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ACTIVE CONSTRAINT STRATEGY FOR FLEXIBILITY ANALYSIS IN CHEMICAL PROCESSES

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Abstract—It is shown in this paper that by exploiting properties of limiting constraints for flexibility in a design, problems for flexibility analysis can be formulated as mixed-integer optimization problems. Formulations are derived when control variables are present or not, and when equalities are eliminated or handled explicitly. These formulations do not rely on the assumption that critical parameter values are vertices, nor do they require exhaustive vertex searches. The case of linear constraints reduces to standard MILP problems, while for the nonlinear case a novel active constraint strategy is proposed and its theoretical properties are analyzed. Examples are presented for both rigorous and screening calculations.

Scope—In the optimal design and synthesis of flexible chemical processes, one of the crucial problems that arises is the one of how to analyze the flexibility of a proposed design. As discussed in Grossmann and Morari [1], this problem can arise in 2 forms. In its simplest form the problem consists in testing the feasibility of operation in a design over a specified range for the uncertain parameters. In its more general form the problem consists in determining the actual parameter range that the design can tolerate for feasible operation. This range can be defined through a scalar, the flexibility index, by specifying expected deviations for each of the parameters [2].

There are several difficulties involved in the above flexibility analysis problems. Firstly, one must anticipate that during plant operation adjustments can be made through the control variables for the infinite number of parameter values that may arise. Secondly, the critical or limiting condition for flexibility is often not obvious. It can in principle occur at any extreme or vertex point of the parameter range, or it can occur at any intermediate point, Morari [3]. Lastly, the rigorous mathematical formulations for these problems involve non-conventional max–min–max optimization problems which cannot be readily solved with standard optimization techniques.

This paper will present novel mathematical formulations that allow the explicit solution of the max–min–max problem that arises in flexibility analysis. The importance of these formulations is that they do not assume that critical points correspond to vertices, and they do not require the exhaustive enumeration of vertex points which can be very large when many uncertain parameters are considered. The main idea of these formulations is based upon the fact that the flexibility analysis can be performed in the space of constraints that can potentially be active in limiting the flexibility in a design. The formulations to be presented involve mixed-integer optimization problems, and 4 numerical examples are presented to illustrate their application.

Conclusions and Significance—This paper has presented new mathematical formulations for the feasibility test and flexibility index problems. These formulations are based upon the property that the number of active or limiting constraints for flexibility is equal to the number of control variables plus one, provided there is linear independence in the active constraints. It has been shown that this property can be exploited so as to reformulate the max–min–max problems for flexibility analysis, as mixed-integer optimization problems. These formulations have the advantage of neither requiring the assumption of vertex critical points nor the exhaustive enumeration of all extreme points. The formulations are quite general since they can cover the following cases: zero or positive number of control variables; handling of reduced inequalities or of process equations and inequalities; treatment of correlated uncertain parameters.

It has been shown that for linear constraints the formulations reduce to mixed-integer linear programming problems that can be solved with standard branch and bound enumeration methods. Also, nonlinear constraints can be linearized to provide approximations that are suitable for screening calculations. For the case when nonlinear constraints are treated explicitly, an active set strategy has been proposed than can identify *a priori* the potential active constraints that limit flexibility. This strategy has been shown to be rigorous for the case of constraints that are quasi-concave in the uncertain parameters. The numerical results that were presented clearly suggest that the new formulations are computationally efficient for the linear case, while for the nonlinear case they offer the possibility of finding non-vertex critical points with modest computational effort.

INTRODUCTION

Flexibility is clearly one of the important components in the operability of chemical plants, since it is related to the capability of a process to achieve feasible operation over a given range of uncertain conditions (e.g. feedstock variations, changes in process parameters). In order to incorporate flexibility in synthesis and design of chemical processes, one of the important problems that arises is the one of analyzing whether the given design is feasible to operate over a

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specified range of conditions; or more generally, establishing how flexible the design really is.

Specifically, 2 types of problems can then be identified in the flexibility analysis of a process:

(1) feasibility test, the objective here is to establish whether a given design is feasible to operate over the specified range of uncertain parameters

$$\theta^L \leqslant \theta \leqslant \theta^u \quad (1)$$

where θ is the vector of n_p uncertain parameters and θ^L, θ^u are fixed lower and upper bounds, respectively. The uncertain parameters θ can in general, either vary independently, or otherwise be correlated in some specified manner. Figures 1 and 2 illustrate the regions of operation of 2 alternative designs which are feasible or infeasible over a specified range of independent parameters.

(2) flexibility index, the objective here is to determine a measure of the flexibility of a design by establishing the maximum parameter range that a design can tolerate for feasible operation. This parameter range can be expressed as

$$\theta^N - F\Delta\theta^- \leqslant \theta \leqslant \theta^N + F\Delta\theta^+ \quad (2)$$

where θ^N is the nominal parameter value, $\Delta\theta^-$, $\Delta\theta^+$ are negative and positive expected parameter deviations, and F is the flexibility index (Swaney and Grossmann [2]). Figure 3 illustrates the actual parameter range for feasible operation that is associated with the flexibility index F for a given design.

It is important to note that the regions of operation depicted in Figs 1, 2 and 3 must in general take into account the fact that the process can be adjusted for the different parameter realizations. This implies that, for the flexibility analysis to be meaningful, one must anticipate that *during plant operation control variables can be adjusted* so as to try to maintain feasible operation for the prevailing conditions. Neglecting this fact can lead to serious underestimation of the inherent flexibility of a process.

In this paper, a new approach is presented for tackling the 2 types of flexibility analysis problems cited above. A brief review of previous work will be presented first, followed by the derivation of new mathematical formulations for the feasibility test and the flexibility index. These formulations, which are based on mixed-integer programming problems, rely on identifying active constraints that limit the flexibility in a design. As will be shown, the formulations allow the handling of large number of uncertain parameters, while at the same time avoiding the assumption that critical points correspond to vertices or extreme values. The special cases when no control variables are present, and when state variables are not eliminated in the formulations are also discussed.

Solution procedures of the new mathematical formulations are presented for the cases of linear and nonlinear constraints. The former involve standard MILP techniques which can also be used for screening calculations. For nonlinear constraints, an *Active Set Strategy* is presented together with theoretical properties that ensure a unique solution. The application of these formulations is illustrated with 4 example problems.

FLEXIBILITY ANALYSIS REVIEW

As discussed in Swaney and Grossmann [2], the physical performance of a chemical process can be described by the following set of constraints

$$\mathbf{h}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) = 0$$
$$\mathbf{g}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) \leqslant 0 \quad (3)$$

where **h** is the vector of equations (e.g. mass and energy balances or equilibrium relations) which hold for steady-state operation of the process, and **g** is the vector of inequalities (e.g. design specifications or

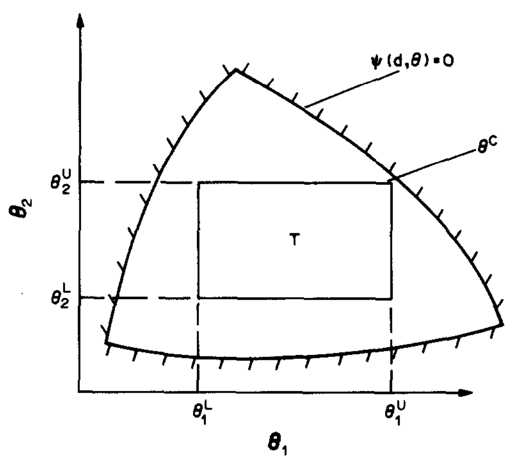

Fig. 1. Region of operation for design with feasible parameter set *T*.

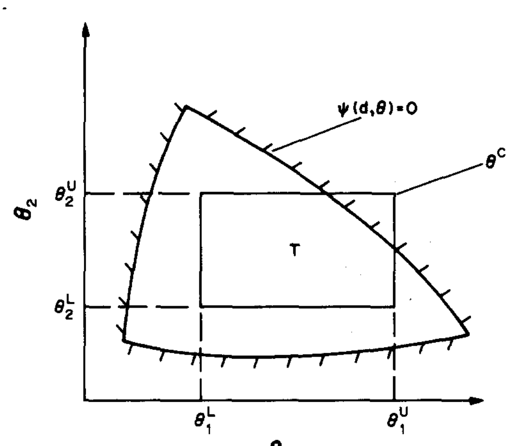

Fig. 2. Region of operation for design with infeasible parameter set *T*.

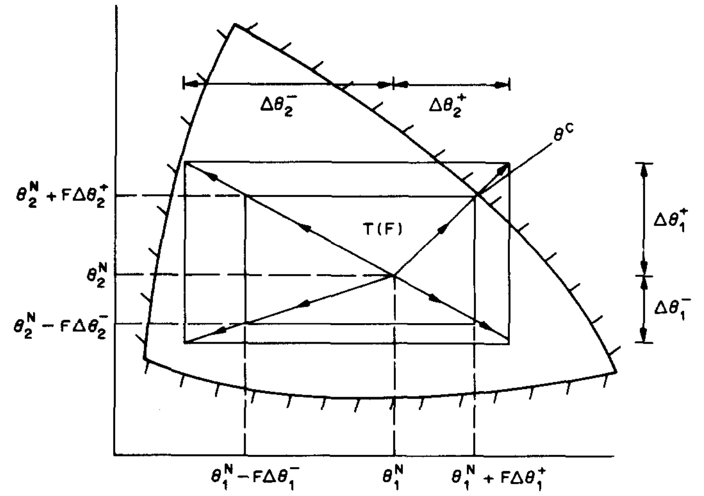

Fig. 3. Maximum feasible parameter set $T(F)$ for flexibility index F.

physical operating limits) which must be satisfied if operation is to be feasible. The variables are classified in the following way: **d** is the vector of design variables that define the structure of the process and equipment sizes. These variables are fixed at the design stage and remain constant during plant operation. $\boldsymbol{\theta}$ is the vector of uncertain parameters. The vector **z** of control variables stands for the degrees of freedom that are available during operation, and which can be adjusted for different realizations of the uncertain parameters $\boldsymbol{\theta}$ during plant operation. Finally, **x** is the vector of state variables which is a subset of the remaining variables, and that has the same dimension as **h**.

For a given plant design **d**, and for any realization of $\boldsymbol{\theta}$ during operation, the state variables can in general be expressed as an implicit function of the control **z** using the equalities **h**,

$$\mathbf{h}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0 \Rightarrow \mathbf{x} = \mathbf{x}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}).$$

This allows the elimination of the state variables, as the performance specifications of the process can be described as the following set of reduced inequality constraints:

$$g_j[\mathbf{d}, \mathbf{z}, \mathbf{x}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}). \boldsymbol{\theta}] = f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leqslant 0 \quad j \in J \qquad (4)$$

where J is the index set for the inequalities. It should be noted that the elimination of the state variables in done at this point for the sake of simplicity in the presentation. The explicit handling of equalities for the flexibility analysis will be treated later in this paper.

As shown in Fig. 4, the inequalities in (4) determine feasibility or infeasibility of operation for a given design **d** for which process adjustments **z** are available to compensate for the effect of the uncertainties $\boldsymbol{\theta}$. Therefore, since the control variables **z** are the degrees of freedom which can be adjusted so as to handle prevailing conditions, feasibility for a given **d** and $\boldsymbol{\theta}$ requires that some **z** exist for which (4) is satisfied.

