^L=1.52\\ F^*=1.52\end{matrix}\right\}\Rightarrow F=1.52 & \end{pmatrix}$$

Graphically this step is given by the segment CD in Figure 3.

The evolution of this example solution and the above steps are graphically presented in Figure 3. Note that all the information with respect to the values of $5^*_{s_j}$ *and* 5^*_u for all the basic variables Sj and u is exact only for 8_c^k and not necessarily for the rest. This is due to the possible existence of multiple basis changes along some of these directions.

Example 3. This is also a heat exchanger problem with four units (Grossmann and Floudas, 1987). The model for this problem in the projected form, with just the inequality constraints and the control variables, has five inequality constraints, one non-negative control variable (Q_c) and four uncertain parameters 6 = [Ti, T2, T3, T_4]^T:

$$f_1: \quad T_2 - 0.667Q_c + 350 + s_1 - u = 0$$
$$f_2: \quad -0.750T_1 - T_2 - T_3 + 0.5Q_c + 1388.5 + s_2 - u = 0$$
J3 1 2 3 · *c $+ 2044 + s_3 - u = 0$ (E3)
/4: -1.57,-2^-73-2^ + ^2830 + ^^ = 0
$$f_5: \quad 1.5T_1 + 2T_2 + T_3 + 3T_4 - Q_c - 3153 + s_5 - u = 0$$
$$U \quad -Q_c + s_6 - u = 0$$

The nominal point is 0" = [620,388,583,313]^r and the expected deviations *Ad* are ±10 for all the uncertain parameters. Our goal is to determine the flexibility index for this structure. The method converges in two iterations and the details are given in Table I. The flexibility index is F = 0.5 and the critical direction D^F = [0, 0, -1, 1]^T. This result verifies the one found in (Grossmann and Floudas, 1987) but here, due to the nature of this method, *all* possible critical directions are identified as opposed to only one reported in the above reference. The multiplicity in the critical direction denotes the fact that there are actually four critical directions with the same flexibility. In other words the displacements to the boundary in the four critical directions are identical, bounded by a single hyperplane at the space of 0.

7. Remarks on the Flexibility Evaluation Methodology

The above method presents several advantages compared to the MILP approach by Grossmann and Floudas (1987). First, the solution yields not a single critical point or active set, but rather it provides all supporting active sets and consequently all critical directions in case there is multiplicity. Second, unlike the above method, the proposed approach does not require the solution of an MILP problem. Instead, a sequence of bounding LP's suffices for the sensitivity based method since the identification of the active sets is essentially done on a need-to-construct basis, as a direct result of the solution of (PI). The solution of a new LP in our method corresponds to a new active set. Hence, the number of the required LP's is bounded by the number of *supporting active sets*, nsAS. Note that all the possible (but not necessary feasible) active set combinations are given by:

$$n_{PAS} = \frac{V}{7 \;,\; IM / \; 777} \qquad (7.1)$$

Therefore, npAS is the number of active sets that the existing methods need to consider in the worst case. In contrast, as it is evident from the construction of the proposed method, only the supporting active sets, nsAS ^wiU be considered. Although this number may still be rather large, the computational complexity of the method may be reduced. On the other hand a disadvantage of the proposed method is that its implementation is not as direct as the mixed-integer approach since its efficient implementation requires that the sensitivity computation in (3.4) be performed as part of the pivot operations in the simplex algorithm. Also the mixed-integer approach can be more readily applied to non-linear problems, it has no difficulties in handling degeneracies in the active sets and it can easily accomodate a wide variety of correlated uncertainties (see Grossmann and Floudas, 1987).

8. Flexible Design for Given Operability Requirements and Uncertainty

After addressing the first important issue in flexibility, which was to determine the flexibility index of an existing design, the next challenging issue is to design (or redesign) a plant so that it will be capable of withstanding some parameter variation expressed in terms of a flexibility index.

Given a model with state and design variables (JC/, *d)* and a set of parameters 0, the goal is to determine a design so that an objective function <^*d)* will be minimal subject to feasibility over a range of values for the parameters 9. Based on the sensitivity analysis procedure for finding the flexibility index for a given design, we describe a method for addressing the problem of designing a plant with a given flexibility and that takes advantage of the fact that all supporting active sets are generated.