Given a nominal parameter value $\boldsymbol{\theta}^N$, and expected deviations $\Delta\boldsymbol{\theta}^+$, $\Delta\boldsymbol{\theta}^-$ in the positive and negative

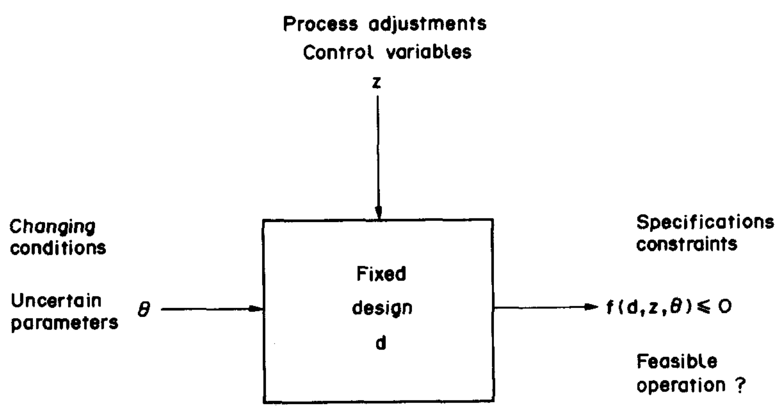

Fig. 4. Representation of flexibility analysis problem.

directions, the specified set of uncertain parameters T will be given by

$$T = (\theta \mid \theta^{L} \leqslant \theta \leqslant \theta^{U})$$

where the lower bound $\theta^{L} = \theta^{N} - \Delta\theta^{-}$, and the upper bound $\theta^{U} = \theta^{N} + \Delta\theta^{+}$. Here it is assumed that the uncertain parameters vary independently; the case of correlated parameters will be treated as a special case later in the paper.

Given this parameter set T, the *Feasibility Test* for a design consists in ensuring that for every $\theta \in T$, there exists a control z that can be selected during plant operation to satisfy each one of the constraint functions f_j, $j \in J$. As has been shown by Halemane and Grossmann [4], this *Feasibility Test* can be formulated mathematically as the max–min–max problem

$$\chi(\mathbf{d}) = \max_{\theta \in T} \min_{\mathbf{z}} \max_{j \in J} f_j(\mathbf{d}, \mathbf{z}, \theta) \tag{5}$$

where $\chi(\mathbf{d})$ can be regarded as a feasibility measure for a given design $\mathbf{d}$. If $\chi(\mathbf{d}) \leqslant 0$, feasibility of operation can be ensured for all $\theta \in T$; if $\chi(\mathbf{d}) > 0$ the design is infeasible for at least some values of $\theta \in T$ since in this case at least one of the constraints in (4) will be violated. Furthermore, the solution θ^{c} of problem (5) defines a critical point for feasible operation; it is the one where the feasible region is the smallest if $\chi(\mathbf{d}) \leqslant 0$ (see Fig. 1), or it is the one where maximum constraint violations occur if $\chi(\mathbf{d}) > 0$ (see Fig. 2). In qualitative terms, the critical points in the feasibility test correspond to the *worst* points for feasible operation.

Alternatively, if it is assumed that θ^{N} is a feasible parameter value, a scalar *Flexibility Index* F, can be defined as the largest scaled deviation δ of any of the expected deviations $\Delta\theta^{+}$, $\Delta\theta^{-}$, that the design can handle for feasible operation. As has been shown by Swaney and Grossmann [2], this *Flexibility Index* can be formulated mathematically as the problem

$$\mathrm{F} = \max \delta$$

$$\text{s.t.} \max_{\theta \in T(\delta)} \min_{\mathbf{z}} \max_{j \in J} f_j(\mathbf{d}, \mathbf{z}, \theta) \leqslant 0 \tag{6}$$

$$T(\delta) = (\theta \mid \theta^{N} - \delta\Delta\theta^{-} \leqslant \theta \leqslant \theta^{N} + \delta\Delta\theta^{+}), \delta \geqslant 0$$

where $T(\delta)$ is a variable parameter set that is defined through the scalar variable δ. This *Flexibility Index* F then defines the maximum parameter set $T(\mathrm{F})$ that a given design can handle for feasible operation. As can be seen in Fig. 3, this set $T(\mathrm{F})$ defines the actual parameter bounds in (2).

Note that the *Flexibility Index* F can be regarded as a quantitative measure of flexibility that is relative to the target (F = 1) specified in the set T. For a value $\mathrm{F} \geqslant 1$, (2) indicates that the flexibility target is clearly satisfied; for $\mathrm{F} < 1$ the index indicates not only that the target is not achieved, but it also gives the maximum fractional deviation that can be allowed for any parameter. The critical prameter θ^{c} that limits the flexibility index in a design is defined through the max–min–max constraint in (6) and lies at the constraint boundary as shown in Fig. 3.

Clearly, the solution of problems (5) and (6) is greatly complicated by the max–min–max problem which in general defines a nondifferentiable global optimization problem Grossmann *et al.*) [5]. Therefore, the natural way to simplify the problem is to decompose it into a two-level optimization problem. In the case of problem (5) this can be done by reformulating it as

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

$$\text{s.t. } \psi(\mathbf{d}, \theta) = \min_{\mathbf{z}} \max_{j \in J} f_j(\mathbf{d}, \mathbf{z}, \theta) \tag{7}$$

where $\psi(\mathbf{d}, \theta)$ corresponds to the nonlinear program

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

$$\text{s.t.} f_j(\mathbf{d}, \mathbf{z}, \theta) \leqslant u \quad j \in J \tag{8}$$

in which u is a scalar variable.

For the case when the constraint functions are jointly 1-D quasi-convex in θ and quasi-convex in $\mathbf{z}$ (e.g. linear in $\mathbf{z}$), it can be proved that the critical point θ^{c} that defines the solution to (7) must lie at one of the vertices of the parameter set T, Swaney and Grossmann [2]. Special types of non-convex functions, however, may lead to nonvertex solutions.

Assuming that critical points correspond to vertices, problem (7) can be simplified as

$$\chi(\mathbf{d}) = \max_{k \in V} \psi(\mathbf{d}, \theta^{k}) \tag{9}$$

where $\psi(\mathbf{d}, \theta^{k})$ is the solution to problem (8) at the parameter vertex θ^{k}, and V is the index set for the 2^{n_p} vertices. In other words, $\chi(\mathbf{d})$ can be determined from (8) by evaluating $\psi(\mathbf{d}, \theta)$ at each vertex so as to select the largest value. In this way, it can be noted that the explicit solution of the max–min–max problem in (5) can be circumvented.

In a similar fashion for the flexibility index, by assuming that the critical points lie at vertices, problem (6) can be simplified as [2]:

$$\mathrm{F} = \min_{k \in V} \delta^{k} \tag{10}$$

where δ^{k} is the maximum deviation along each vertex direction $\Delta\theta^{k}$, $k \in V$, and it is given by the nonlinear program

$$\delta^{k} = \max_{\delta, \mathbf{z}} \delta$$

$$\text{s.t.} f_j(\mathbf{d}, \mathbf{z}, \theta) \leqslant 0 \quad j \in J \tag{11}$$

$$\theta = \theta^{N} + \delta\Delta\theta^{k}, \quad \delta \geqslant 0.$$

Problems (9) and (10) constitute the basic formulations for flexibility analysis by Halemane and

Grossmann [4], and Swaney and Grossmann [2]. Although these problems lead to rigorous methods for the type of constraint functions assumed above, they have the difficulty that their computational effort is in general proportional to the number of vertices, 2^{n_p}. Swaney and Grossmann [6], have proposed 2 algorithms, a heuristic vertex search and an implicit enumeration scheme, that avoid the exhaustive enumeration of all vertices. Nevertheless, these algorithms rely on the assumption that critical points correspond to vertices. Therefore, the main question that will be addressed in this paper is on how to solve explicitly the max–min–max problems without relying on the assumption that the solution lies at a vertex, as well as avoiding the exhaustive enumeration of vertices. It will be shown that the answer to this question requires the development of new mathematical formulations for the *Feasibility Test* and the *Flexibility Index* which will exploit effectively the candidate sets of active constraints that limit flexibility in a design. In the next sections the new mathematical formulation of the *Feasibility Test* will be presented, as well as the treatment of special cases.

ACTIVE CONSTRAINTS IN FLEXIBILITY ANALYSIS

As indicated previously, the mathematical formulation of the *Feasibility Test* given by the max–min–max problem (5) is equivalent to the 2-level optimization problem

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

$$\text{s.t. } \psi(\mathbf{d}, \boldsymbol{\theta}) = \min_{\mathbf{z}} \max_{j \in J} f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}). \tag{7}$$

It will be shown in this section that this 2-level optimization problem can be simplified by exploiting the fact that limiting or active constraints characterize the function $\psi(\mathbf{d}, \boldsymbol{\theta})$, which in turn represents the feasibility of operation for a given $\boldsymbol{\theta}$.

In order to gain some insight on the nature of the function $\psi(\mathbf{d}, \boldsymbol{\theta})$, consider an example where the specifications of a given design are represented by the inequalities

$$f_1 = \mathbf{z} - \boldsymbol{\theta} \leqslant 0$$

$$f_2 = -\mathbf{z} - \boldsymbol{\theta}/3 + 4/3 \leqslant 0$$

$$f_3 = \mathbf{z} + \boldsymbol{\theta} - 4 \leqslant 0. \tag{12}$$

These inequalities involve a single control variable $\mathbf{z}$ and a single uncertain parameter $\boldsymbol{\theta}$ that is specified within the range $0 \leqslant \boldsymbol{\theta} \leqslant 4$. Figure 5a shows the feasible region of operation in the $\mathbf{z} - \boldsymbol{\theta}$ space. As can be seen, by proper selection of the control variables $\mathbf{z}$, the design is feasible for the range $1 \leqslant \boldsymbol{\theta} \leqslant 4$, while it is infeasible for the range $0 \leqslant \boldsymbol{\theta} < 1$. Solving for the function $\psi(\mathbf{d}, \boldsymbol{\theta})$ as given in (8) for the 3 constraints in (12), the following result is obtained:

(1) for $0 \leqslant \boldsymbol{\theta} \leqslant 2$, f_1 and f_2 are active constraints in (8), which then leads to $\psi(\mathbf{d}, \boldsymbol{\theta}) = 2(1 - \boldsymbol{\theta})/3$.
(2) for $2 \leqslant \boldsymbol{\theta} \leqslant 4$, f_2 and f_3 are active constraints in (8), which then leads to $\psi(\mathbf{d}, \boldsymbol{\theta}) = (\boldsymbol{\theta} - 4)/3$.

By plotting the above function $\psi(\mathbf{d}, \boldsymbol{\theta})$ in Fig. 5b, it can be seen that it reflects precisely the fact that the feasible range of operation is given by $1 \leqslant \boldsymbol{\theta} \leqslant 4[\psi(\mathbf{d}, \boldsymbol{\theta}) \leqslant 0]$, while the infeasible range is given by $0 \leqslant \boldsymbol{\theta} < 1[\psi(\mathbf{d}, \boldsymbol{\theta}) > 0]$. Furthermore, $\psi(\mathbf{d}, \boldsymbol{\theta})$ attains its maximum value at $\boldsymbol{\theta} = 0$, which corresponds to the critical point with largest constraint violations.

It can also be seen in Fig. 5b, that $\psi(\mathbf{d}, \boldsymbol{\theta})$ is a piecewise linear function. The reason for this is that each segment is characterized by different active or "limiting" constraints. In particular, as was found previously, the segment on the left $(0 \leqslant \boldsymbol{\theta} \leqslant 2)$ is characterized by constraints f_1 and f_2 which are precisely the constraints that limit the flexibility as $\boldsymbol{\theta} \to 0$. The segment on the right $(2 \leqslant \boldsymbol{\theta} \leqslant 4)$ is characterized by constraints f_2 and f_3 which are the constraints that limit the flexibility as $\theta \to 4$. This observation would suggest that the 2-level optimization problem in (7) could be simplified by expressing the feasibility function $\psi(\mathbf{d}, \boldsymbol{\theta})$ in terms of those active constraints that limit flexibility in a design.

In order to show how this simplification can be

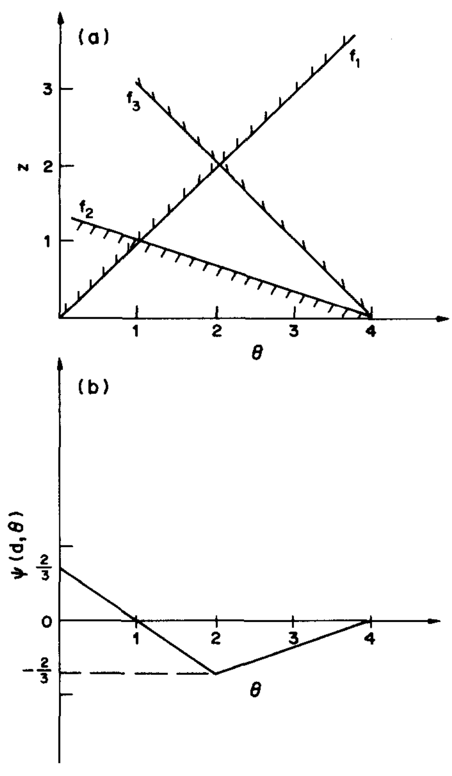

Fig. 5. (a) Region of feasible operation in $\mathbf{z} - \boldsymbol{\theta}$ space; (b) Feasibility function $\psi(\mathbf{d}, \boldsymbol{\theta})$.

achieved, consider the following property of the function $\psi(\mathbf{d}, \boldsymbol{\theta})$ when expressed as

$$\psi(\mathbf{d}, \boldsymbol{\theta}) = \min_{\mathbf{z}, u} u$$
$$\text{s.t.} f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leqslant u \quad j \in J. \tag{8}$$

Property 1—If each square submatrix of dimension $(n_z \times n_z)$ of the partial derivatives of the constraints $f_j\ j \in J$ with respect to the control $\mathbf{z}$,

$$\left(\frac{\partial f_1}{\partial \mathbf{z}}, \frac{\partial f_2}{\partial \mathbf{z}}, \ldots \frac{\partial f_m}{\partial \mathbf{z}}\right), \quad m \geqslant n_z + 1$$

is of full rank, then the number of active constraints $(f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, j \in J_A)$ is equal to $n_z + 1$, where n_z is the number of control variables $\mathbf{z}$.

The proof of this property can be found in Madsen and Schjaer-Jacobsen [7], and in Swaney and Grossman [2]. Notice also that this property is consistent with the example given by constraints (12) which involve one control variable, and where 2 active constraints were found for the function $\psi(\mathbf{d}, \boldsymbol{\theta})$. Also, from a qualitative standpoint, property 1 can be expected to hold since limits of feasible operation are often given by intersection of constraints (e.g. see Fig. 5a). However, exceptions may be found especially with nonlinear constraints.

There are 2 important implications that follow from the property of having $n_z + 1$ active constraints. Firstly, for a given $\boldsymbol{\theta}$ the optimal solution u', z' of $\psi(\mathbf{d}, \boldsymbol{\theta})$ in (8) can be determined from a square system of equations. This follows from the fact that the active constraints $(f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, j \in J_A)$ define $n_z + 1$ equations in $n_z + 1$ unknowns $(u, \mathbf{z})$. With this, the feasibility function is determined directly by these equations; namely $\psi(\mathbf{d}, \boldsymbol{\theta}) = u'$. The second implication is that the 2-level optimization problem in (7) reduces then to the problem

$$\chi(\mathbf{d}) = \max_{\boldsymbol{\theta} \in T} u' \tag{13}$$

where u' is determined from the system of equations for the corresponding active set at the given $\boldsymbol{\theta}$.

Although (13) leads to a simplification of the 2-level optimization problem, the remaining difficulty, however, is that the active set of constraints can change with different $\boldsymbol{\theta}$. Therefore, it is necessary to develop a system of equations in which $\psi(\mathbf{d}, \boldsymbol{\theta}) = u$ is expressed parametrically in terms of $\boldsymbol{\theta}$.

MIXED-INTEGER FORMULATION FOR THE FEASIBILITY TEST

The required system of equations that can determine the optimal value u in (13) for different values of $\boldsymbol{\theta}$ (and hence different possible active sets), can be expressed in terms of the Kuhn–Tucker conditions [8] of problem (8) as follows:

$$\begin{aligned}
&\text{(a)} \quad \sum_{j \in J} \lambda_j = 1, \\
&\text{(b)} \quad \sum_{j \in J} \lambda_j \frac{\partial f_j}{\partial \mathbf{z}} = 0, \\
&\left.\begin{aligned}&\text{(c)} \quad s_j = u - f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \\ &\text{(d)} \quad \lambda_j s_j = 0\end{aligned}\right\} j \in J, \\
&\text{(e)} \quad \lambda_j \geqslant 0, \quad s_j \geqslant 0 \quad j \in J,
\end{aligned} \tag{14}$$

where s_j and λ_j are the slack variables and the Kuhn–Tucker multipliers for constraint j. Equations (14a) and (14b) represent the stationary conditions of the lagrangian with respect to u and $\mathbf{z}$, respectively; (14c) defines the slack variables, and (14d), (14e) represent the complementarity conditions.

For the case when $n_z + 1$ constraints are active, such as when the conditions of Property 1 are satisfied, the equations in (14) can be shown to be necessary and sufficient for a local minimum in (8) (see Madsen and Schjaer-Jacobsen [7]). This applies to both convex and nonconvex constraints. Furthermore, for the case when the constraints are quasiconvex in $\mathbf{z}$ (e.g. linear in $\mathbf{z}$). the equations in (14) will define the global minimum solution. Also, note that for a given set of $n_z + 1$ active constraints $(s_j = 0, j \in J_A; \lambda_j = 0, j \notin J_A)$, (14) leads to a system of $2 + 2n_z$ unknowns $(u, \mathbf{z}, \lambda_j, j \in J_A)$ and $2 + 2n_z$ equations (stationary conditions (14a) (14b) and $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, j \in J_A)$.

The advantage of the equations in (14) is that they provide a way to determine the value of u for the set of active constraints that result for every parameter value $\boldsymbol{\theta}$. However, it should be noted that in the above Kuhn–Tucker conditions discrete decisions are involved in the complementarity conditions (14d), (14e), since they define the selection of active sets of constraints. To express explicitly these discrete decisions, a set of binary variables $y_j, j \in J$, will be defined which are equal to one when constraint j is active, and zero otherwise (Clark [9]). Thus, the complementarity conditions (14d), (14e) can be replaced by:

$$\begin{aligned}
&\text{(a)} \quad \lambda_j - y_j \leqslant 0 \quad j \in J \\
&\text{(b)} \quad s_j - U(1 - y_j) \leqslant 0 \quad j \in J \\
&\text{(c)} \quad \sum_{j \in J} y_j = n_z + 1 \\
&\text{(d)} \quad y_j = 0, 1; \quad \lambda_j, s_j \geqslant 0 \quad j \in J
\end{aligned} \tag{15}$$

where U represents an upper bound for the slacks, and where equation (15c) has been included to reflect the property that $n_z + 1$ constraints must be active under the assumption that each square submatrix in the Jacobian of the constraints with respect to the control variables is of full rank. From (15) it is apparent that the following relations hold:

(i) if $y_j = 1$, then $\lambda_j \geqslant 0$, $s_j = 0$, which indicates that constraint j is active.

(ii) if $y_j = 0$, then $\lambda_j = 0$, $s_j \geq 0$, which indicates that constraint j is inactive.

Since $\psi(\mathbf{d}, \boldsymbol{\theta}) = u'$ can be determined through the Kuhn–Tucker conditions (14) with the complementarity conditions expressed in discrete form as in (15), these equations can be introduced as constraints in the 2-level optimization problem (13). This then leads to the following mixed-integer maximization problem,

$$\begin{aligned} \chi(\mathbf{d}) = & \max_{\boldsymbol{\theta}, \mathbf{z}, u, s_j, \lambda_j, y_j} u \\ \text{s.t. } & s_j + f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) - u = 0 \quad j \in J \\ & \sum_{j \in J} \lambda_j = 1 \\ & \sum_{j \in J} \lambda_j \frac{\partial f_j}{\partial \mathbf{z}} = 0 \\ & \left. \begin{aligned} \lambda_j - y_j \leq 0 \\ s_j - U(1 - y_j) \leq 0 \end{aligned} \right\} j \in J \\ & \sum_{j \in J} y_j = n_z + 1 \\ & \boldsymbol{\theta}^L \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^U \\ & y_j = 0, 1; \quad \lambda_j, s_j \geq 0 \quad j \in J. \end{aligned} \tag{P1}$$

In this way, for any combination of $n_z + 1$ binary variables that is selected in this formulation (i.e. for a given set of $n_z + 1$ active constraints), all the other variables u, $\mathbf{z}$, λ_j, s_j can be determined as a function of $\boldsymbol{\theta}$. However, a feasible selection of $n_z + 1$ binaries is the one where λ_j and s_j satisfy the nonnegativity constraints in (P1). It should also be noted that although $\mathbf{z}$ appears as a variable for maximization of the objective function u, it will actually be selected to minimize u. This follows from the fact that the equations in (14), which are included as constraints in (P1), define the minimization of u with respect to $\mathbf{z}$.

The mathematical formulation of the *Feasibility Test* in (P1) is a mixed-integer optimization problem since it contains continuous and integer variables. If the constraints $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ are linear in $\mathbf{z}$ and $\boldsymbol{\theta}$, then since the partial derivatives for the control variables are constant, (P1) reduces to a mixed-integer linear programming (MILP) problem. If the constraints $f_j(\mathbf{d}, \mathbf{z},, \boldsymbol{\theta})$ are nonlinear then (P1) results in a mixed-integer nonlinear programming (MINLP) problem.

A very important feature of the formulation in (P1) is that it does not assume the critical points to be vertices since the max–min–max problem in (5) is solved explicitly. Also, for the case when critical points do correspond to vertices due to the nature of the constraint functions, the formulation in (P1) avoids the combinatorial problem of having to analyze 2^{n_p} vertices. The combinatorial problem is only dependent on the number of possible active sets in (8). Actually, the maximum number of assignments of $n_z + 1$ active constraints is given by:

$$\frac{m!}{(n_z + 1)!\,(m - n_z - 1)!} \tag{16}$$

where $m\,(m \geq n_z + 1)$ is the number of inequalities. However, the nonnegativity constraints on λ_j, s_j in problem (P1), severely restrict the number of feasible assignments of active sets. This observation has been confirmed by many problems (see Grossmann and Floudas [10]).

Finally, it should also be noted that in the formulation (P1) it is straightforward to handle correlated uncertain parameters that can be expressed through algebraic equations, $r(\boldsymbol{\theta}) = 0$. These equations would simply be included as constraints in (P1).

SPECIAL CASES FOR THE FEASIBILITY TEST

The formulation (P1) for the *Feasibility Test* that was presented above assumes that there is at least one control variable, and that the reduced set of inequalities $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$, $j \in J$, is given by eliminating the state variables $\mathbf{x}$. These 2 restrictions can easily be relaxed in the new formulation as will be shown in this section.

For the case when it is desired to handle explicitly the equalities and inequalities in (3), the function $\psi(\mathbf{d}, \boldsymbol{\theta})$ in (8) can be redefined as follows:

$$\begin{aligned} \psi(\mathbf{d}, \boldsymbol{\theta}) = & \min_{\mathbf{z}} u \\ \text{s.t. } & h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0 \quad i \in I \\ & g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq u \quad j \in J \end{aligned} \tag{17}$$

where I is the index set for the equalities.

By defining for the equalities h_i, $i \in I$, the multipliers μ_i which are unrestricted in sign, and the nonnegative multipliers λ_j for the inequalities g_j, $j \in J$, then by applying the Kuhn–Tucker conditions to (17), it is easy to show that the corresponding mixed-integer programming formulation for the *Feasibility Test* is given by:

$$\begin{aligned} \chi(\mathbf{d}) = & \max_{\boldsymbol{\theta}, \mathbf{x}, \mathbf{z}, u, s_j, \mu_j, \lambda_j, y_j} u \\ \text{s.t. } & h_i(\mathbf{d}, \mathbf{x}, \mathbf{z}, \boldsymbol{\theta}) = 0 \quad i \in I, \\ & s_j + g_j(\mathbf{d}, \mathbf{x}, \mathbf{z}, \boldsymbol{\theta}) - u = 0 \quad j \in J, \\ & \sum_{j \in J} \lambda_j = 1 \\ & \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial \mathbf{z}} + \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} = 0 \\ & \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial \mathbf{x}} + \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial \mathbf{x}} = 0 \\ & \left. \begin{aligned} \lambda_j - y_j \leq 0 \\ s_j - U(1 - y_j) \leq 0 \end{aligned} \right\} j \in J \end{aligned} \tag{P2}$$

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

$$\theta^L \leqslant \theta \leqslant \theta^U$$

$$y_j = 0, 1; \quad \lambda_j, s_j \geqslant 0 \quad j \in J; \quad \mu_i \in R^1 \quad i \in I.$$

Note that although the advantage in (P2) is that the elimination of state variables is not required, it involves as additional variables $\mathbf{x}$ and μ_i $i \in I$, and as additional constraints the system of equations $h_i(\mathbf{d}, \mathbf{x}, \mathbf{z}, \theta)$, $i \in I$, as well as the stationary conditions with respect to the state variables.