Based on the linear model (PI), formulation (F3) yields:

$$\begin{aligned} &\min\ c^T d \\ &s.L\quad A[x^T \backslash z^T f + Bd + C0 + a = 0 \\ &\qquad D[x^T \backslash z^T]^T + Ed + F6 + b + s = u \qquad\qquad (P3) \\ &\qquad .y \geq 0 \qquad ueR^{\{} \\ &V0\ e\ T(F) = \{01\ 0'' - FAO' \leq 0 \leq 9^N + FA6^+\} \end{aligned}$$

In this problem a set of uncertain parameters with nominal values 0^N, is given along with positive and negative expected deviations A0+ and A0~ and a desired degree of flexibility F.

The idea in the design procedure is to solve problem (P3) through a relaxation of (F3) in which all the supporting \|/'s are generated. This approach follows an evolutionary scheme in which the \|/'s are defined at each point from the solution of (PI). In particular, starting with a design d^N and the nominal 0^N we find the corresponding flexibility index. From the above procedure a set of *projectedfeasibilityfunctions* y/* is determined. These functions are expressed in terms of G and d. Maximizing each *f* over 8 (with fixed d), we reduce \|/ to a function of d only. As shown by Pistikopoulos and Grossmann (1988) this can be accomplished by analyzing the sign of the gradients of y at any arbitrary design. A new design can be found based on the minimization of (|>(d) subject to these *projected feasibility constraints yf(dft,* as seen below in problem (P4). The algorithm, summarized below, consists of the iterative solution of the above scheme until a specified flexibility index F* is achieved.

Algorithm II - Design for Fixed Flexibility F*.

Step 0: Set iteration count M = 1. Select d^1 setting $d^l = \min_d$ *<t>(d)*.

Step 1: a. Evaluate the flexibility index F^M (using Algorithm I in section 5).

b. If $F^M \geq F^*$ terminate with optimum design *(PP** = d^M. If $F^M < F^*$, based on the examined active sets determine all the *supporting feasibility functions* $y/^{kht}$, k\i = 1, . KM, given by either (2.2) or (8.2) depending on whether explicit equalities are present. (Note that 1CM is the iteration index of Algorithm I).

c. Determine the critical parameters 0*" that will solve $\max_o y/^{kM}(0_9 d^M)$. This can be accomplished by evaluating the signs at $dy/^{k}"/dO$.

Step 2: Solve design problem (P4) to find the optimal design *d** for all the accumulated projected constraints k_m=l, K_m; m=l, M.

$$\min_d <j>(d)$$

$$s.t.\quad yA(</,0*")<O \quad fc_m=l, \quad K_m\backslash \quad m = lM \tag{P4}$$

Set M <- M+l. Update d^M by setting d^M <- d*. Go to step 1.

The above algorithm provides the optimal solution for the design problem (P3) for fixed flexibility F*. On the one hand, from step 1 the optimal design solution d^M has an associated flexibility index $F^M \geq F^*$, so that at the conclusion of the algorithm we have a feasible design solution with flexibility at least F*. On the other hand, this solution is the minimum since all the constraints in (P4) are valid projected feasibility constraints, according to (F2).

Note that in step l.a of Algorithm II all supporting active sets are generated, *all* the *limiting* \|/'s are systematically identified *(limiting y/s* are the ones that define the design for a given flexibility F* at the optimum). The set of all limiting $i[^f$s consists of all *yfi* for which

$\psi^k(d^{opt}) = 0$. Note also, as it is evident from the structure of (P4), that the maximum number of limiting flexibility constraints is *rid* = dim{d}. A similar result was also independently developed through bottleneck period arguments for multiperiod design problems (Varvarezos et al., 1993). In order to illustrate the above method, we present the following example problem.

Example 4. This is an analytical design problem (from Pistikopoulos and Grossmann, 1988) with one uncertain parameter, two design variables, a single unbounded control variable and three inequalities:

$$
\begin{aligned}
f_1 &= z - \theta + d_1 - 3d_2 \le 0 \\
f_2 &= -z - \frac{\theta}{3} + d_2 + \frac{1}{3} \le 0 \\
f_3 &= z + \theta - d_1 - 1 \le 0
\end{aligned}
\tag{E4}
$$

The uncertain parameter has a nominal value $0^N = 2$, and expected deviations $A0^+ = A0'' = 2$. Our goal is to design this process (find the values of di and d2) so that the above model is feasible for the entire uncertain range ($0 \le 0 \le 4$; $F^* = 1$), with the minimal investment cost. The cost is given by the following objective function: *(/> = l0d_x + \0d_2.*