For the particular case when there are no control variables ($n_z = 0$), or alternatively when these are assumed to remain constant during operation, it follows that the constraints f_j are independent of the controls, i.e.

$$\frac{\partial f_j}{\partial \mathbf{z}} = 0 \quad j \in J.$$

This implies that the stationary conditions and the multipliers λ_j, $j \in J$, can be eliminated from (P1), which then leads to the formulation:

$$\begin{aligned} \chi(\mathbf{d}) = &\max_{\theta, u, s_j, y_j} u \\ \text{s.t. } &\left.\begin{aligned} s_j + f_j(\mathbf{d}, \theta) - u &= 0 \\ s_j - U(1 - y_j) &\leqslant 0 \end{aligned}\right\} j \in J \\ &\sum_{j\in J} y_j = 1, \\ &\theta^L \leqslant \theta \leqslant \theta^U, \\ &y_j = 0, 1, s_j \geqslant 0 \quad j \in J, \end{aligned} \tag{P3}$$

Since in this formulation only one constraint is allowed to be active, (P3) can be decomposed in terms of each individual constraint $j \in J$ by solving:

$$u^j = \max_{\theta^j \in T} f_j(\mathbf{d}, \theta^j), \tag{18}$$

with which

$$\chi(\mathbf{d}) = \max_{j\in J} u^j. \tag{19}$$

Finally, if equality constraints are explicitly handled for the case $n_z = 0$, the corresponding formulation for the *Feasibility Test* is given by:

$$\begin{aligned} \chi(\mathbf{d}) = &\max_{\theta, \mathbf{x}, u, s_j, y_j} u, \\ \text{s.t. } &h_i(\mathbf{d}, \mathbf{x}, \theta) = 0 \quad i \in I, \\ &\left.\begin{aligned} s_j + g_j(\mathbf{d}, \mathbf{x}, \theta) - u &= 0 \\ s_j - U(1 - y_j) &\leqslant 0 \end{aligned}\right\} j \in J, \\ &\sum_{j\in J} y_j = 1, \\ &\theta^L \leqslant \theta \leqslant \theta^U, \\ &y_j = 0, 1 \quad s_j \geqslant 0 \quad j \in J, \end{aligned} \tag{P4}$$

where this problem can be similarly decomposed by maximizing individual constraints as in (P3). Obviously, the formulations that have been presented for special cases in this section can also easily handle the case of correlated parameters.

MIXED-INTEGER FORMULATION FOR THE FLEXIBILITY INDEX

Using a similar approach for the active sets of constraints as for the *Feasibility Test*, the problem of the *Flexibility Index* in (6) can also be formulated as a mixed-integer optimization problem as will be shown in this section.

As has been shown by Swaney and Grossmann [2], the condition $\psi(\mathbf{d}, \theta^c) = 0$ holds at the solution of problem (6). Furthermore, equation (10) implies that F is given by the smallest δ that lies on the boundary of the parameter region of feasible operation ($\psi(\mathbf{d}, \theta) = u = 0$). Therefore, the problem for determining the *Flexibility Index* F can be formulated as the mixed-integer minimization problem:

$$\begin{aligned} F = &\min_{\theta, \mathbf{z}, \delta, s_j, \lambda_j, y_j} \delta, \\ \text{s.t. } &s_j + f_j(\mathbf{d}, \mathbf{z}, \theta) - u = 0 \quad j \in J, \\ &u = 0, \\ &\sum_{j\in J} \lambda_j = 1, \\ &\sum_{j\in J} \lambda_j \frac{\partial f_j}{\partial \mathbf{z}} = 0, \\ &\left.\begin{aligned} \lambda_j - y_j &\leqslant 0 \\ s_j - U(1 - y_j) &\leqslant 0 \end{aligned}\right\} j \in J, \\ &\sum_{j\in J} y_j = n_z + 1, \\ &\theta^N - \delta\Delta\theta^- \leqslant \theta \leqslant \theta^N + \delta\Delta\theta^+, \\ &\delta \geqslant 0; \quad y_j = 0, 1; \quad \lambda_j, s_j \geqslant 0 \quad j \in J, \end{aligned} \tag{P5}$$

where the constraint $u = 0$ is strictly redundant as it can be substituted in the first equation, but it has been included for comparison with (P1). In a similar fashion as in problem (P1), the mathematical formulation in (P5) does not require the examination of all possible vertices, nor does it assume that critical points must correspond to vertices. Correlated uncertain parameters can also be handled easily. The special cases of handling explicitly the equalities, and of no control variables are essentially similar to problems (P2), (P3), (P4) of the *Feasibility Test*. The corresponding formulations [(P6), (P7), (P8)] can be found in Floudas [11].

LINEAR CONSTRAINT FUNCTIONS

The new formulations for the *Feasibility Test* (P1)–(P4) and for the *Flexibility Index* (P5)–(P8), correspond to mixed-integer optimization problems that involve the integer variables y_j with the remaining variables being continuous. For the case when the constraint functions $(h_i(\mathbf{d}, \mathbf{x}, \mathbf{z}, \boldsymbol{\theta})\, i \in I, g_j(\mathbf{d}, \mathbf{x}, \mathbf{z}, \boldsymbol{\theta})\, j \in J)$ are linear in **x**, **z** and $\boldsymbol{\theta}$, problems (P1)–(P8) lead to mixed-integer linear programming MILP problems for which the global optimum solution can be obtained with standard branch and bound enumeration procedures. Alternatively, the active set strategy presented in the section of nonlinear constraints can also be used, in which case the problem reduces to a sequence of linear programs. It should be recalled that in the linear case the critical points $\boldsymbol{\theta}^c$ will correspond to vertices due to the convexity of the linear functions. Also, in the linear case the constraint on the sum of the integer variables y_j can be relaxed to an inequality less or equal than $n_z + 1$ since the Kuhn–Tucker conditions in (14) are necessary and sufficient for linear constraints. In this way the assumption of linear independence of the active constraints can be relaxed.

For process synthesis applications, where approximate solutions would be suitable for screening purposes, a quicker way to solve the nonlinear versions of problems (P1)–(P8) is to linearize the constraint functions. For example, the constraints $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ could be approximated by

$$f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = f_j(\mathbf{d}, \mathbf{z}^N, \boldsymbol{\theta}^N) + \left(\frac{\partial f_j}{\partial \boldsymbol{\theta}}\right)^T (\boldsymbol{\theta} - \boldsymbol{\theta}^N) + \left(\frac{\partial f_j}{\partial \mathbf{z}}\right)^T (\mathbf{z} - \mathbf{z}^N) \quad (20)$$

where $(\mathbf{z}^N, \boldsymbol{\theta}^N)$ corresponds to the nominal point. In this way, problems (P1)–(P8) can also be solved as MILP problems. As discussed by Grossmann and Floudas [10], these linearizations can often yield good approximations. To illustrate the application of the new formulations to linear constraints, the 2 following examples are considered.

Example 1

In the heat exchanger network shown in Fig. 6, the inlet temperatures of the 2 hot and two cold process streams are regarded as uncertain parameters. Given the nominal values of the temperatures and the flowrates shown in Fig. 6 and assuming expected deviations of the temperatures of ± 10 K, the objective is to determine if the network is feasible for the specified range of inlet temperatures.

Applying the energy balances in the heat exchanger units yields the following set of linear equations:

$$\begin{aligned} 1.5\,(T_1 - T_2) &= 2(T_4 - T_3) \\ T_5 - T_6 &= 2\,(563 - T_4) \\ T_6 - T_7 &= 3(393 - T_8) \\ Q_c &= 1.5\,(T_2 - 350) \end{aligned} \quad (21)$$

Assuming a minimum temperature approach, $\Delta T_{min} = 0$ K, the 5 following linear inequalities are

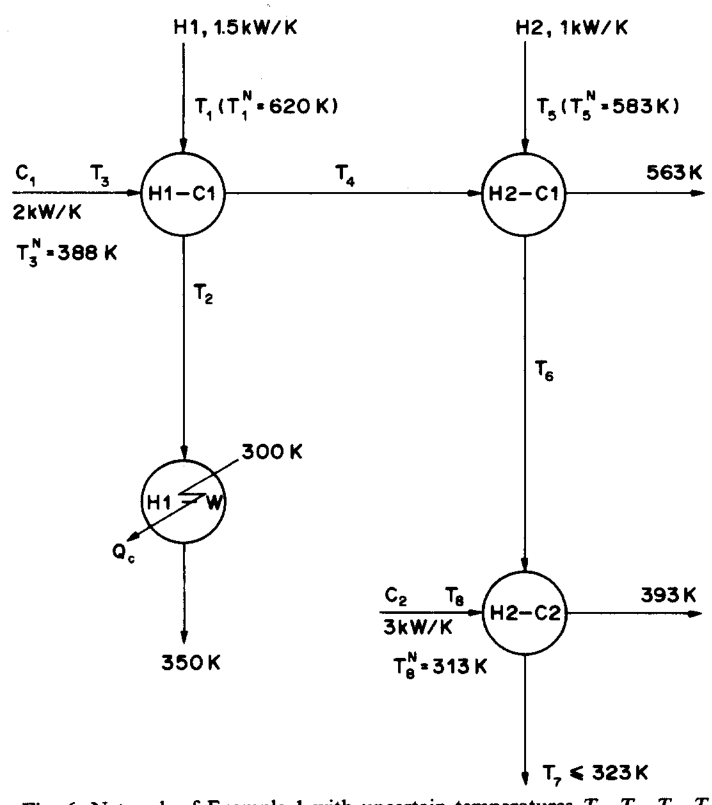

Fig. 6. Network of Example 1 with uncertain temperatures T_1, T_3, T_5, T_8.

considered for feasible operation of this heat exchanger network.

$$T_2 - T_3 \geq 0$$
$$T_6 - T_4 \geq 0$$
$$T_7 - T_8 \geq 0$$
$$T_6 - 393 \geq 0$$
$$T_7 \leq 323 \qquad (22)$$

The first 4 inequalities ensure feasible heat exchange in units H1–C1, H2–C1, H2–C2, while the last inequality is a specification on the outlet temperature of H2, as shown in Fig. 6.

The system of equations in (21) involves one degree of freedom since there are 4 equations and 5 unknowns. Therefore, the temperatures T_2, T_4, T_6, T_7 can be regarded as state variables, while the heat load in the cooler (Q_c) can be regarded as a control variable. Using equations (21), the state variables can be expressed as linear functions of the uncertain parameters (temperatures T_1, T_3, T_5, T_8) and the nonnegative control variable (Q_c). Then, the inequality constraints take the following form:

$$f_1 = -0.67Q_c + T_3 - 350 \leq 0$$
$$f_2 = -T_5 - 0.75T_1 + 0.5Q_c - T_3 + 1388.5 \leq 0$$
$$f_3 = -T_5 - 1.5T_1 + Q_c - 2T_3 + 2044 \leq 0$$
$$f_4 = -T_5 - 1.5T_1 + Q_c - 2T_3 - 2T_8 + 2830 \leq 0$$
$$f_5 = T_5 + 1.5T_1 - Q_c + 2T_3 + 3T_8 - 3153 \leq 0. \qquad (23)$$

To test if this network is feasible for specified variations of ± 10 K in the inlet temperatures, the MILP versions of the *Feasibility Test* (P1) (elimination of equations) and (P2) (without elimination of equations), were applied. The resulting formulation of (P1) has 5 integer variables, 16 continuous variables and 27 rows, and required 4.5 s of CPU-time(DEC-20) with the computer code LINDO (Schrage [12]). The resulting formulation of (P2) has 5 integer variables, 24 continuous variables and 35 rows, and required 4.9 s of CPU-time. The solution found in both problems was $u = +8.7425$ indicating therefore, that the network is infeasible to tolerate simultaneous variations of up to ± 10 K in the temperatures of the inlet streams. The critical point was located at the upper bound of T_8 and the lower bounds of T_1, T_3, T_5.

The formulations (P5), (P6) for the *Flexibility Index* were also applied to this network. The MILP for (P5) involved 5 binary variables, 16 continuous variables, 27 rows and required 7.18 s of CPU-time; problem (P6) involved 5 binary variables, 24 continuous variables, 34 rows and required 7.6 s of CPU-time. With both formulations it was found that the flexibility index is F = 0.5, which means that the network of Fig 6 can tolerate simultaneous variations in the inlet temperatures up to ± 5 K. The critical point was located at the upper bound of T_8 (318 K), and at the lower bounds of T_1, T_3, T_5 (615 K, 383 K, 578 K).

To illustrate the case of correlated uncertain parameters, suppose that the inlet temperatures T_3, T_8 of cold stream C1 and cold stream C2, respectively, are correlated according to the following relationships:

$$T_3 = T_3^N + \theta,$$
$$T_8 = T_8^N + 0.8\theta, \qquad (24)$$

where θ in an independent parameter.
The above 2 equations can be simplified into one equation that correlates T_3 and T_8 as follows

$$0.8\ T_3 - T_8 = -2.6. \qquad (25)$$

Applying formulation (P6) with the additional constraint (25) that correlates T_3 and T_8, results in a flexibility index F = 0.58824, which as expected is a higher value than the case when the 4 inlet temperatures vary independently. It can therefore be seen that the case of correlated parameters can be handled very easily in the proposed formulations.

Example 2

The heat exchanger network of Fig. 7 is shown with nominal conditions for the heat capacity flowrates and temperatures. If uncertainties are considered for the 7 inlet temperatures, then the inequalities for feasible heat exchange in every exchanger can be shown to be linear (see Saboo *et al.* [13]). Given the expected deviations of ± 10 K for each inlet stream, and specifying fixed values for the outlet temperatures given in Fig. 7, it is desired to determine the flexibility index for this network. Temperature z_1 will be treated as a control variable, and 19 inequalities for temperature differences ($\Delta T_{min} = 0$) and positive heat loads are considered for feasible heat exchange.

The MILP version of (P5) for the *Flexibility Index* involves 19 binary variables, 48 continuous variables and 83 rows. The flexibility index obtained with this formulation is F = 0.75, which implies that the network of Fig. 7 can tolerate simultaneous variations in the inlet temperatures up to ± 7.5 K. The solution to this problem required 31 s of CPU-time (DEC-20) with the computer code LINDO, Schrage [12].

This problem was also solved with the direct search over all vertex directions as given by equation (10). This required the solution of $2^7 = 128$ linear programming problems as given by (11), yielding also a flexibility index of F = 0.75. The computer time required with this approach, however, was 227 s, which clearly shows the advantage of not having to analyze the parameter vertices with the new formulation.

It is also interesting to compare the result obtained for the *Flexibility Index* with the case when the control variable z is assumed to remain constant during operation. In this case, formulation (P7) in-

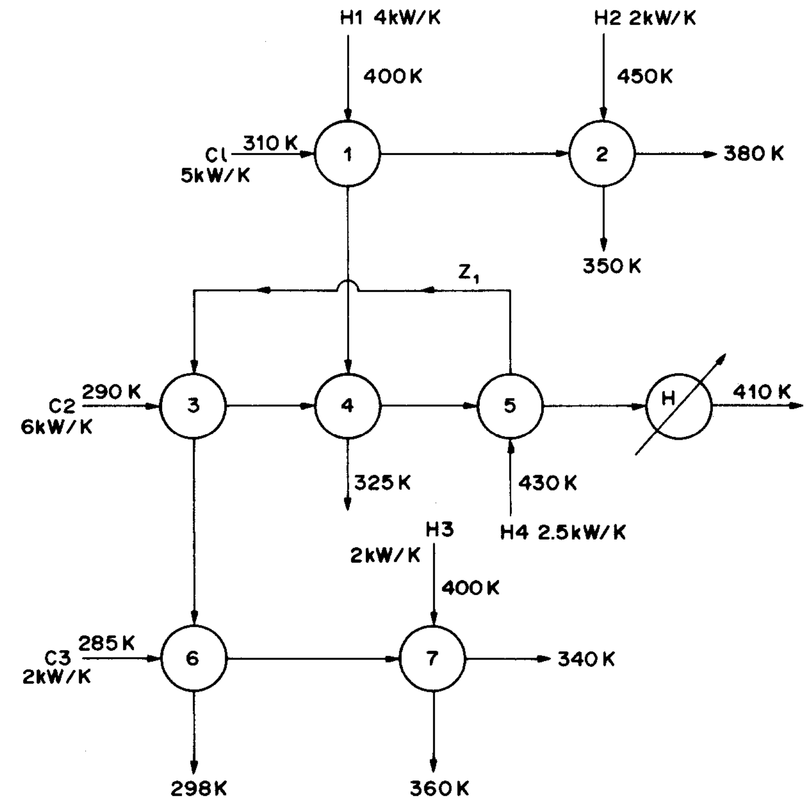

Fig. 7. Network of Example 2 with uncertain inlet temperatures.

volves 19 binary variables, 29 continuous variables and 62 rows. Table 1 shows values of the flexibility index for several fixed values of the control variable $\mathbf{z}_1$. As can be seen, very conservative results can be obtained when the flexibility analysis does not account for the adjustment of the control variables (e.g. $F = 0.114$ for $\mathbf{z}_1 = 390$ K).

Table 1. Flexibility index for fixed z_1 in Example 2

z_1 (K)	310	334	350	390
F	0.167	0.265	0.532	0.114

NONLINEAR CONSTRAINT FUNCTIONS

In the case when the constraint functions are nonlinear in $\mathbf{z}$ and $\boldsymbol{\theta}$, problems (P1)–(P8) become mixed-integer nonlinear programming MINLP problems. A major difficulty, however, that arises in these formulations is that they involve as constraints the stationary conditions with respect to the control variables [e.g. equation (14b) in problem (P1)]. These stationary conditions involve partial derivatives, which unlike the linear case, are not constant since they are in general a function of the uncertain parameters and the control variables. Handling the derivatives for the control variables in (14b) as constraints in a general purpose MINLP algorith (see Geoffrion [14]; Duran and Grossman [15]), can be a very difficult task, apart from the fact that rigorous solutions with these methods can only be guaranteed for restricted types of constraint functions Floudas [11]. Therefore, this section will present an *Active Set Strategy* that decomposes the solution of the MINLP problem into NLP subproblems that avoid the explicit handling of the stationary conditions. As will be shown, the proposed active set strategy is rigorous for special types of constraints that are monotonic in the control variables, and it has the capability of finding nonvertex critical points.

The basic idea in the proposed active set strategy consists in identifying from the stationary conditions in (14b), the potential candidates for the active sets that can lead to the correct solution of the corresponding flexibility analysis problem. Assuming that the constraint functions $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}), j \in J$ are monotone in $\mathbf{z}$ (in the sense that every component of the gradients $\nabla_z f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ remains one-signed for all $\boldsymbol{\theta}$), the potential active sets can easily be determined from (14b) and (15a, 15c):

$$\sum_{j\in J} \lambda_j \frac{\partial f_j}{\partial \mathbf{z}} = 0; \quad (14b)$$

$$\lambda_j - y_j \leqslant 0 \quad j \in J; \quad (15a)$$

$$\sum_{j\in J} y_j = n_z + 1. \quad (15c)$$

Since $\lambda_j \geqslant 0$ must hold for each constraint $j \in J$, then if the components of

$$\frac{\partial f_j}{\partial \mathbf{z}}$$

are one-signed, equation (14b) will indicate the different combinations of $n_z + 1$ active constraints that can satisfy this equation. As an example, assume the case of one control variable and three constraints for which

$$\frac{\partial f_1}{\partial \mathbf{z}} > 0, \quad \frac{\partial f_2}{\partial \mathbf{z}} > 0, \quad \frac{\partial f_3}{\partial \mathbf{z}} < 0.$$

It is then clear that for (14b) to be satisfied for two nonzero multipliers, either $\lambda_1 > 0$, $\lambda_3 > 0$, $\lambda_2 = 0$, or $\lambda_2 > 0$, $\lambda_3 > 0$, $\lambda_1 = 0$. In other words, the only candidates for the active sets are (1, 3) and (2, 3) respectively.

It is important to note, that special consideration must be provided for the case when in a given candidate active set constraints are present that are lower and upper bounds on the same function. For example, assume that a and b ($a < b$) are the lower and upper bound of the function g, that is:

$$a \leqslant g(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leqslant b. \tag{26}$$

Then, the constraints for the *Feasibility Test* take the following form:

$$f_1 = a - g(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leqslant u;$$
$$f_2 = g(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) - b \leqslant u. \tag{27}$$

Assuming that both f_1 and f_2 are active, it can be easily shown that $u = (a - b)/2$, which is always negative. This result can be generalized for any combination of active constraints, that contains constraints which are lower and upper bounds on the same function. As shown in Appendix A, the value u^k for an active set k of this type is given by the following equation:

$$u^k = \frac{1}{\alpha_k}\left(\sum_{j(l) \in AS(k)} a_{j(l)} - \sum_{j(u) \in AS(k)} b_{j(u)}\right) \tag{28}$$

where the indices $j(l)$, $j(u)$ correspond to those pairs of constraints representing lower and upper bounds on the same function, and α_k is the total number of this type of constraints. Therefore, by using the expression u^k in (28) the solution of the NLP problem that corresponds to that active set can be obtained analytically. It should also be noted that since u^k is always negative here, then for the *Flexibility Index* those active sets containing lower and upper bound constraints can be excluded *a priori*. This follows from the fact that the *Flexibility Index* requires a solution with $u^k = 0$ for a given active set as can be seen in (P5).

Having identified the combinations of different potential active sets of constraints, the corresponding NLP that arises for a fixed choice of an active set k in the MINLP formulation, can be solved to determine its corresponding maximum u^k (*Feasibility Test*) or its corresponding minimum δ^k (*Flexibility Index*). The final solution is then just simply given by the largest value of u^k, or the smallest value of δ^k that is obtained among the candidate active sets.

As an example, for the *Feasibility Test* in (P1), the steps of the algorithm are as follows:

1. Identification of the possible active sets
   (a) For every $j \in J$ compute $\nabla_z f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ and determine the signs of each component of the gradients.
   (b) Identify the n_{AS} combinations of active sets of constraints from equation (14b) based on the signs of the gradients $\nabla_z f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ and considering (15a) and (15c). Also, identify lower and upper bound constraints that might be present.
   (c) For each combination $k = 1, 2, \ldots n_{AS}$, define the set $AS(k) = (j \mid j \in J$, and j is one of the $n_z + 1$ active constraints)

2. Determine the value of u^k for each candidate active set $k = 1, 2, \ldots n_{AS}$.
   (a) If $AS(k)$ involves lower and upper bound constraints, then u^k is given by:

$$u^k = \frac{1}{\alpha_k}\left(\sum_{j(l) \in AS(k)} a_{j(l)} - \sum_{j(u) \in AS(k)} b_{j(u)}\right).$$

   (b) Otherwise, solve the nonlinear programming (NLP) problem:

$$u^k = \max_{\boldsymbol{\theta}, \mathbf{z}, u} u,$$
$$\text{s.t.}\, f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) - u = 0 \quad j \in AS(k) \quad (NP^k),$$
$$\boldsymbol{\theta}^L \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^U,$$

(3) The solution of the *Feasibility Test* problem is given by:

$$\chi(\mathbf{d}) = \max_{k \in AS(k)} u^k.$$

Similar algorithms can be developed for the formulations (P2)–(P4) of the *Feasibility Test*, and for the formulations (P5)–(P8) of the *Flexibility Index*. In the case of (P2) and (P6) where equalities are explicitly handled and $n_z \geqslant 1$, step 1 requires the elimination of the multipliers μ_i from the stationary conditions in order to obtain equation (14b). In the case of (P3), (P4), (P7), (P8) where $n_z = 0$, step 1 is replaced by setting AS(j) = j, $j \in J$, since in this case each constraint becomes a candidate active set. For example, for problem (P3), the algorithm just simply reduces to equations (18) and (19).