Iteration 1. Following the initialization procedure in Algorithm II, we start with $d^1 = [0,0]^T$.

$$
\left.\begin{array}{l} d^1 = [0,0]^T \\ \theta^N = 2 \end{array}\right\} \overset{(P1)}{\Rightarrow} \left\{\begin{array}{l} s_2 = 0 \backslash X_2 = 0S \\ s_3 = 0;\ \lambda_3 = 0.5 \\ « = 0.33 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} y/^1_Y = \frac{—L}{2} + \frac{-2-}{2} + \frac{}{3} \frac{}{3} \\ F' < 0 \end{array}\right\}
$$

$$
\left.\begin{array}{l} \min\limits_d \phi = 10(d_1 + d_2) \\ s.t. \max\limits_{9} w^1_T < 0 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \text{mmlO}(d_{1+} d_2) \\ \text{s.r.-34+3</}_2\text{+6<0j} \end{array}\right. \quad \text{U} \wedge = \text{p l} \quad \text{L°J}
$$

Iteration 2. We start with $d^2 = [2,0]^T$

$$
\left.\begin{array}{l} d^2 = [2,0]^T \\ 6^N = 2 \end{array}\right\} \overset{(P1)}{\Rightarrow} \left\{\begin{array}{l} s_1 = 0:\ \lambda_1 = 0.5 \\ s_2 = 0; A_2 = 0.5 \\ w = -0.167 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \psi^2 = \frac{d_1}{2} - d_2 - \frac{26}{3} + \frac{1}{6} \\ F^2 = 0.125 \end{array}\right\}
$$

$$
\left.\begin{array}{l} \min\limits_d \phi = 10(d_1 + d_2) \\ s.t. \max y/^1 \le 0 \\ \quad \max\limits_\theta y/^2 \le 0 \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \min\limits_d 10(d_1 + d_2) \\ s.t. -3d_1 + 3d_2 + 6 < 0 \\ \quad 3d_x - 6d_2 + l \le 0 \end{array}\right\} \Rightarrow d^* = \begin{array}{l} J4.3331 \\ [2.333] \end{array}
$$

Iteration 3. We start with $d^3 = [4.333,2.333]^T$

$$d^3 = [4.333, 2.333]^T \\ \theta^N = 2 \Bigg\} \overset{(P1)}{\Rightarrow} \begin{Bmatrix} s_2=0; X_2=0.5 \\ \wedge_3=0; A_3=0.5 \\ w=-0.667 \end{Bmatrix} \Rightarrow \{F^3 = 1.0\} \Rightarrow d^{opt} = \begin{bmatrix} 4.333 \\ 2.333 \end{bmatrix}$$

An alternative design procedure could involve the initial sampling of the parameter space, by solving (PI) and (P2) for different G^N. This can produce different active sets to start off problem (P4), and amounts to a "warm start". Also, while the above example can be solved in one iteration with the analytical method by Pistikopoulos and Grossmann (1988), it requires in general the a-priori identification of all feasible active sets.

Another important issue particularly relevant to larger scale problems is the direct use of the process model without projecting it on the space of control variables. Although this projection has been quite popular in the past mainly due to its simplicity for the presentation, it can become troublesome and unrealistic for large scale models. The proposed method was developed without any projection simplifications. Although the construction of the projected feasibility functions \|/(G, d) can be done in principle by using (2.2), in general we have to account for the state variables as well. This can be accomplished by applying the Lagrangian function in the full space and making use of all the multipliers in (PI) which leads to:

$$\psi^k(\theta,d) = \sum_i \mu \mathrm{fo}(*.0,d) + \text{£}_J \mathrm{Afo}(x, 0_9 d) \tag{8.1}$$

An alternative way to construct the projected feasibility functions \|/(6, d) is based on the sensitivity information with respect to both the uncertain parameters and the design variables. This leads to formulation (8.2):

$$\psi^k(\theta,d \quad {}^{T} \quad yde) \quad {}^{*T} \quad ydd) \tag{8.2}$$

The following example problem addresses the above issues and demonstrates the use of a full process model without the elimination of state variables.

Example 5. **This is the problem of estimation and possible redesign of a chemical complex that processes 10 chemicals, and involves 6 processing units and 22 process streams, based on the model presented in Grossmann et al., 1982. The flowsheet for this complex is presented in Figure 4. The complete model for this complex is given below.**

Process Material Balances

$$w_2 - 1.2w_3 = 0$$
$$w_3 - 0.8w_4 = 0$$
$$w_4 - 1.8w_5 = 0$$
$$w_8 - 0.3w_{13} = 0$$
$$w_9 - 0.7w_5 = 0$$
$$w_{10} - 0.2w_3 = 0$$
$$w_{11} - 0.3w_{16} = 0$$
$$w_{12} - 1.1w_{13} = 0$$
$$w_{15} - 1.3w_{16} = 0$$
$$w_{18} - 1.1w_{19} = 0$$
$$w_{20} - 0.5w_4 = 0$$

Node Material Balances

$$w_1 - w_2 - w_8 = 0$$
$$w_{20} - w_{21} - w_{22} = 0$$
$$w_5 - w_6 - w_7 = 0$$
$$w_{15} - w_{13} - w_{14} = 0$$
$$w_{16} - w_{17} - w_{18} = 0$$
$$w_9 - w_{10} - w_{11} = 0$$

Design Equations

$$w_3 - d_1 + s_1 = u$$
$$w_4 - d_2 + s_2 = u$$
$$w_5 - d_3 + s_3 = u$$
$$w_{13} - d_4 + s_4 = u$$
$$w_{16} - d_5 + s_5 = u$$
$$w_{19} - d_6 + s_6 = u$$

Process Bounds

$$w_6 - \theta_1 + s_7 = u$$
$$w_1 - \theta_2 + s_8 = u$$
$$w_{2l} — \theta_3 + s_9 = u$$
$$w_{l7} - 0_4 + s_{l0} = u$$
$$—W_7 + 0_5 + £,, = W$$
$$W_{12} - H£ + 5_{12} = K \qquad (<_2 = 120)$$
$$w_{14} - w_{14}^U + s_{l3} = II \qquad (<_4 = 50)$$
$$-w_i + w_i^L + s_{i+1}2 = w \qquad ï = 1,22$$
$$s_j \geq 0 \qquad j = 1, 35$$

The existing design is d^N = [100,150,80,120,100,30]^r. Additional data on this problem are presented in Tables II and HI. Using Algorithm I, the flexibility index for the above process was determined being F = 0.47. During this phase two supporting active sets were determined. However, since one of them had a zero sensitivity with respect to the feasibility variable u, $(\frac{du}{d\{d)}$^- = [0,0,0,0,0,-0.227f;$\frac{du}{d(d)}$^- = 0), only the first is relevant in the design phase. The corresponding projected feasibility function, y^1, is determined using (8.2). Using Algorithm II, we solve a minimization problem with only one constraint *(\\f^d)* that involves only one design variable (d6) and results into a new design for process 6 (from d6 = 30 to d6 = 45, kg h"^{1}). Note that due to the fact that there is only one constraint involving one variable *(6$)* in a linear form, any monotonic objective function (strictly a function of design variables) will give the same optimum design (that is \\f^d $\leq$ 0 => *d$* $\geq$ 45 => d6* = 45). However, in the general case problem (P4) should be solved with an appropriate objective function. Finally, using Algorithm I, for this new design we confirm the flexibility index for the redesigned process to be 1.

9. Conclusions

In this paper we have presented a novel solution approach to the systematic evaluation and design of flexible linear processes. In particular, a sensitivity based method that uses a bounding search procedure was proposed for the evaluation of the flexibility index of an existing design. This approach is computationally competitive compared to existing methods as it can effectively address the dimensionality problem in terms of both the number of the uncertain parameters as well as the number of the model constraints. The method also has the interesting feature of generating all the supporting feasibility projected functions given the constructive element of the search procedure. This property is directly utilized in the optimal design model by Pistikopoulos and Grossmann (1988), thus providing a systematic framework for generating flexibility constraints in the design of linear processes under uncertainty. Finally, examples have been presented to illustrate the steps of the methods and their performance.