It should be noted that the above algorithm is equivalent to an enumeration of all feasible candidate active sets. As was indicated before, when control variables are involved, this number can be expected to be relatively small, especially when compared to the number of vertices involved in problems with many uncertain parameters. Also, it should be noted

Table 2. Sufficient conditions for global optimality in the NLP subproblems of active constraint strategy

	Feasibility Test	Flexibility Index
	(P1) ($n_z \geqslant 1$)	(P5) ($n_z \geqslant 1$)
$\psi(\mathbf{d}, \boldsymbol{\theta})$	Quasi-concave in $\boldsymbol{\theta}$ (Theorem 1)	Quasi-concave in $\boldsymbol{\theta}$ (Theorem 3)
$f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$	Jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and strictly quasi-convex in $\mathbf{z}$ for fixed $\boldsymbol{\theta}$. (Theorem 2)	Jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and strictly quasi-convex in $\mathbf{z}$ for fixed $\boldsymbol{\theta}$.
	(P3) ($n_z = 0$)	(P7) ($n_z = 0$)
$f_j(\mathbf{d}, \boldsymbol{\theta})$	Quasi-concave in $\boldsymbol{\theta}$	Quasi-concave in $\boldsymbol{\theta}$

that the above algorithm does not assume vertex solution, and that for the linear case it can be used instead of a direct MILP solution.

An important question in the proposed algorithm for active sets is what assumptions are required for the constraint functions so as to guarantee the global optimal solution of the NLP corresponding to each active set of constraints. Table 2 presents sufficient conditions that are required for the feasibility function $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ and for the constraint functions $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}), j \in AS(k)$, corresponding to the kth active set in the formulations (P1), (P3), (P5), (P7). The theorems are presented in Appendix B.

The geometrical interpretation of the sufficient conditions for a unique global solution for u^k in the *Feasibility Test* are illustrated in Figs 8a–c in which 1-D plots of $\mathbf{z}$ vs $\boldsymbol{\theta}$ and $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ vs $\boldsymbol{\theta}$ are depicted. In Fig. 8a, the constraint functions f_1, f_2 are jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and strictly quasi-convex in $\mathbf{z}$ for fixed $\boldsymbol{\theta}$. Therefore, $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave (see theorem 2) and, hence, u^k corresponds to a unique global solution (see theorem 1). To show that the conditions in Table 2 are sufficient, consider in Fig. 8b the constraint functions f_1, f_2 which are jointly quasi-convex in $\mathbf{z}$ and $\boldsymbol{\theta}$, and therefore do not satisfy the conditions of theorem 2. However, as can be seen in Fig. 8b, $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$, and u^k is a unique solution. On the other hand, in Fig. 8c, f_1 and f_2 are also quasi-convex in $\mathbf{z}$ and $\boldsymbol{\theta}$, but these result in $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ which is quasi-convex, leading to 2 local maxima for $u^k = 0$ as shown in this figure.

The geometrical interpretation of the sufficient conditions for a unique global solution for the *Flexibility Index* are similar to the above cases. An example where these conditions are satisfied is illustrated in Fig. 9, in which 1-D plots of $\mathbf{z}$ vs $\boldsymbol{\theta}$ and $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ vs $\boldsymbol{\theta}$ are presented. In this figure, f_1, f_2 are jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and therefore, $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$ (see theorem 2). As shown in theorem 3, if the NLP subproblem for the *Flexibility Index* is solved by relaxing the constraint on the boundary as $\psi^k(\mathbf{d}, \boldsymbol{\theta}) \geqslant 0$, it will have a unique solution (point F_1 in Fig. 9.) It is interesting to note that if the constraint on $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is not relaxed, then as seen in Fig. 9, there are 2 local solutions, F_1 and F_2, which correspond to the intersection points $\psi^k(\mathbf{d}, \boldsymbol{\theta}) = 0$.

It should be pointed out that even though for practical design problems it might be difficult to establish whether the active constraints belong to the class of functions described above, the theoretical results presented here describe precisely the sufficient conditions for which a unique global solution can be guaranteed for the problem formulations (P1), (P3), (P5), (P7). An example where the knowledge of the theoretical properties has been useful is in the flexibility analysis of heat exchanger networks with uncertain flowrates and temperatures, a problem that has been shown to satisfy the conditions in Table 2 (see Floudas and Grossmann [16]).

Example 3

A slightly modified version of the heat exchanger network given in Grossmann and Morari [1], is shown in Fig. 10; in this network the outlet temperature of stream H1 is specified to be cooled down to at least 323 K. The uncertain parameter is the heat capacity flowrate of stream H1 which has a nominal value of 1 kW/K and an expected deviation of +0.8 kW/K. This network is feasible for the extreme values (1, 1.8), but it is infeasible for some intermediate values. It will be shown that the *Active Set Strategy* used in the formulation for the *Feasibility Test* (P1) can identify the nonvertex critical point.

The 4 following inequalities are considered for feasible operation of this network.

$$\begin{aligned} &\text{Feasibility in exchanger 2: } t_2 - t_1 \geqslant 0 \\ &\text{Feasibility in exchanger 3: } t_2 - 393 \geqslant 0 \\ &\text{Feasibility in exchanger 3: } t_3 - 313 \geqslant 0 \quad (29) \\ &\text{Specification in outlet temperature: } t_3 \leqslant 323. \end{aligned}$$

By eliminating the state variables, these 4 inequalities can be written as a function of the control variable Q_c (cooling load) and the uncertain parameter F_{H1} as follows:

$$\begin{aligned} f_1 &= -25 + Q_c[(1/F_{H1}) - 0.5] + (10/F_{H1}) \leqslant 0 \\ f_2 &= -190 + (10/F_{H1}) + (Q_c/F_{H1}) \leqslant 0 \\ f_3 &= -270 + (250/F_{H1}) + (Q_c/F_{H1}) \leqslant 0 \\ f_4 &= 260 - (250/F_{H1}) - (Q_c/F_{H1}) \leqslant 0. \end{aligned} \quad (30)$$

The feasible region for these constraints is shown in Fig. 11.

To test for feasibility of operation in this network for the parameter range $F_{H1} \in (1, 1.8)$, the *Active Set Strategy* will be applied to the formulation (P1). From the constraint on the Lagrange multipliers λ_1, λ_2, λ_3, λ_4 of the Kuhn–Tucker conditions we have:

$$[(1/F_{H1}) - 0.5]\lambda_1 + (1/F_{H1})\lambda_2 + (1/F_{H1})\lambda_3 - (1/F_{H1})\lambda_4 = 0. \quad (31)$$

Since $(1–0.5\,F_{H1})$ is greater than zero for the parameter range of F_{H1}, and there exists one control variable (i.e. 2 active constraints), there are 3 active

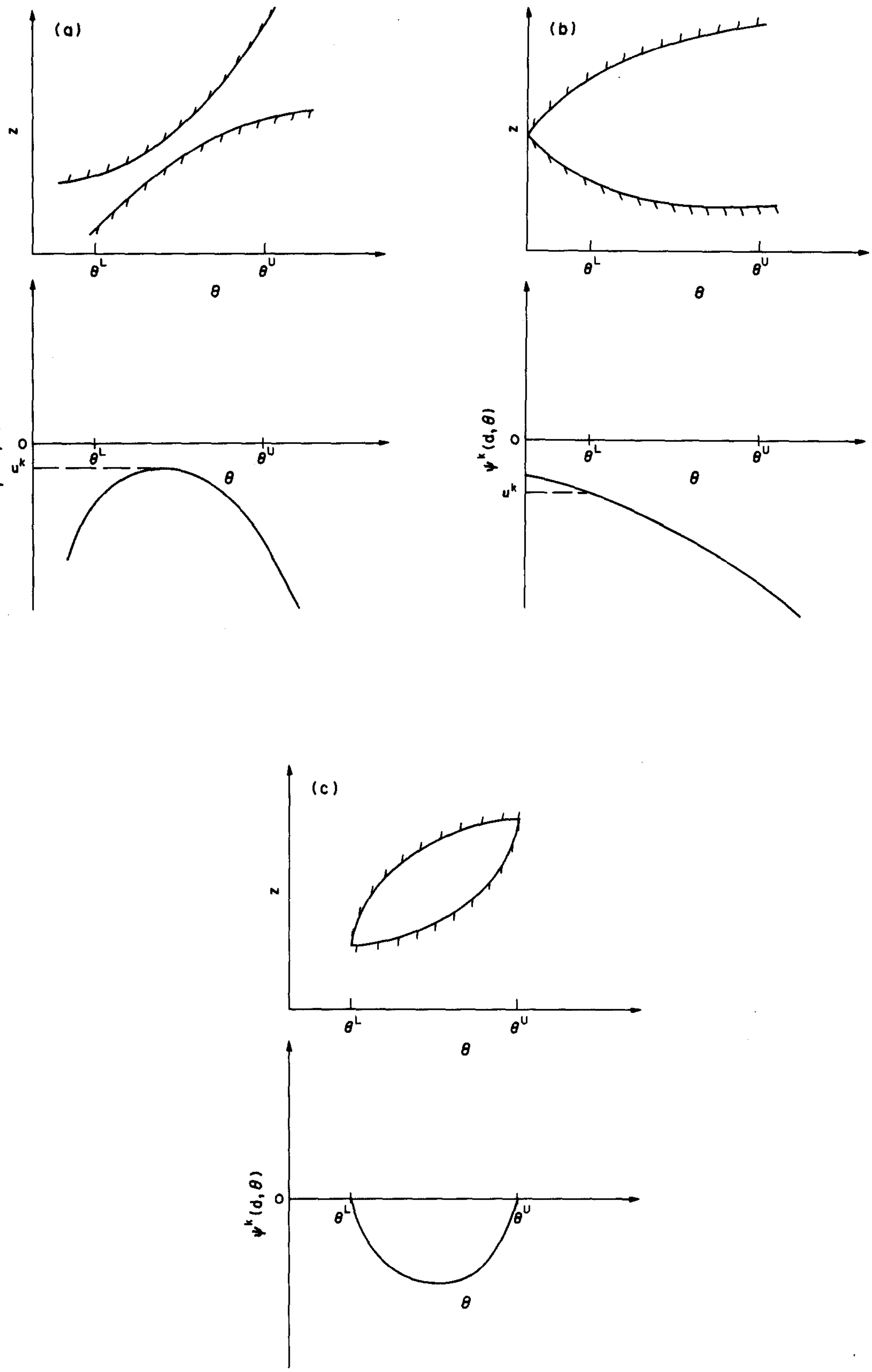

Fig. 8. (a) $\psi(\mathbf{d}, \boldsymbol{\theta})$ quasi-concave in $\boldsymbol{\theta}$; (b) $\psi(\mathbf{d}, \boldsymbol{\theta})$ quasi-concave in $\boldsymbol{\theta}$; (c) $\psi(\mathbf{d}, \boldsymbol{\theta})$ quasi-convex in $\boldsymbol{\theta}$.

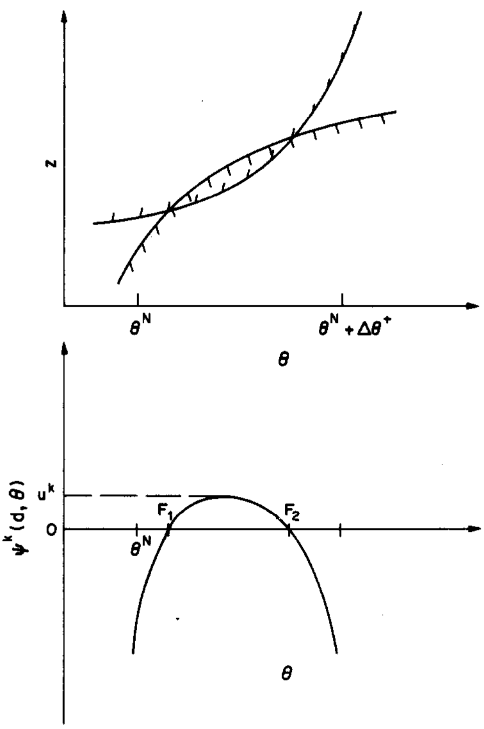

Fig. 9. Example of concave ψ (**d**, $\boldsymbol{\theta}$) for the flexibility index.

sets satisfying $\lambda \geqslant 0$; Active set 1: constraints 1 and 4; Active set 2: constraints 2 and 4; and Active set 3: constraints 3 and 4. All active sets will be examined below.

Active set 2 implies that solving the system of $f_2 = u, f_4 = u$; the following expression is found for u:

$$u = 35 - (120/\mathrm{F_{H1}}). \tag{32}$$

Since u is monotone in the uncertain parameter, a unique global solution exists for u in Active set 2 (see theorem 1). This solution is $\mathrm{F_{H1}} = 1.8$, $Q_c = 275$, and $u^2 = -31.667$, thus indicating that these 2 constraints are feasible at the upper limit of $\mathrm{F_{H1}}$. It should be noted, however, that constraint f_3 is violated for this active set.

Active set 3 involves the lower and upper bounds on t_3 (313 K, 323 K respectively). Thus, from (28) it follows that $u^3 = (313 - 323)/2 = -5$, which indicates that f_3 and f_4 are feasible constraints.

Finally, solving the system of equalities $f_1 = u$, $f_4 = u$ for Active set 1, it is found that:

$$u = 260 - (250/\mathrm{F_{H1}}) + \frac{520 - 570\,\mathrm{F_{H1}}}{\mathrm{F_{H1}}(4 - \mathrm{F_{H1}})}. \tag{33}$$

The above expression for u attains a maximum at the nonvertex value $\mathrm{F_{H1}} = 1.3722813$ with $u^1 = +5.10875$ (infeasible), $Q_c = 99.7825$. It should be noted that

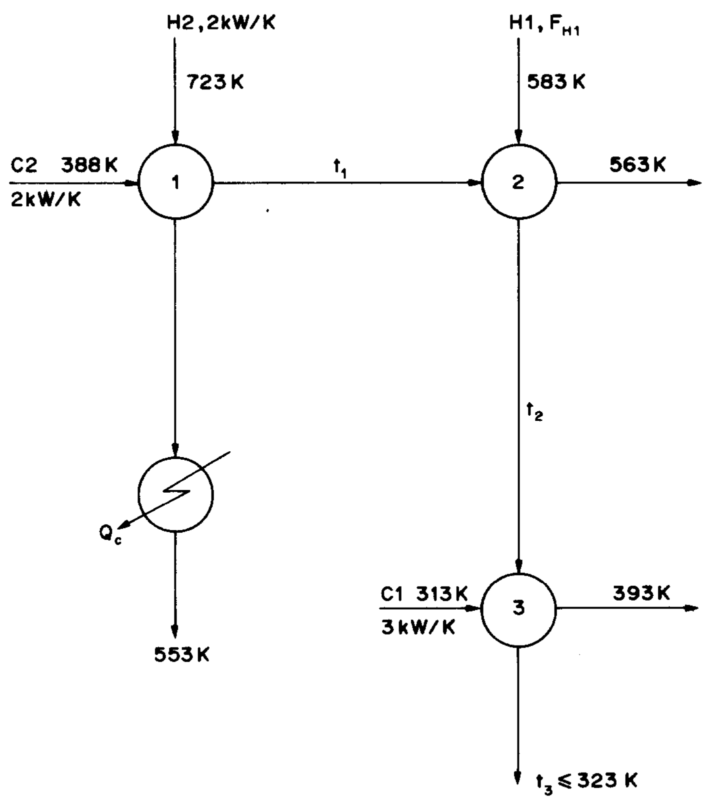

Fig. 10. Network of Example 3 with uncertain flowrate $\mathrm{F_{H1}}$.

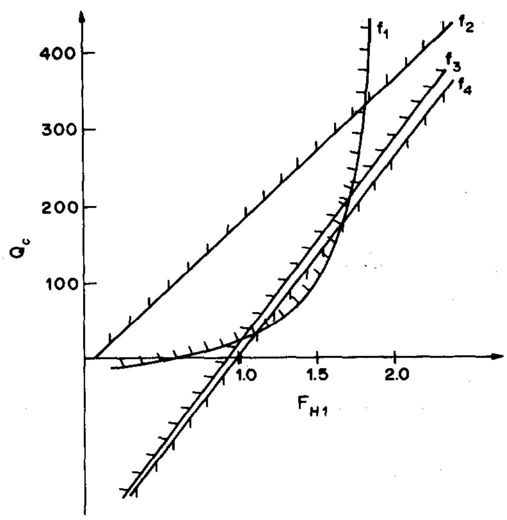

Fig. 11. Feasible region for constraints for Example 3.

since $\psi(\mathbf{d}, \boldsymbol{\theta}) = u$ is quasi-concave a unique maximum solution exists for u at this active set (see theorem 1).

Since the value u^1 for the Active set 1, is the largest, it then follows that $\chi(\mathbf{d}) = +5.10875$, which defines the global solution of problem (P1) at the nonvertex critical point $F_{H1} = 1.3722813$. This corresponds precisely to the point of largest constraint violations in the range (1, 1.8). Specifically, at this point the temperatures are $t_1 = 508.11$ K, $t_2 = 503$ K and $t_3 = 328.11$ K, which clearly violate the first and fourth feasibility constraint (f_1, f_4). Thus, as shown in this example, the formulation (P1) has the capability of predicting critical points that do not correspond to vertices or extreme values.

To illustrate the application of the *Flexibility Index*, formulation (P5) was applied to this problem. The nominal value for F_{H1} was taken as 1 kW/K with a positive expected deviation of 0.8 kW/K. It should be noted that the calculation of the *Flexibility Index* for Active set 3 is excluded, since constraints 3 and 4 can not be simultaneously active with $u^3 = 0$. Also, when applying problem formulation (P5) to the different active sets, the constraint $u = 0$ is reformulated as $u \geqslant$ as implied by theorem 3 to ensure uniqueness of the solution.

Testing for Active set 2, it was found that $\delta^2 = 3.0357$, which implies a maximum value of $F_{H1} = 3.428$ for feasible operation of constraints 2 and 4. This solution of (P5) is unique global solution since $\psi^2(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$.

Testing for Active set 1 in problem formulation (P5), the solution is $\delta^1 = 0.1476825$ for $F_{H1} = 1.118146$. By similar arguments as above, this is also a unique solution.

Since the flexibility index $F = \min \delta^k$, the flexibility index for this heat exchanger network is $F = 0.1476825$, $k \in AS(k)$ which implies that this network remains feasible only for the range $F_{H1} \in [1, 1.118146]$.

Finally, the quality of the approximation of the nonlinear constraints with the linearized ones at the nominal point ($F_{H1} = 1, Q_c = 10$) for the *Flexibility Index* will be illustrated in this example problem. Using the MILP version of (P5), it was found that $F = 0.125$ which implies a range for the flowrate F_{H1} of [1, 1.1] in which feasible operation is guaranteed. Therefore, it is apparent that the quality of the linear approximation is very good in this case.

Example 4

This example problem, which is an extended version of the problem in Swaney and Grossmann [2], will illustrate the application of the formulation (P8) for the *Flexibility Index*. In this example, a centrifugal pump (see Fig. 12) must transport liquid at a flowrate m from its source at pressure P_1 through a pipe run to its destination at pressure P_2'. The flowrate m, the pressure P_2', the pump efficiency η, the pressure drop constant in the pipe k, and the liquid density ρ are treated as uncertain parameters. The design variables $\mathbf{d}$, are the pipe diameter D, the pump head H, the driver power W, and the control valve size C_v^{MAX}. The control variable is the valve coefficient C_v, while P_2 is a state variable. Nominal values and expected deviations for the uncertain parameters are shown in Table 3. P_1 is fixed at 100 kPa. The problem then consists of determining the *Flexibility Index* for the design for which $W = 31.2$ kW, $H = 1.3$ kJ/kg, $D = 0.0762$ m and $C_v^{MAX} = 0.039673$.

The corresponding inequalities that apply for this problem in terms of the control variable C_v and the uncertain parameters P_2', m, η, k, ρ are given by Swaney and Grossmann [12]:

$$f_1 = P_1 + \rho H - \epsilon - \frac{m^2}{\rho C_v^2} - k m^{1.84} D^{-5.16} - P_2' \leqslant 0.$$

$$f_2 = -P_1 - \rho H - \epsilon + \frac{m^2}{\rho C_v^2} + k m^{1.84} D^{-5.16} + P_2' \leqslant 0$$

$$f_3 = m H - \eta W \leqslant 0$$

$$f_4 = C_v - C_v^{MAX} \leqslant 0$$

$$f_5 = -C_v + r C_v^{MAX} \leqslant 0 \tag{34}$$

where r is the control valve range ($r = 0.05$) and $\epsilon = 20$ kPa is a tolerance for the delivery pressure.

To identify the possible active sets, equation (14b) is used in conjunction with the number of active constraints (2 active constraints for this example, since there is one control variable). Equation (14b) takes the following form for the above set of inequalities:

$$\frac{2m^2}{\rho C_v^3}\lambda_1 - \frac{2m^2}{\rho C_v^3}\lambda_2 + \lambda_4 - \lambda_5 = 0. \tag{35}$$

From (35), the active sets of constraints can be identified easily since the partial derivatives of the constraints with respect to the control variable C_v do

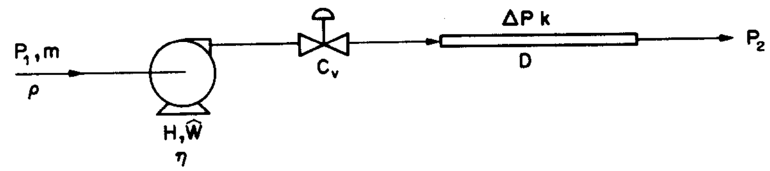

Fig. 12. Pump and pipe run of Example 4 with P_2', m, η, k, ρ uncertain parameters.

not change sign because of the nonnegativity of the uncertain parameters and the control variable. Then, the possible active sets of constraints identified from equation (35) are:

Active set 1: Constraints f_1, f_5;

Active set 2: Constraints f_2, f_4;

Active set 3: Constraints f_1, f_2;

Active set 4: Constraints f_4, f_5.

Since active sets 3 and 4 are lower and upper bounds on the same function, they can be excluded from the calculation of the *Flexibility Index* as was indicated previously in the paper. Therefore, only active sets 1 and 2 have to be considered, which implies the solution of 2 NLP problems in formulation (P5). In contrast, the vertex enumeration would require the solution of 32 NLP's since there are 5 uncertain parameters, and therefore 32 vertices.

Solving the NLP for active set 2, leads to $\delta^2 = 0.40765$ at $P_2' = 881.5297$, $m = 10.8153$, $\eta = 0.479618$, $k = 9.2865 \times 10^{-6}$, and $\rho = 979.6175$. Solving the NLP for active set 1, it was found that $\delta^1 = 1.50437$ at $P_2' = 0$, $m = 2.4781$, $\eta = 0.4247$, $k = 8.4164 \times 10^{-6}$, and $\rho = 1075.22$. Notice that the solutions of the NLP's for each active set are unique global solutions since the constraint functions are monotone and satisfy the conditions of theorem 2. Since the *Flexibility Index* is given by the minimum of δ^1, δ^2, the flexibility index for this example problem is F = 0.40765 which implies that the uncertain parameters can vary in the ranges $P_2' \in [596.17, 881.53]$, $m \in [7.962, 10.815]$, $\eta \in [0.4796, 0.5204]$, $k \in [8.9155, 9.2865] \times 10^{-6}$, $\rho \in [979.62, 1020.38]$. The solution of the 2 NLP's required a total of 4.7 s of CPU-time(DEC-20) with the computer code MINOS/AUGMENTED Murtagh and Saunders [17].