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Appendix A - Dependencies Between the Uncertain Parameters

The case of dependencies between the uncertain parameters can be addressed within a sensitivity analysis framework as follows. Assume that there is a dependency among the uncertain parameters 0, described by:

$$0 \bullet FM:H:;] \tag{A.1}$$

where 0i and 0D are the independent and dependent parameters respectively. In that case the sensitivities with respect to the uncertain parameters are estimated based on (3.4) and in addition, for the independent uncertainty parameters we have:

$$\frac{db\wedge}{dOj} = \frac{db\wedge}{d0_D}\frac{de\wedge\wedge}{dO,} db\_ = \frac{db\wedge}{dd_t}\frac{HT}{dd_D} \tag{A.2}$$

In the case where the parameter dependency comes through inequalities, the latter can be transformed into inequalities with the addition of a new uncertain parameter:

$$\bar{H}\theta + \bar{h} \le 0 \Rightarrow \begin{cases} \bar{H}\theta + \bar{h} + \theta_s = 0 \\ 0 \le \theta_s \end{cases} \tag{A3}$$

The above can be addressed within the proposed framework (eq. (3.4)).

Appendix B - Flexibility Index and Sensitivity Analysis

In order to show that the combined solution of (PI) and (P2) will determine the lower bound on the flexibility index for a given active set we need to show that the optimal (as well as any feasible) solution *8* of (P2) will always be a feasible solution of the flexibility problem (PI). If we project the equalities out in (PO) and express the uncertainty domain parametrically in 8 through set T(5), we have:

$$
\begin{aligned}
F = \max 8 \quad & \\
\text{s.t.} \quad & fj(z,0,d^N) \leq 0 \qquad jeJ \\
& \theta \in T(\delta) = \{\theta \mid \theta^N - \delta\Delta\theta^- \leq 6 \leq d^N + SA6^+\} \\
& zeZ = \{z \backslash z^L \leq z \leq z^u\} \\
& 8 \geq 0
\end{aligned}
\tag{Bl}
$$

where *J* is the set of all projected inequalities/ The above can be also expressed equivalently in a minimax form:

$$
\begin{aligned}
F = \max \delta \quad & \\
\text{s.t.} \quad & \max_{0eT(8^c)} \min_{z} \; m d x_{j} f_i(z,0,d^N) < 0\_
\end{aligned}
\quad \wedge 2)
$$

The solution of the above problem will also give the flexibility index of our design d^N over the uncertain parameter space T(9). Note that all the functions involved are considered linear.

Property Bl. Any feasible solution of (P2), *8,* is a feasible solution of (B1).

<u>Proof</u>: It has been shown (Halemane and Grossmann, 1983), that the constraint in problem (B2) is equivalent to the following logical constraint (for a fixed value of *8= fr):*

$$
V8eT(8^c)\{3z(VjeJ\backslash fj(z,0,d^N)<0)\} \tag{B.3}
$$

From the solution of (PI) and the sensitivity analysis in (P2) for any feasible *8,* and for all 0 G $T(8^C)$ there is always a $z = \dot{z} + \frac{dz}{dO}(0 - 9^N)8^C$ that yields a feasible (u≤0) solution of (PI) and therefore satisfies: $/_y(z, 6, d^N) < 0$ V·/ G /, or in other words:

$$
V0G7T<5^C):
$$

$$
\exists z \in Z: z = z^* + \frac{dz}{d\theta}(\theta - \theta^N)\delta^c
$$

and therefore: $\qquad V0 \in T(S^C); \; 3z \; \mathbf{e} \; ZI \; /_j(z, 6, d^N) \leq 0; \; V; \; \mathbf{e} \; J \qquad$ r.

Corollary Bl. Any feasible solution of (P2), 5, is a lower bound F^L to the flexibility index F.

<u>Proof:</u> Since 8 is a feasible solution of (Bl) it follows trivially that it corresponds to a lower bound to F r.

List of Tables

Table I. Detailed solution of Example 2, where the solution of problems (PI) and (P2) are presented in a condensed form.

Iteration	1					2				
AS-Non-basic v.	s_4 s_5					s_2 s_5				
Basic Variables	s_1	s_2	s_3	s_6	u	s_1	s_3	s_4	s_6	u
	10.6	2.5	160	15	-5	10.9	156	e	72	-4
Sensitivity $\frac{db_j}{d\theta}$	$\begin{pmatrix} \text{[illegible]} \\ 0.34 \\ 0.67 \\ 2.18 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0.5 \\ -0.8 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ -2 \end{pmatrix}$	$\begin{pmatrix} 1.5 \\ 2.0 \\ 1.0 \\ 3.0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0.5 \end{pmatrix}$	$\begin{pmatrix} 1.01 \\ 0.34 \\ 0.56 \\ 2.34 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ -0.7 \\ -1.0 \end{pmatrix}$	$\begin{pmatrix} \text{[illegible]} \\ 0 \\ -0.7 \\ 1.0 \end{pmatrix}$	$\begin{pmatrix} 1.5 \\ 2.0 \\ 1.0 \\ 3.0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ -0.3 \\ 1.0 \end{pmatrix}$
Projected $\theta^k_{b_j}$	0.25	**0.20**	8.0	1.0	1.0	∞	∞	(a)	24.0	**0.5**
Direction ξ_j	$\begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ -1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$	(a)	$\begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ -1 \\ 1 \end{bmatrix}$