Finally, equation (20) was utilized for the linearization of the nonlinear constraints to yield the MILP formulation of (P5) for the *Flexibility Index*. The result obtained is F = 0.4656, which is the nonlinear solution $F = 0.40765$. The CPU-time (DEC-20) required for the MILP with the LINDO code (Schrage [12]) was 1.57 s.

DISCUSSION

As has been illustrated with example problems 1 and 2, when the constraints are linear the formulations (P1)–(P8) become mixed-integer linear programming (MILP) problems which can be readily implemented in computer software and solved with standard branch and bound enumeration techniques. (MILP) formulations also result from linearizations performed on nonlinear functions which can be used to obtain estimates of flexibility for screening purposes. These linear estimates are of course not guaranteed to be always very accurate. However, they would seem to be particularly suitable for estimating the flexibility index since quite often the actual parameter deviations will be rather small. It is interesting to note that since measures of controllability or dynamic resiliency rely on function linearizations of the process, Grossmann and Morari [1], one can use this common information to characterize both the flexibility and controllability of chemical processes.

For the case, when the constraints are nonlinear, an *Active Set Strategy* has been presented for the solution of the mixed-integer nonlinear programming (MINLP) problems. In this strategy, the potential active sets of constraints are identified, and a nonlinear programming NLP problem is solved for each active set of constraints. Automating this strategy should in general not be too difficult given a suitable NLP routine. As was shown with Examples 3 and 4, the proposed strategy offers the possibility of identifying nonvertex critical points if they exist, and furthermore the number of NLP's that have to be solved is very often much smaller than the number of vertices. Sufficient conditions that guarantee global solutions for this strategy have been investigated. For processes not satisfying these conditions rigorous guarantees are not possible. However, results of the examples, the study on heat exchanger networks by the authors Floudas and Grossmann [6], and pre-

Table 3. Nominal values and deviations of the uncertain parameters in Example 4

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

liminary experience on process flowsheets by the first author have been very encouraging.

Finally, it is interesting to note the differences and similarities of this work with the one by Swaney and Grossmann, [2, 6]. In their work, the solution of the max–min–max problem is simplified by the assumption that the critical points for feasible operation correspond to vertices or extreme values of the uncertain parameters. In this paper, however, the max–min–max problem is solved explicitly, without making any assumptions on the critical points, except for the linear independence of the constraint gradients. In the work of Swaney and Grossmann, sufficient conditions for a global solution are that the constraint functions must be jointly quasi-convex in $\mathbf{z}$ and one dimensional quasi-convex in $\boldsymbol{\theta}$, which guarantees that the critical points lie at the vertices. In this work, however, the main sufficient conditions for a global solution are that the constraint functions must be jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and strictly quasi-convex in $\mathbf{z}$ for fixed $\boldsymbol{\theta}$ (see Table 2). Therefore, it can be seen that the 2 works are complementary to each other in terms of the type of nonlinear functions that can be handled. There is, however, also an overlap on the type of functions that can be handled, as for instance the case of linear functions.

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APPENDIX A

Proposition: Let problem

$$u^k = \max_{\theta, z, u} (u \,|\, f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, j \in AS(k))$$

be such that a subset of the constraints $AS'(k)$ is given by $g_{j(u,l)}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leq b_{j(u)}$, $a_{j(l)} \leq g_{j(u,l)}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$, $j(l), j(u) \in AS'(k)$. Then u^k is given by:

$$u^k = \frac{1}{\alpha_k}\left(\sum_{j(l) \in AS(k)} a_{j(l)} - \sum_{j(u) \in AS(k)} b_{j(u)} \right)$$

where $\alpha_k = |AS'(k)|$

Proof: The constraints in the active set can be written as:

$$g_{j(u,l)}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) - b_{j(u)} = u, \quad j(u) \in AS'(k),$$
$$a_{j(l)} - g_{j(u,l)}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, \quad j(l) \in AS'(k),$$
$$f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, \quad j \notin AS'(k).$$

By adding the above equations, it follows that:

$$u|AS'(k)| + \sum_{j \notin AS'(k)} u = \sum_{j(l) \in AS'(k)} a_{j(l)} - \sum_{j(u) \in AS'(k)} b_{j(u)} + \sum_{j \notin AS'(k)} f_j.$$

But, since $u = f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$, $j \notin AS'(k)$,

$$u = \frac{1}{|AS'(k)|}\left(\sum_{j(l) \in AS'(k)} a_{j(l)} - \sum_{j(u) \in AS'(k)} b_{j(u)} \right).$$

Since u is a constant, its maximum has the same value; that is

$$u^k = \frac{1}{\alpha_k}\left(\sum_{j(l) \in AS(k)} a_{j(l)} - \sum_{j(u) \in AS(k)} b_{j(u)} \right).$$

APPENDIX B

Definitions, theorems and proofs of theorems

Definition 1: $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ for the k'th active set is given by:

$$\psi^k(\mathbf{d}, \boldsymbol{\theta}) = \min_{u, z} [u \,|\, f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = u, j \in AS(k)].$$

Definition 2: $\psi(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$ if and only if for $\boldsymbol{\theta}^1, \boldsymbol{\theta}^2 \in R$, the following condition holds:

$$\psi[\mathbf{d}, \lambda\boldsymbol{\theta}^1 + (1 - \lambda)\boldsymbol{\theta}^2] \geq \min[\psi(\mathbf{d}, \boldsymbol{\theta}^1), \psi(\mathbf{d}, \boldsymbol{\theta}^2)]$$

for each $\lambda \in (0, 1)$.

Theorem 1: If $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$, then the subproblem for active set k in (P1),

$$u^k = \max_{\theta \in T} [\psi^k(\mathbf{d}, \boldsymbol{\theta})]$$

has a unique global solution.

Proof: It is well known [1] that if $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave function of $\boldsymbol{\theta}$, then every strict local maximum problem over the convex set T will also be a strict global maximum.

Theorem 2: If the constraint functions $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$, $j \in AS(k)$, are jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$, and strictly quasi-convex in $\mathbf{z}$ for any fixed $\boldsymbol{\theta}$, then the function $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$.

Proof: (a) It will be proved first that $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is uniquely defined for the given active set.

$$\text{Let } \psi(\mathbf{d}, \boldsymbol{\theta}) = \min_z \phi(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$$

where

$$\phi(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) = \max_{j \in AS(k)} [f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})].$$

Since $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ is strictly quasi-convex in $\mathbf{z}$

$$f_j(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}) < \max[f_j(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta}), f_j(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta})]$$

where $\mathbf{z}^3 = \alpha \mathbf{z}^1 + (1-\alpha)\mathbf{z}^2, \alpha \in (0, 1)$. It then follows that

$$\begin{aligned}\phi(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}) &= \max_{j \in AS(k)} [f_j(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta})] \\ &< \max_{j \in AS(k)} \{\max[f_j(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta}), f_j(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta})]\} \\ &= \max\left\{\max_{j \in AS(k)} [f_j(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta})], \max_{j \in AS(k)} [f_j(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta})]\right\}\end{aligned}$$

Hence,

$$\phi\, \mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}) < \max[\phi(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta}), \phi(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta})].$$

Therefore, since $\phi(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ is also strictly quasi-convex in $\mathbf{z}$ it implies that $\psi(\mathbf{d}, \boldsymbol{\theta})$ has a unique solution [8].

(b) In the second part it will be proved that $\psi(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave.

Consider any 2 points $\boldsymbol{\theta}^1$, $\boldsymbol{\theta}^2$, such that $\psi(\mathbf{d}, \boldsymbol{\theta}^1) \leqslant \psi(\mathbf{d}, \boldsymbol{\theta}^2)$. From definition 1,

$$\psi(\mathbf{d}, \boldsymbol{\theta}^1) = f_j(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta}^1) \quad j \in AS(k),$$

$$\psi(\mathbf{d}, \boldsymbol{\theta}^2) = f_j(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta}^2) \quad j \in AS(k),$$

From the above this implies that

$$\psi(\mathbf{d}, \boldsymbol{\theta}^1) = \min[f_j(\mathbf{d}, \mathbf{z}^1, \boldsymbol{\theta}^1), f_j(\mathbf{d}, \mathbf{z}^2, \boldsymbol{\theta}^2)] \quad j \in AS(k). \tag{A1}$$

Furthermore, since $f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta})$ is jointly quasi-concave in $\mathbf{z}$ and $\boldsymbol{\theta}$

$$\psi(\mathbf{d}, \boldsymbol{\theta}^1) \leqslant f_j(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}^3) \quad j \in AS(k) \tag{A2}$$

where

$$\mathbf{z}^3 = \alpha \mathbf{z}^1 + (1-\alpha)\mathbf{z}^2, \quad \boldsymbol{\theta}^3 = \alpha \boldsymbol{\theta}^1 + (1-\alpha)\boldsymbol{\theta}^2, \quad \alpha \in (0, 1).$$

If the solution $\mathbf{z}'$ to $\psi(\mathbf{d}, \boldsymbol{\theta}^3) = f_j(\mathbf{d}, \mathbf{z}', \boldsymbol{\theta}^3)$, $j \in AS(k)$, is given by $\mathbf{z}^3$, then it clearly follows from (A2) that $\psi(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave since $\psi(\mathbf{d}, \boldsymbol{\theta}^3) \geqslant \psi(\mathbf{d}, \boldsymbol{\theta}^1) = \min[\psi(\mathbf{d}, \boldsymbol{\theta}^1), \psi(\mathbf{d}, \boldsymbol{\theta}^2)]$.

For the case when $\mathbf{z}' \neq \mathbf{z}^3$, $\psi(\mathbf{d}, \boldsymbol{\theta}^3)$ is not identical to $f_j(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}^3)$ for all $j \in AS(k)$. Hence, there will exist a constraint j' such that $f_{j'}(\mathbf{d}, \mathbf{z}^3, \boldsymbol{\theta}^3) < \psi(\mathbf{d}, \boldsymbol{\theta}^3)$. Applying (A2) to j' it follows that

$$\psi(\mathbf{d}, \boldsymbol{\theta}^3) > \psi(\mathbf{d}, \boldsymbol{\theta}^1) = \min[\psi(\mathbf{d}, \boldsymbol{\theta}^1), \psi(\mathbf{d}, \boldsymbol{\theta}^2)]$$

which then proves that $\psi(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$.

Theorem 3: If the function $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$, then the subproblem for active set k in (P5)

$$\begin{gathered}\delta^k = \min \delta \\ \text{s.t. } \psi^k(\mathbf{d}, \boldsymbol{\theta}) = 0 \\ \boldsymbol{\theta}^N - \delta \Delta \boldsymbol{\theta}^- \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^N + \delta \Delta \boldsymbol{\theta}^+, \delta \geqslant 0\end{gathered}$$

has a unique global solution.

Proof: Since by definition of the *Flexibility Index*, $\delta = 0$ implies that $\psi(\mathbf{d}, \boldsymbol{\theta}) \leqslant 0$, the above problem for δ^k is equivalent to:

$$\begin{gathered}\delta^k = \min \delta \\ \text{s.t. } \psi^k(\mathbf{d}, \boldsymbol{\theta}) \geqslant 0 \\ \boldsymbol{\theta}^N - \delta \Delta \boldsymbol{\theta}^- \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^N + \delta \Delta \boldsymbol{\theta}^+, \delta \geqslant 0.\end{gathered}$$

Since $\psi^k(\mathbf{d}, \boldsymbol{\theta})$ is quasi-concave in $\boldsymbol{\theta}$, the constraint $\psi^k(\mathbf{d}, \boldsymbol{\theta}) \geqslant 0$ and the linear constraints for $\boldsymbol{\theta}$ define a convex feasible region. Hence, this problem has a unique global solution [8].

The proofs of the rest of the properties listed in Table 2, are similar to those presented in this Appendix.