([a]) **This variable is not considered in the sensitivity analysis since it corresponds to the active set in iteration 1 that is already explored.**

Table H Nominal values and deviations of the uncertain parameters in Example 5.

Uncertain Parameter	Nominal Value (kg. hr^{1})	Positive Deviation (kg. hr^{1})	Negative Deviation (kg. hr^{1})
θ_1	10	5	5
ℓ_2	200	50	50
ℓ_3	50	10	10
ℓ_4	50	10	10
%	50	15	15

Table HI. Bounds on the process streams for Example 5.

Process Stream	Lower Bound (kg hr^{1})	Upper Bound (kg hr^{1})
w_3	10	-
$W4$	10	-
$W5$	10	-
w_{12}	-	120
w_{13}	10	-
w_{14}	20	50
w_{16}	10	-
vv/9	10	-
w_{22}	20	20

List of Figures

Figure 1. Illustration of the concepts of supporting and redundant active sets in flexibility analysis for a given design.

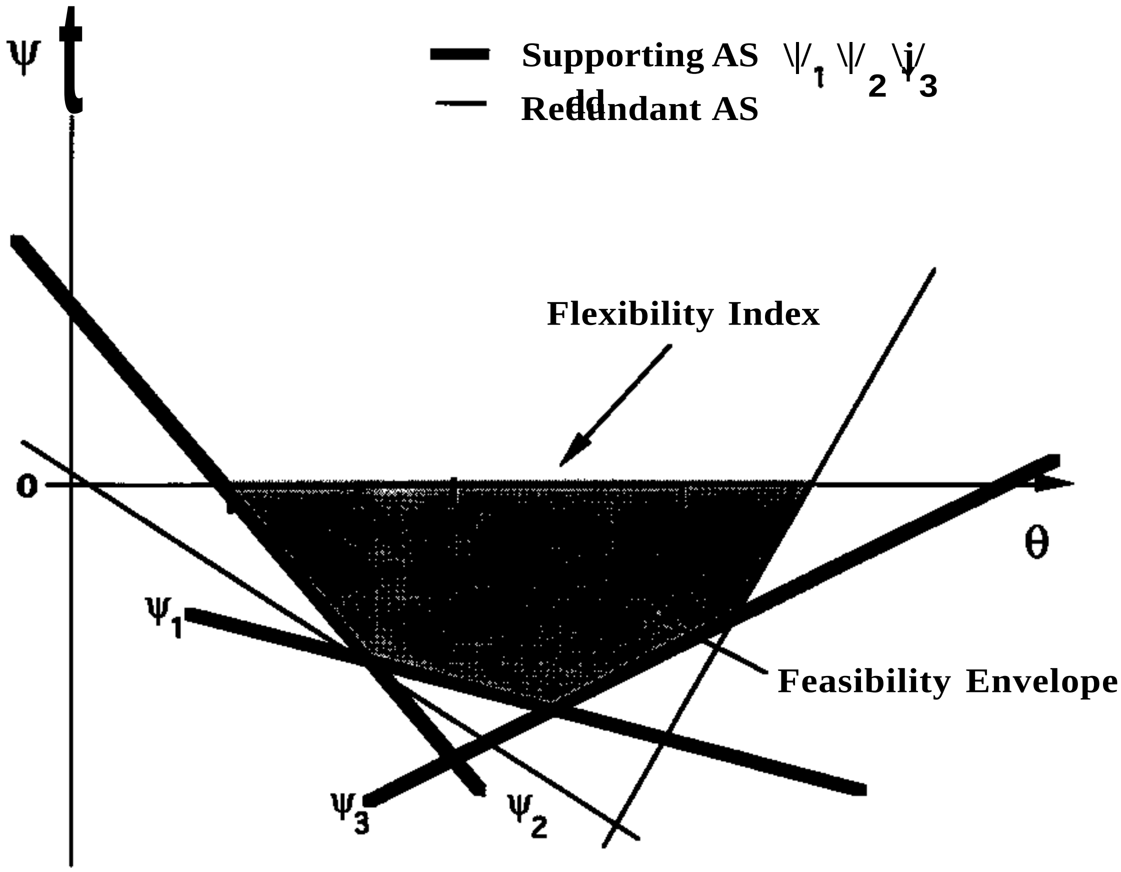

Figure 2. The two active sets projected in z - 6 and \\f - 8 space. The active sets and the procedure path are denoted by the dark lines - Example 1.

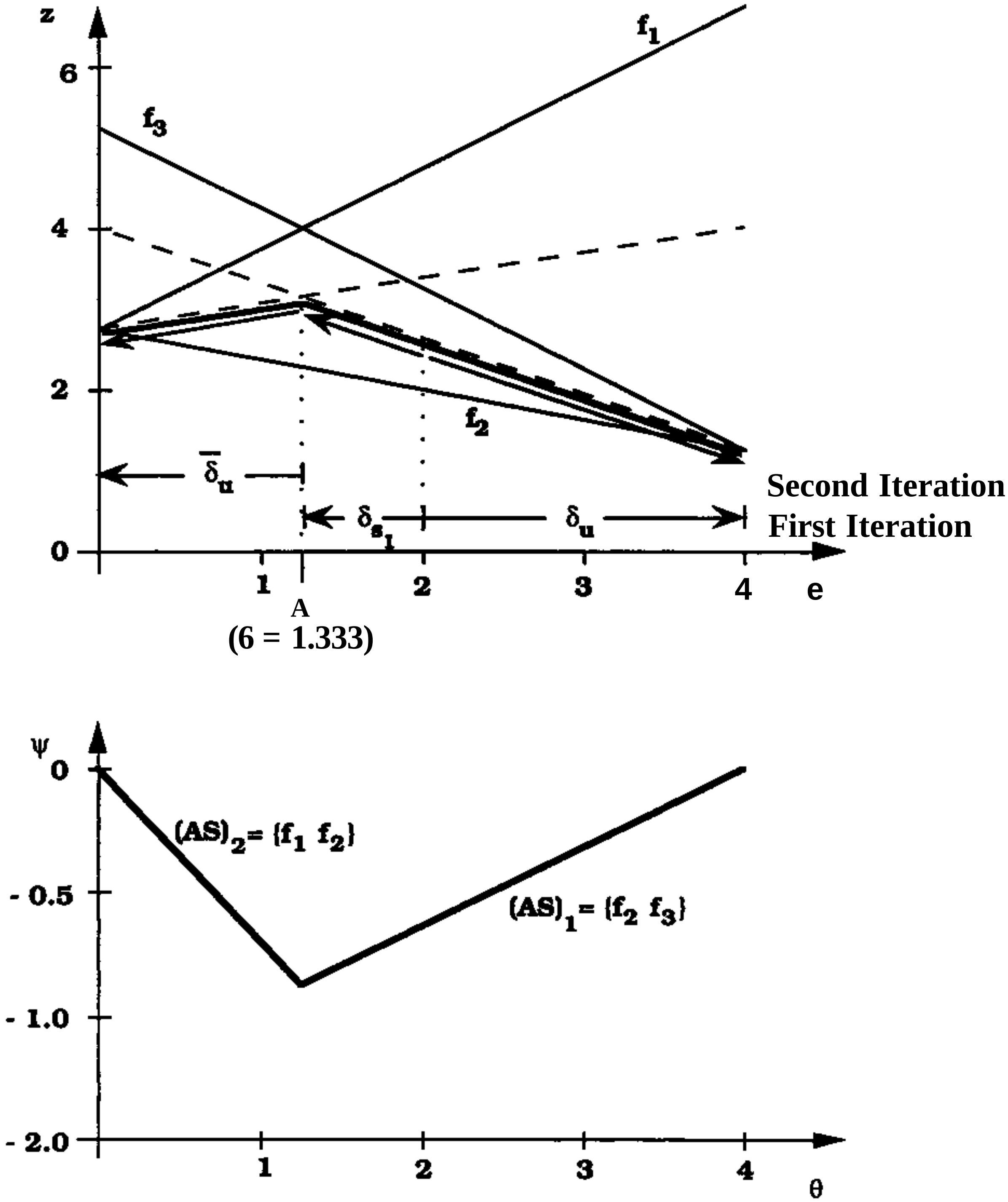

Figure 3. Graphical representation of the procedure for evaluating the flexibility index. Areas with different shade represent different active sets - Example 2.

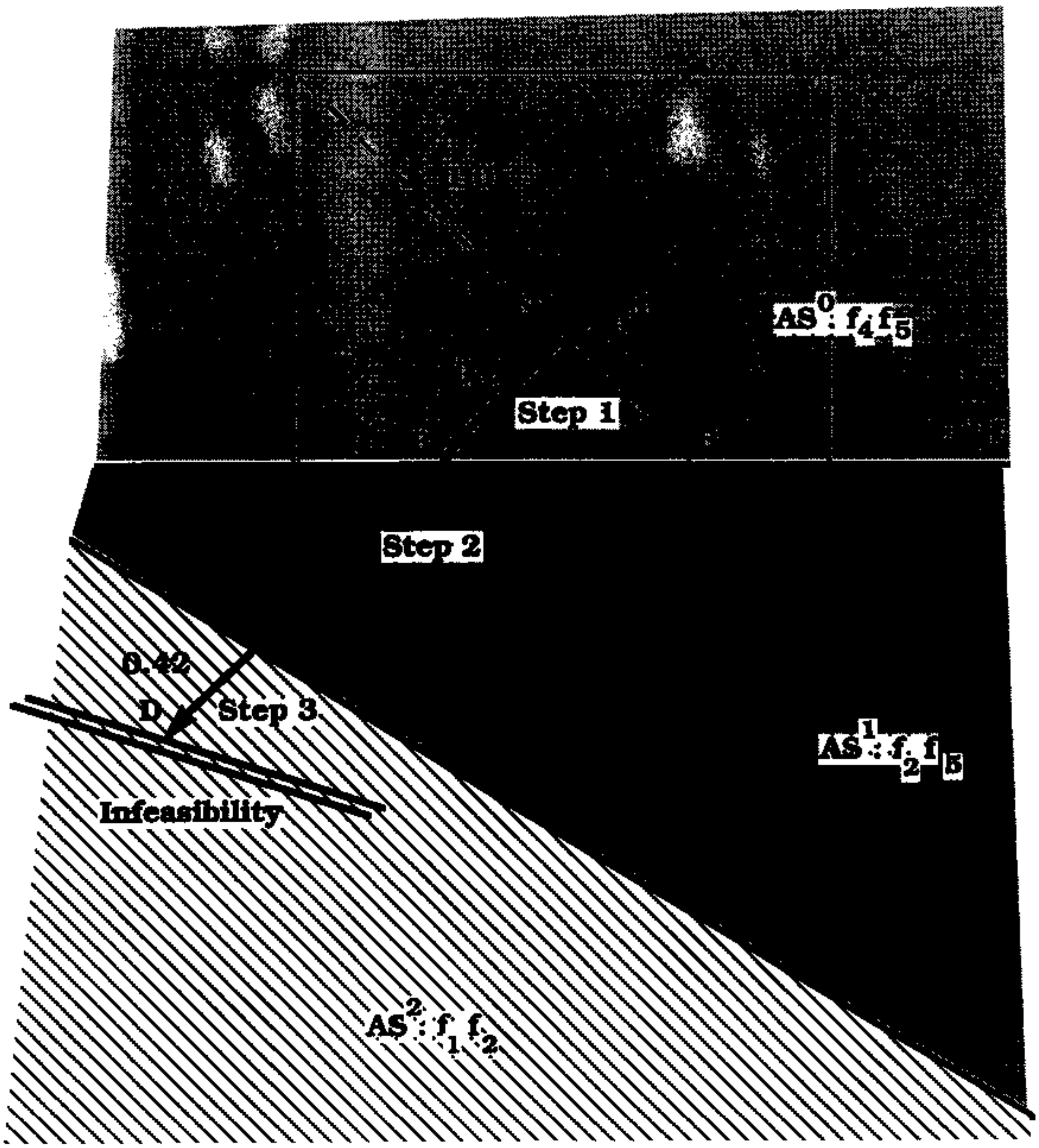

Figure 4. Process Flowsheet for the Chemical Complex in Example 5.